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

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

Abstract: Over the last decade, 4D printing paradigm has received intensive research efforts, whether from researchers in additive manufacturing (AM) or in smart materials (SMs) development. Related research works have thereby generated a large number of *ad-hoc* solutions with relevant disparate and scattered knowledge. This lack of common core knowledge is mainly due to the multiple involved expertise for fabricating stimulus-reactive structures. The scientific issue of federating and reconciling knowledge is also reinforced especially if such technology **must** be integrated into the product design **process**, falling under the field of design for 4D printing. To tackle this challenge, it becomes crucial to formalize and represent knowledge relating AM processes/techniques, SMs behaviours, stimuli and transformation functions with the variety of design objects. In such a context, the paper aims at developing an ontology-based framework for the semantic and logical description of transformable objects in the era of 4D printing for product-process design related purposes. This framework – which is built upon a foundational ontology associated **with** mereotopology for describing dynamical phenomena called basic formal ontology – consists in introducing a domain ontology equipped with reasoning capabilities supported by description logics for SMs selection and distribution, transformation sequence planning and AM process planning purposes.

Keywords: 4D Printing, Smart materials, Additive manufacturing, Design for 4D printing, Ontology, Description logics

1. Introduction

Since the beginning of the 1980's, rapid prototyping – which is also known as three-dimensional (3D) printing or additive manufacturing (AM) – has received growing attention from academia and industry (about 150.000 scientific papers), mostly federating a wide spectrum of scientific domains (André *et al.*, 1984; Rengier *et al.*, 2010; Manfredi *et al.*, 2013). Beyond engineering opportunities and challenges offered by this manufacturing technology, two emerging and interrelated paradigms have been derived, namely 4D printing and bio-printing (André, 2017). Both technologies aim at integrating transformation capabilities into manufactured parts. By relating **AM** techniques and smart materials (SMs), 4D printing can play a crucial role for fabricating transformable, deployable and adaptive

structures that carry out a predictable shift (Ge *et al.*, 2013; Tibbits, 2014). This challenging association provides a temporal dimension in which transformation is triggered via stimuli. The development of 4D printing applications therefore requires **taking** advantages of AM techniques capacity and also multi-material printing ability (Vaezi *et al.*, 2013; Gibson *et al.*, 2015; Momeni *et al.*, 2017). With both capabilities, parts are henceforth designed and manufactured as alive objects able to shift into different physical states or geometric configurations with respect to its trigger conditions (Choi *et al.*, 2015). **Indeed**, stimuli are required to activate changes at different levels such as structure, shape, properties and functionalities. For all the above reasons, 4D printing is seen as a promising manufacturing technology and a booming cross-disciplinary research field to deliver next generation of alive products (Tibbits, 2014; André, 2017; Kuang *et al.*, 2019). To achieve this objective, the related multi-perspective knowledge needs to be formalized and represented in order to be properly reused in the product development phases.

Over the last decades, efforts have been made towards integrating a wide range of manufacturing technologies as well as lifecycle purposes in product design. As such, several methods and tools falling under the concept of design for X (DFX) (Holt and Barnes, 2010) have been proposed. DFX aims to concurrently consider lifecycle purposes like assembly, manufacturing, recycling, etc. and product design, therefore delivering lifecycle friendly designed definitions. In a similar way and 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 **and related proof-of-concepts showing** scattered and disparate knowledge due to the multiple involved expertise.

In such a context, the main research objective is to formalize and represent 4D printing knowledge related to AM processes and techniques, SMs, stimuli and transformation issues.

Such critical knowledge requires to be properly described and computer interpretable in order to be reused along the product design stages. In other words, by following such an objective, product architects and designers will be aided to make right decisions during the design process of alive and transformable objects. To do so, an ontology-based framework is proposed to ensure the semantic and logical description of transformable objects in the era of 4D printing.

The structure of the paper is as follows. Section 2 addresses relevant research works in the fields of 4D printing and ontology models for design with a special emphasis on product, process and material, on which motivation is highlighted. Section 3 establishes the ontological framework with the underlying philosophical/epistemic, scientific hypotheses and the support of the basic formal ontology (BFO) (Arp *et al.*, 2015), along with the use of 4D printing knowledge in design. Built on this, Section 4 presents the proposed ontology for formalizing and representing 4D printing knowledge. The proposed ontology embeds reasoning capabilities supported by mereotopological relationships and description logics for further design for 4D printing purpose. Two case studies are introduced in the last section to illustrate the relevance of the proposed knowledge base.

2. Literature Review

This section gives an overview on the significant published research works on 4D printing and ontology models for design. It also highlights current challenges in these fields to be tackled in the specific context of the paper.

2.1 4D Printing

This research domain has initially been addressed by polymer scientists with the development of shape morphing structures and shape memory polymers or artificial muscles (Kang *et al.*, 2007; Woodruff and Hutmacher, 2010; Nakano, 2010). Pioneer works set up behavioural

studies of glass transition temperature, magnitude of stress and elasto-viscoplasticity deformation (Yakacki *et al.*, 2008; Qi *et al.*, 2008a; Nguyen *et al.*, 2008; Anand *et al.*, 2009; Xie, 2010; Yu *et al.*, 2012), whose applications are scattered in different domains (Lebel *et al.*, 2010; Roy *et al.*, 2010; Stuart *et al.*, 2010; Hu *et al.*, 2012; Zarek *et al.* 2016). These efforts also have investigated fabrication techniques (e.g. direct ink writing, material jetting), smart materials (e.g. nanocomposites polymers, polymeric hydrogels) and emerging applications have been developed like organic reactions, digital composites, tissue engineering, biomimicry, biomedical applications and jewellery to name a few (Lebel *et al.*, 2010; Roy *et al.*, 2010; Stuart *et al.*, 2010; Hu *et al.*, 2012; Sun *et al.*, 2012; Gong *et al.*, 2016; Zarek *et al.*, 2016). Along with the cited works, some material embedding active behaviours were developed to fulfil transformation primitives such as bending, twisting and folding – once exposed to solvent, light, magnetic and electric fields (Holmes *et al.*, 2011; Laflin *et al.*, 2012; Ryu *et al.*, 2012; Ahmed *et al.*, 2013). In addition, shape memory composites and pH-responsive materials like hydrogels were developed for self-folding transformation, which were presented in many experiments using origami hinges or multi-layered materials (Best *et al.*, 2013; Demaine and Wood, 2013; Jamal *et al.*, 2013; Krogsgaard *et al.*, 2013; Stoychev *et al.*, 2013; Thérien-Aubin *et al.*, 2013). Accordingly, the aforementioned research progresses have initiated the opportunity to program materials by tuning constitutive laws (Knaian, 2013; Meng and Li, 2013).

Consequently, 4D printing has been coined to cover these efforts with AM technologies, particularly material jetting (Ge *et al.*, 2013; Tibbits, 2013). Most of their proposed works have addressed *ad-hoc* experiments entailed by multi-materials directly off the print bed, whether dipped in water (e.g. hydrophilic polymer material) or triggered with electricity. Similarly, for folding application cases, researchers have demonstrated various programs depending on stimuli, materials, material distributions and shapes. Subsequently,

4D printing enables transformation based-sequence over spatial dimensions (i.e. 2D and 3D) from one state to another in terms of shapes, properties and functions (Khoo *et al.*, 2015; Khare *et al.*, 2017). Built on the above, Baker *et al.* (2016) have programmed a sequential actuation of 2D hydrogel membranes into 3D folded architecture. Raviv *et al.* (2014) have also demonstrated a linear stretching structure (from 1D to 1D), a 2D folding and stretching structure and a 3D topographical surface change. Then multiple transformation-dimensions possibilities were illustrated and multiple research niches have been opened. Other researchers have focused their efforts on controlling the bending and folding primitives by using reverse engineering and monitoring some parameters like fibre length, hinge length and location, strain, temperature, deformation behaviours and activation processes (Ge *et al.*, 2014; Lauff *et al.*, 2014; Naficy *et al.*, 2016). Peraza-Hernandez *et al.* (2014) have addressed kinematic studies of different bending configurations and folding patterns activated by several stimuli (e.g. thermal, chemical, optical and magnetic). 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 (Hager *et al.*, 2015; Kokkinis *et al.*, 2015; Kuksenok and Balazs, 2015; Lee *et al.*, 2015).

Henceforth, one can state that the main artefacts shaping 4D printing technology are stimuli, geometry, AM processes and techniques, SMs and transformation functions (Truby and Lewis, 2016; Momeni *et al.*, 2017). Almost all the research works have considered proof-of-concept machines/devices and several AM processes, ranging from material extrusion (fused filament fabrication and direct ink writing), photopolymerization (stereolithography, digital light processing) to material jetting (drop-on-demand and PolyJet[®]), just to name a few (Gao *et al.*; Gong *et al.*; Khademhosseini and Langer; Miao *et al.*; Sydney Gladman *et al.*; Wu *et al.*; Zarek *et al.*, 2016). Such ongoing developments therefore demand to be considered beforehand in the design process, whether to control self-folding materials (Tao *et al.*, 2018),

evaluate and determine SMs distributions in the early design stages of 4D printed structures by considering a voxel-based modelling approach coupled with genetic algorithms (Sossou *et al.*, 2019a; Sossou *et al.*, 2019b). In a same way, optimization approaches for 4D printing oriented design have been conducted. Paz *et al.* (2017) have pointed out parametric optimization techniques via Kriging metamodel and genetic algorithms to find the best combination of design variables to reduce weight and manufacturing costs for shape-changing printed parts using shape memory polymers. More recently, Zolfagharian *et al.* (2020) have applied topology optimization to obtain a soft actuator with an optimal structure to achieve a bending function.

2.2 Ontology models for product/process/material design

With the introduction of semantic web in the early 2000s in the field of computer science, a wide spectrum of ontologies has been developed to formally and explicitly describe concepts within a specific knowledge domain. 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 (Gruber, 1993; Borst 1997; Studer *et al.*, 1998). As a whole, an ontology can represent knowledge according to the triplet subject-predicate-object. The backbone of an ontology is composed of a concept hierarchy linked by a subtype relationship. The latter – once built with axioms and constraints – makes explicit domain assumptions and provides a common understanding of the knowledge domain. An ontology can then be either informal or formal with a systematic and axiomatic development of logic for all forms and modes of existence (Cochiarella, 1991; Guarino, 1995). In such a context, OWL (Web Ontology Language) and DL (Description Logics) rules provides a strong 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, intersection of concepts, value

restrictions for concepts, universal and existential quantification restrictions. Axioms such as disjunctions and equivalences may be represented as well as the instantiation of concepts and roles assertions. More details are given in [Section 4.5](#).

Among the investigated engineering domains, Dartigues *et al.* (2007) have created a feature-based ontology able to capture semantic information for integrating computer-aided design (CAD) and computer-aided process planning. The interoperable protocol was for an exchange purpose between current and next generation CAD systems. Grüninger and Delaval (2019) have proposed an ontology to support a first-order process planning for sheet lamination technology. For the same manufacturing process, Bateman *et al.* 2011 have developed an ontology embedding manufacturing rules for further automatic features recognition procedure. Kim *et al.* (2019) have [proposed a design for AM ontology to product a structure for information on part design, AM processes and capabilities to represent design rules. Reasoning is then possible to evaluate design features against manufacturing constraints](#). In the same context, Liang (2018) has created an informal generative ontology model for AM process planning.

From a material perspective, Biswas *et al.* (2008) have captured the properties of heterogeneous materials to the core product model developed at National Institute of Standards and Technologies (NIST), which initially was [a generic product model](#) (Fenves *et al.*, 2004). In addition, Zhang *et al.* (2015) have presented an ontology-based framework for selecting material in a domain-oriented knowledge and semantically retrieving and querying it. Among the numerous published materials ontologies (Ashino, 2010; Zhang *et al.*, 2015; Zhang *et al.*, 2015; Zhao and Qian, 2017), Ghedini *et al.* (2017) have recently developed a materials ontology at the European level called European Materials Modelling Ontology (EMMO), which covers materials, physics laws [and physical model](#). EMMO is built upon an upper ontology, BFO (Arp *et al.*, 2015). In this context, Hagedorn *et al.* (2019) 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 (Gruhier *et al.*, 2015). In summary, we can see that many challenges in 4D printing and ontology-oriented design have not been addressed yet.

2.3 *Synthesis*

The aforementioned study of significant research works in 4D printing has highlighted a wide spectrum of knowledge over the multiple involved domains and scales. This provides an abundant body of knowledge with spectacular results, but also leads to difficulties if they have to be integrated over a complete 4D printed structures development process including design, modelling, simulation and manufacturing (Hu *et al.*, 2016; Demoly, 2019). Indeed, product architects and designers still cannot take profits of the capabilities of this trendy technology; dissimilarly from conventional manufacturing processes and some AM techniques (e.g. selective laser sintering) that already have guidelines and rules for design and process planning nowadays (Seepersad *et al.*, 2012; Dinar and Rosen, 2017; Jee and Witherell, 2017). Since 4D printing encompasses large number of scattered artefacts and little is known about how these factors influence a “4D printed” part, its future use requires distinguished design and process planning knowledge. In order to specifically address a design problem, it is crucial to establish a classified and structured knowledge base that such a software invokes in its libraries and querying it fluently. Hence a description for the dynamical phenomena at various scales is strongly needed to formalize the knowledge behind for logical continuity over the design stages.

Based on the study in Section 2.2 highlighting the importance of ontologies in

establishing a prior level in DFX, ontology development **is a required phase to formalize the aforementioned knowledge behind such a paradigm**. A key step is bringing relevant knowledge to designer in order to make 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.

3. Ontology construction and utilization framework

The formalization and representation of 4D printing knowledge for design related purposes requires beforehand a dedicated framework built upon foundational hypotheses and theories. The objectives of such an ontological framework are then twofold: (i) providing a domain ontology construction strategy and (ii) clarifying the ontology usage scenarios.

Since the investigated knowledge domain highlights objects transformation over time (Al-Debei *et al.*, 2012), it seems convenient to address three-dimensionalism (Hales and Johnson, 2003) and four-dimensionalism (Sider, 2001) theories to describe materials objects with temporal and spatiotemporal parts. For such representation issue, BFO as upper ontology has been adopted to reconcile both mentioned visions through endurants and occurrents concepts (Arp *et al.*, 2015). In its actual shape BFO itself is not enough suitable to cover the semantic articulation between the material objects, immaterial objects and processes participating in design for 4D printing process. In such a context, mereotopology is considered as a complementary theory relating mereology (**i.e.** part-whole theory) and topology **to** introduce specific relationships and then object's properties between the aforementioned classes. 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 (Pittet *et al.* 2014). On the other hand, such critical 4D printing knowledge cannot be described from scratch, it is indeed important to consider current existing information and data sources ranging from AM processes and techniques standard, materials database and proof-of-concept experiments 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.

By following such a combined construction strategy, the framework should also clarify the design purposes and scope. 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 paper, the knowledge domain will be limited to product/part design although each design scale merits to be investigated. Actually, the introduced artefacts provided by 4D printing issues can be considered as 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, potential utilization purposes can be ranged over transformation sequence planning, smart materials selection, smart material distribution, AM process planning to name a few and will require dedicated application programming interfaces (APIs) related to the involved stakeholders.

As result, this framework (shown in Fig. 1) places the HERMES ontology (under the supervision of the ontology specialist) as a central and hermetic semantic silos where multiple rules-based reasoning and queries can be made from multiple actors (i.e. product architect, product design, material expert, process planner) with diverse concerns in the design process.

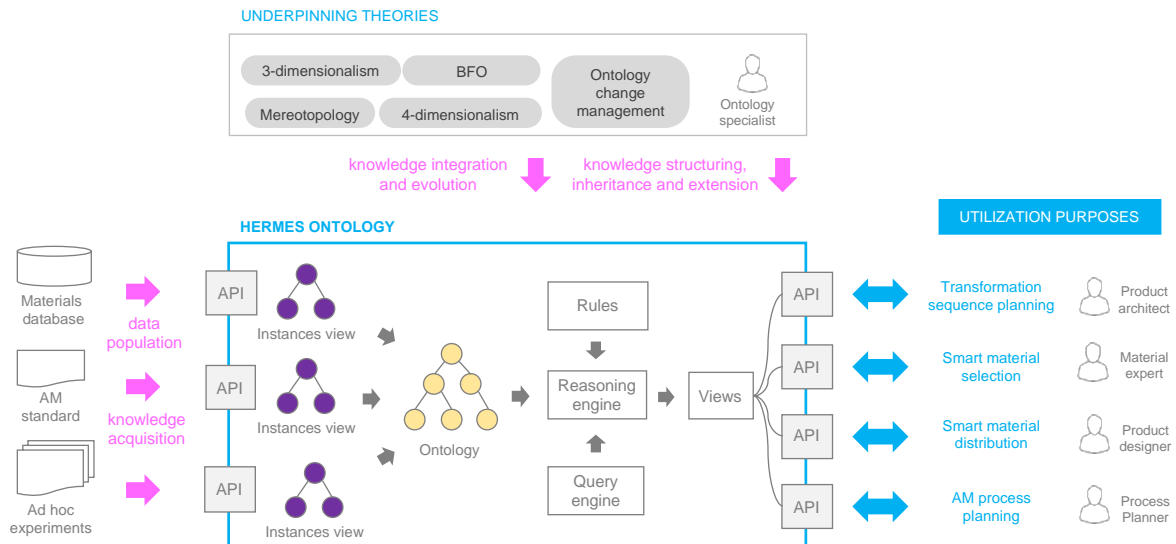


Fig. 1. HERMES ontology-based construction and utilization framework

4. HERMES ontology development

With respect to the aforementioned framework, this section presents the HERMES ontology development. For the sake of clarity, a labelling convention has been adopted as follows: the names of classes are written in capitalised/lower case Arial (i.e. **Part**), the names of attributes and relationships are capitalised/lower case Courier New (i.e. `isParentOf`) while names of instances are in italics Arial (i.e. *Part_1*).

4.1 Classes definition and modelling

As the HERMES ontology has been built 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 Fig. 2). The latter opens great perspective to gather and align multiple domain ontologies with the support of Industry Ontology Foundry (IOF) community and is suitable to apply 3- and 4-dimensionalism theories. The objective of formalizing and representing design for 4D printing knowledge therefore requires **mapping** concepts (later called classes) and properties of the investigated domain, but also to provide formal specifications in order to be computer-interpretable. Figure 2 presents the top-level concepts

of the HERMES ontology built from the upper ontology BFO over continuant and occurrent entities. For the sake of clarity, the upcoming subsections highlight the ontology model through several concerned views such as design and engineering, material, AM process and transformation process.

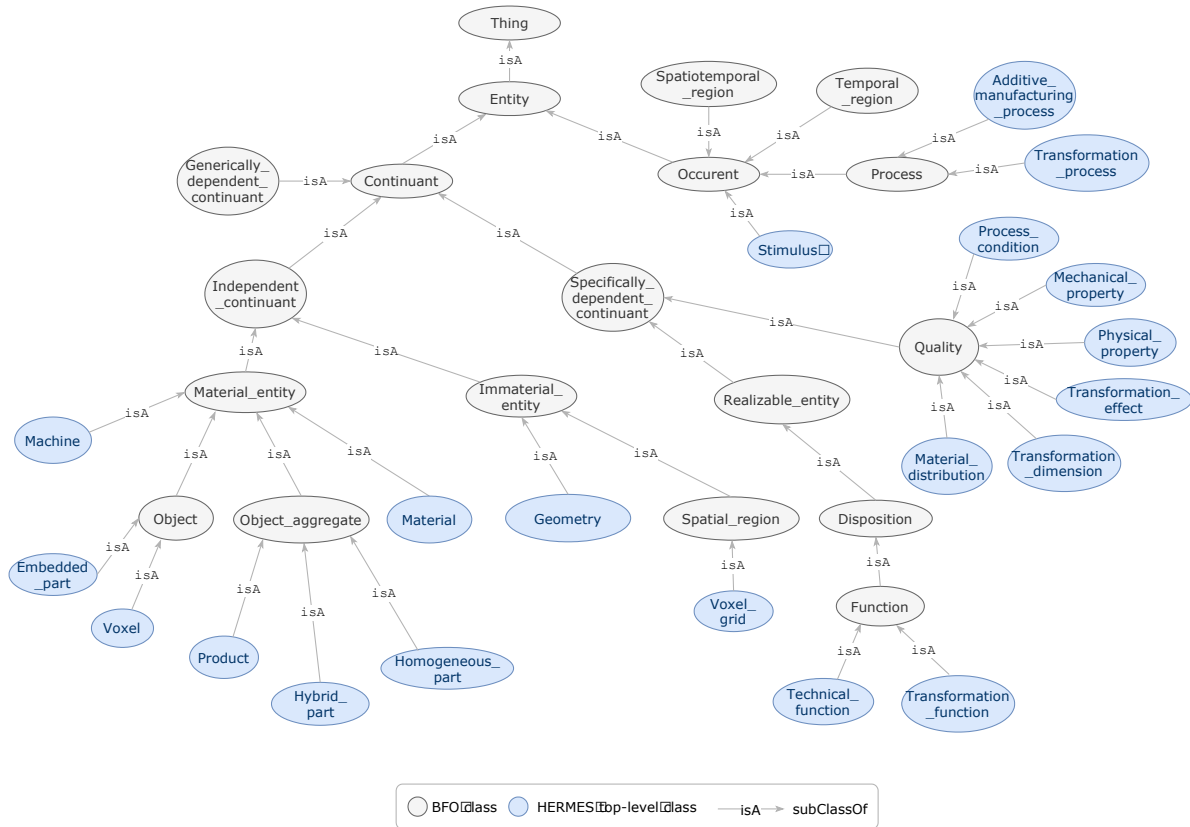


Fig. 2. Top-level concepts of the HERMES Ontology built from BFO

Design and engineering view

The integration of 4D printing knowledge in **mechanical** design requires changes in traditional product models. As this technology mainly features shape, function and property transformations and multi-material printing capabilities, it is indeed important to rethink **about** current established design and engineering models to support multi-perspective knowledge and rules over space and time. Therefore, this view – presented in Fig. 3 – can be considered as an integration driver to connect all 4D printing surrounding aspects. Designing a product/object 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, but not roughly; thus, it provides an interesting knowledge modelling strategy to represent objects with different points of view. For the actual purpose, Object class can concern 4D printed part as a whole with multiple states (e.g. manufacturing state denoted Initial_state, use state denoted Final_state) over space and time, but also 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. The different states and related geometric definitions of the 4D printed objects – which can be either 1D, 2D or 3D – are enabled by the transformation function.

Hence, according to spatiotemporal modelling, 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 for a set of objects. Thus spatiotemporal modelling is a quite heterogeneous domain that supports identifying generic characteristics identification for modelling an entity over time. A spatiotemporal entity is obviously a representation of 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 dynamic part. When the identity of an entity varies, there is a particular evolution of where the spatiotemporal entity is transformed into a new one. It can be defined as the uniqueness of an object, regardless of its attributes or values. It is the feature that distinguishes one object from all others. The identity is essential in the conceptualization and modelling of a phenomenon (Muller, 2002; Del Mondo *et al.*, 2010). 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 aforementioned 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. colour, position and scale in terms of size in a

grid), multiple mechanical properties and multiple materials. It may be refined within a specific spatial resolution and appropriately subdivided with quadtree and/or octree related data structures for numerical analysis or machine learning based reasoning purposes. Voxel can be considered as an enabler to decompose any 3D object in multiple sub-objects to allocate materials, simulate their behaviour or even to increase AM printing capabilities.

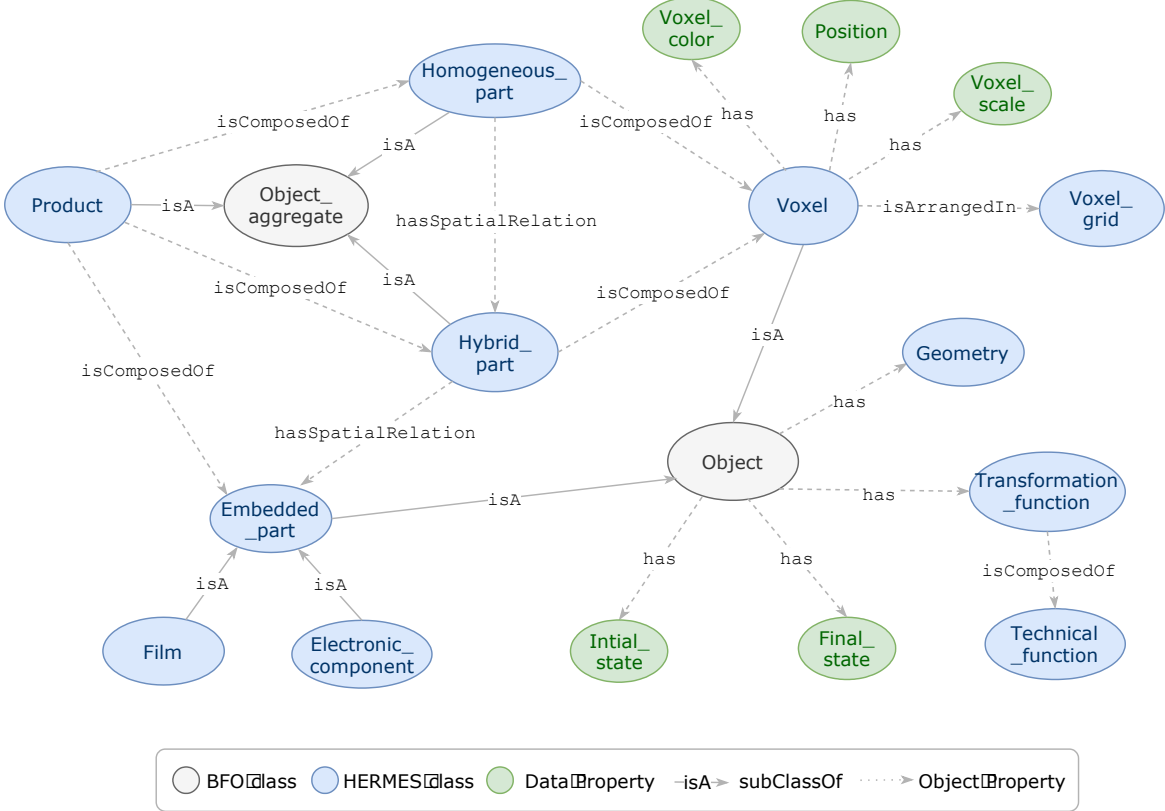


Fig. 3. Design and engineering view with classes and object properties

To meet 4D printing requirements in terms of multi-material product and multi-material printing, such above-mentioned singular objects must be spatially organised to build a 4D printed product/part. As such, Product, Homogeneous_part and Hybrid_part classes have been specified to address different compositions. Homogeneous_part is exclusively composed of one kind of material either active, structural or sacrificial as explicitly presented in Fig. 7. The material typology – partially covered here – will be further defined in the material view. The Hybrid_part class described a part of an object which is composed of at

least two Homogeneous_part(s), therefore providing multi-material modelling capacity. Both classes are obviously composed of set of voxels. Since 4D printing related literature has showed the introduction of embedded parts to enhance transformability with dedicated smart materials, it seems necessary to introduce the Product class. Referring to mechanical design, this class has disposition to gathers material entities like embedded, homogeneous and hybrid parts through spatial and mereotopological relationships. The latter denotes multiple semantic description ranging from topological relations to direction and distance relations, and therefore provides suitable semantics for further qualitative spatial reasoning.

This view exhibits semantically relationships with material and AM process views, whether in the association of objects with materials or AM processes and related machines. In such a context, the design/engineering view is a strategic place with dedicated classes to articulate 4D printing related knowledge (see Fig. 4).

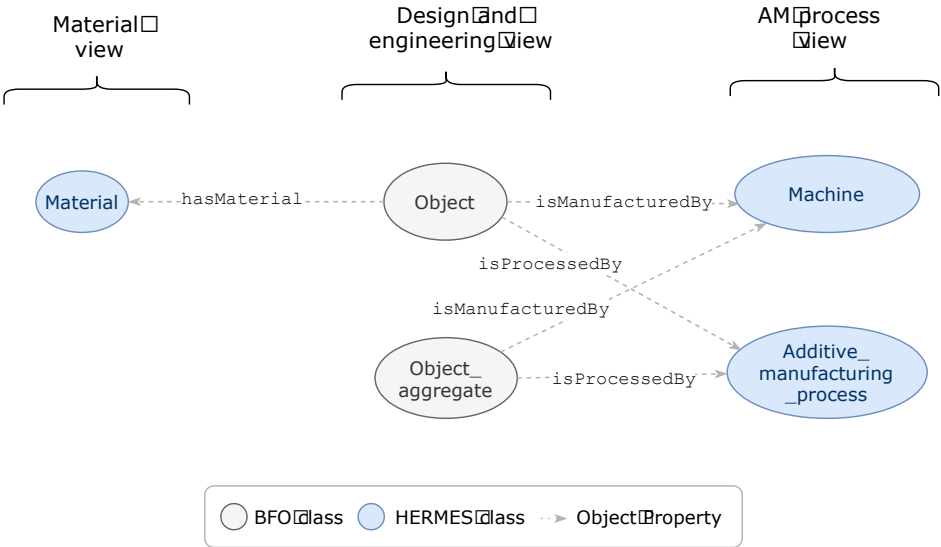


Fig. 4. Semantic associations between Design/engineering view and material and AM process views

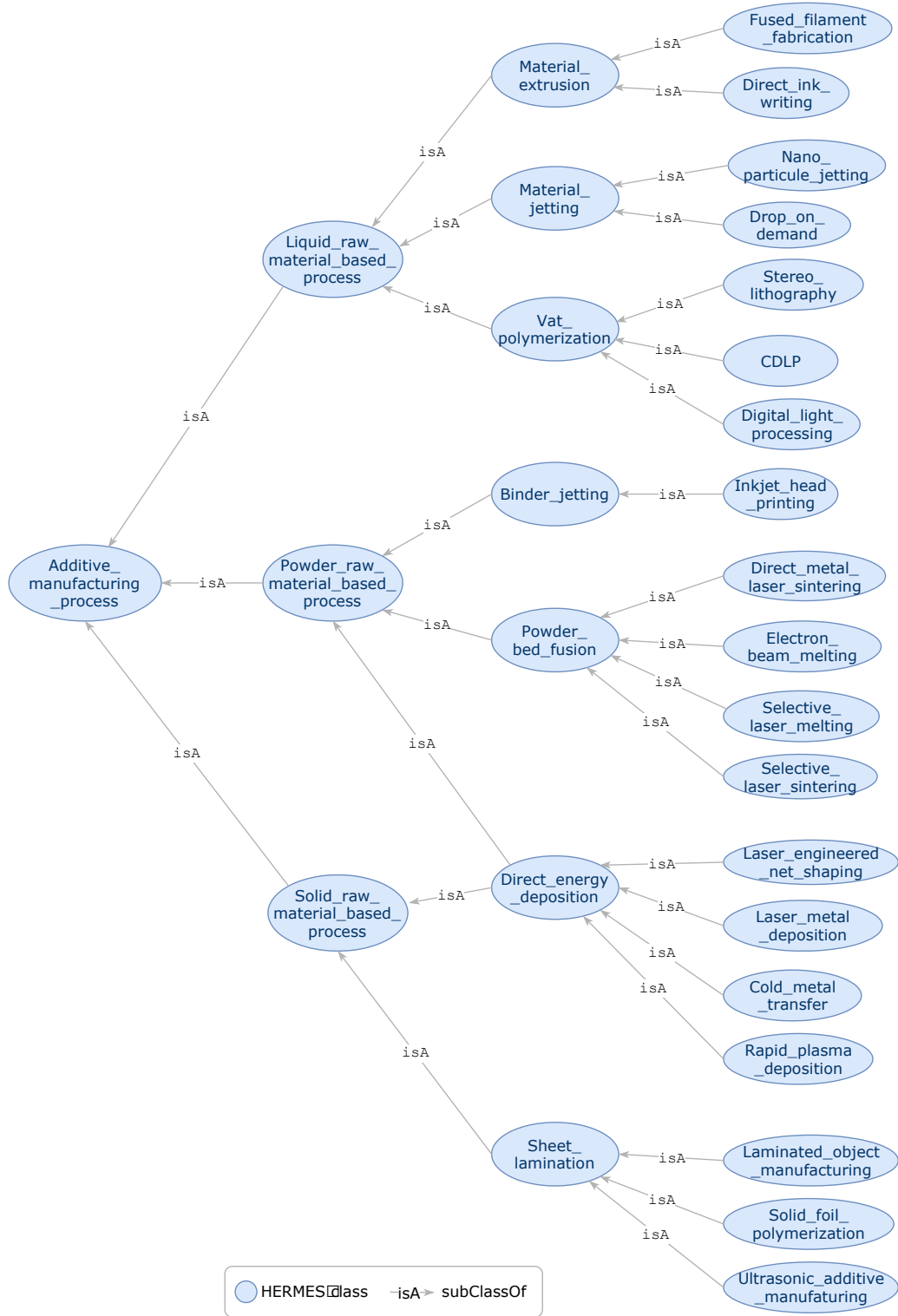


Fig. 5. Part of the AM process view describing AM technologies and techniques

AM process view

Designing for 4D printing demands beforehand to consider **existing** AM process knowledge.

As AM has already been covered by taxonomies and standards (American Society for Testing

and Materials – ASTM Committee F42, Kruth *et al.*, 1998 and Internal Organization for Standardization – ISO Technical Committee 261, ISO/ASTM 52900), this view aims at gathering – through Additive_manufacturing_process class as a subclass of BFO Process class – AM technologies and techniques that could be allocated to stimulus-responsive materials deposition, but also machines and process conditions. As illustrated in Fig. 5, this class has many subclasses in view of different rules likewise the used raw material (solid, liquid and powder) and the applicable technique (Blatteis *et al.*, 2003).

In addition, Machine class – that is a subclass of BFO Material_entity class – enables the elicitation of commercial multi-material printers and **customised** ones. Process_condition class specifies machine control parameters aligning machine capability and material forming requirements. **Among the AM parameters that affects the 4D printing process, one can cite the printing speed, printing path orientation, layer height or even hot end temperature. A variation of these parameters can actually influence object’s geometry quality, mechanical behaviour or even transformation capability.** Fig. 6 presents the view with top-level concepts relating machine, parameters and AM processes and technique, which can be semantically associated with design and engineering objects (as shown Fig. 4).

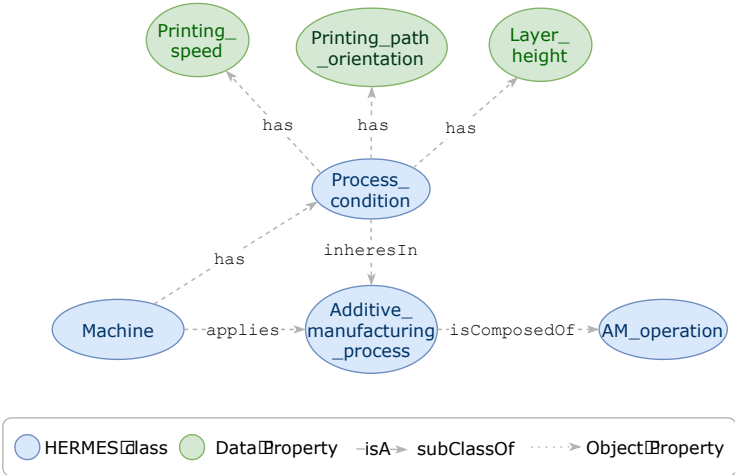


Fig. 6. AM process view with top-level concepts

Material view

In addition to the previous views, material related knowledge can also be seen as a pillar of 4D printing paradigm. Material selection is always addressed to embody the desired mechanical properties, it is indeed a supplementary step to define structure and shape. This is still valid with 4D printing technology; nevertheless, in this actual context, the role of materials is augmented with technical functions or functionalities with respect to the actual aim (i.e. active, structural and sacrificial) in order to cover transformation issue (this aspect will be discussed in the next section). Figure 7 presents the Technical_function class as well as its subclasses that can be used to express technical requirements of transformable systems. Beyond their traditional structural role, materials – covering metal, alloy, composite, polymer and ceramic – from now on embodies smart behaviours. This entails the consideration of SMs from the conceptual design stage in order to define 4D printed parts which can be either composed of a single material (i.e. homogeneous part) or multiple materials (i.e. hybrid part). A material can fulfil a sacrificial function where 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 wide spectrum of stimulus.

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 the next view. In order to carry out a desired transformation of a product/part/structure and also to take advantage of the multi-material printing capabilities, 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 Fig. 8). Here the materials distribution provides design flexibility to distribute mechanical property change within the structure for 3D shape 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 (see Fig. 9).

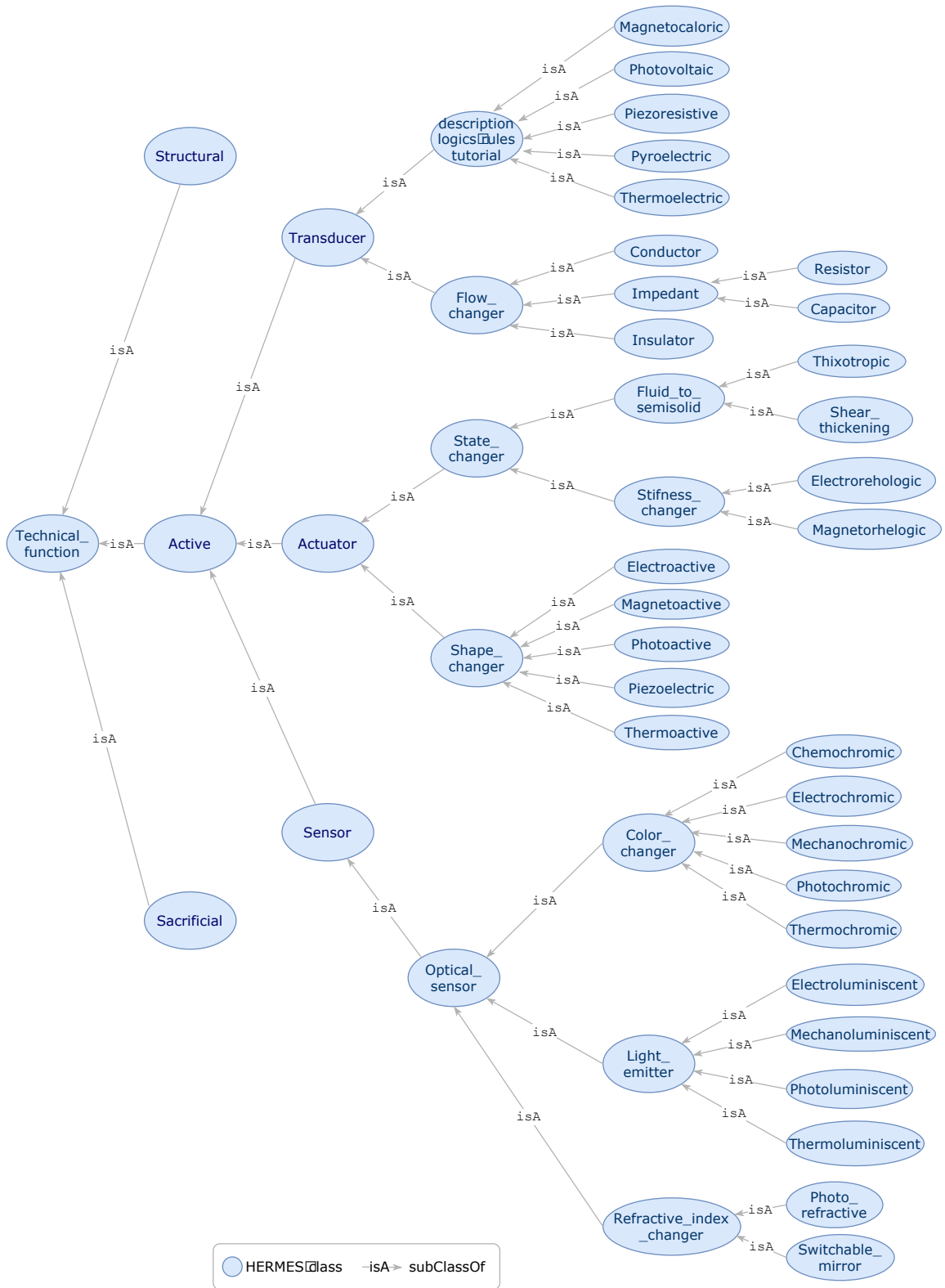


Fig. 7. Definition of the Technical_function taxonomy

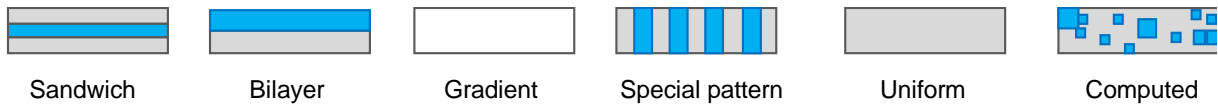


Fig. 8. Material distributions extended from (Momeni *et al.*, 2017)

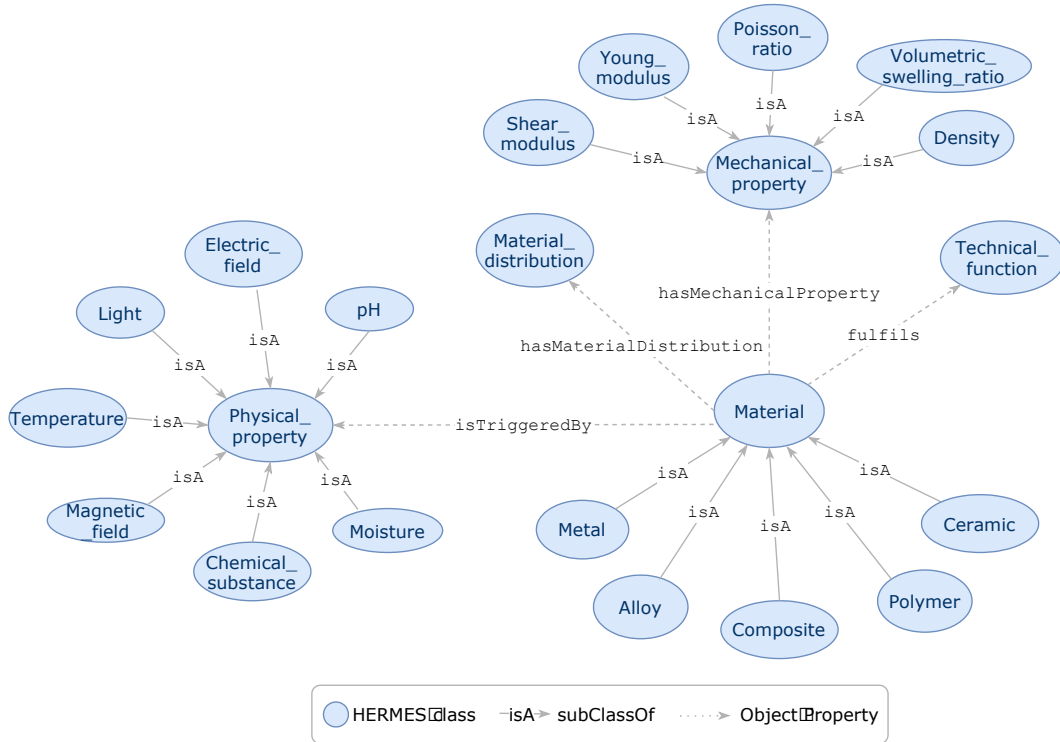


Fig. 9. Material view with classes and object properties

Transformation process View

This view refers to the **inherent** temporal dimension that is inherent to 4D printing. Current product design practices are focused on building static geometric definition related to a specific physical state. In the present objective, it is needed to capture additional knowledge to enable the description of transformable objects over time in terms of shape, functions or property. Thereupon, designing disruptive object requires **beforehand specifying** functional requirements and technical functions as part of inherent transformation function in addition to traditional service and constraint functions that a system/product/part must fulfil. As such, Fig. 10 delineates the transformation process view featuring the key transformation functions

as initiated in (Nam and Pei, 2019).

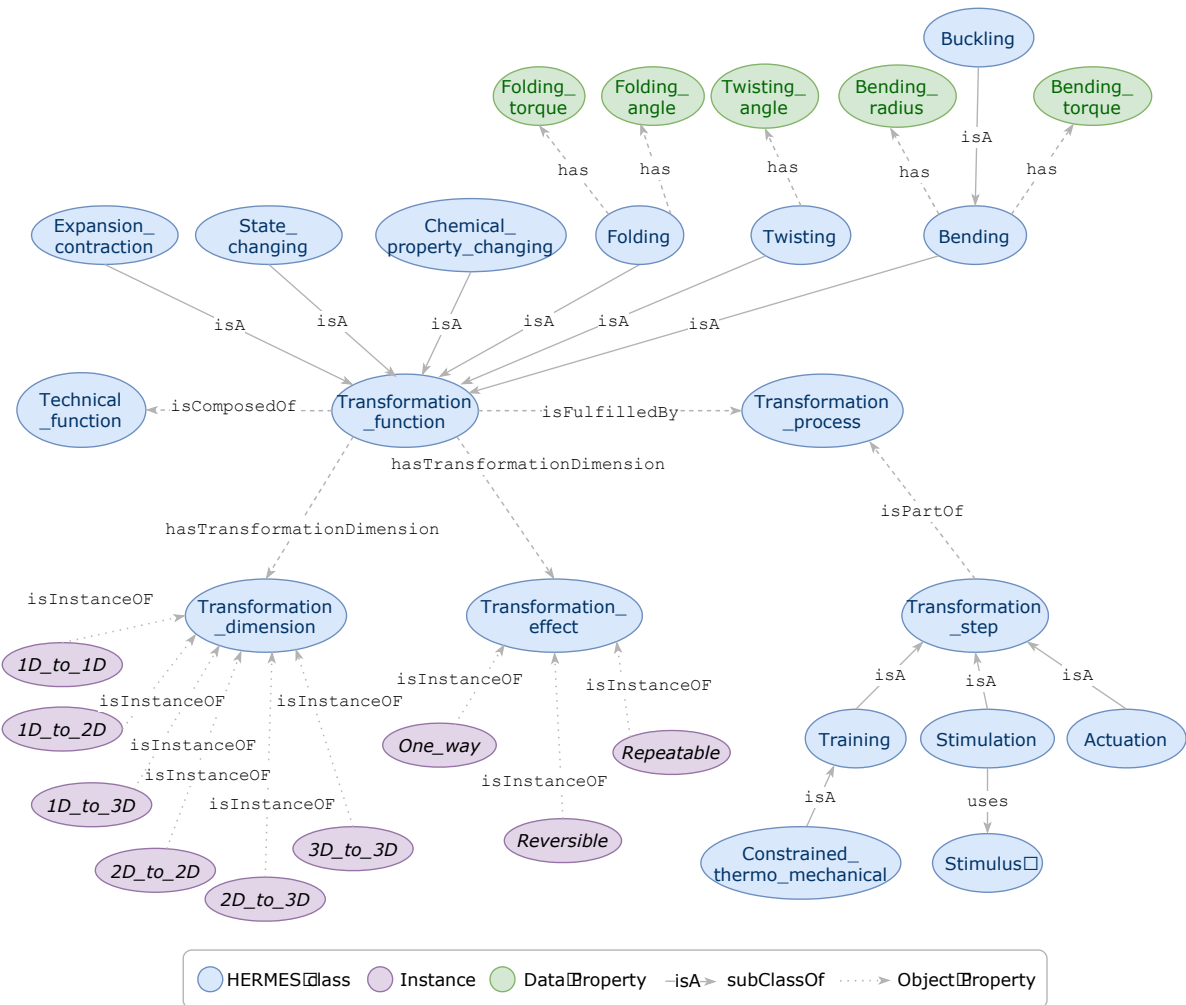


Fig. 10. Transformation process view with classes and object properties

Among such functions (such as illustrated in Fig. 11), one can firstly describe Expansion/Contraction, Twisting, Bending and Folding classes for shape transformations. Chemical_properties_changing is about changesets in colour, swelling ratio, stress or stiffness of such a part/product/structure; and State_changing represents a change of a material state (i.e either liquid or solid).

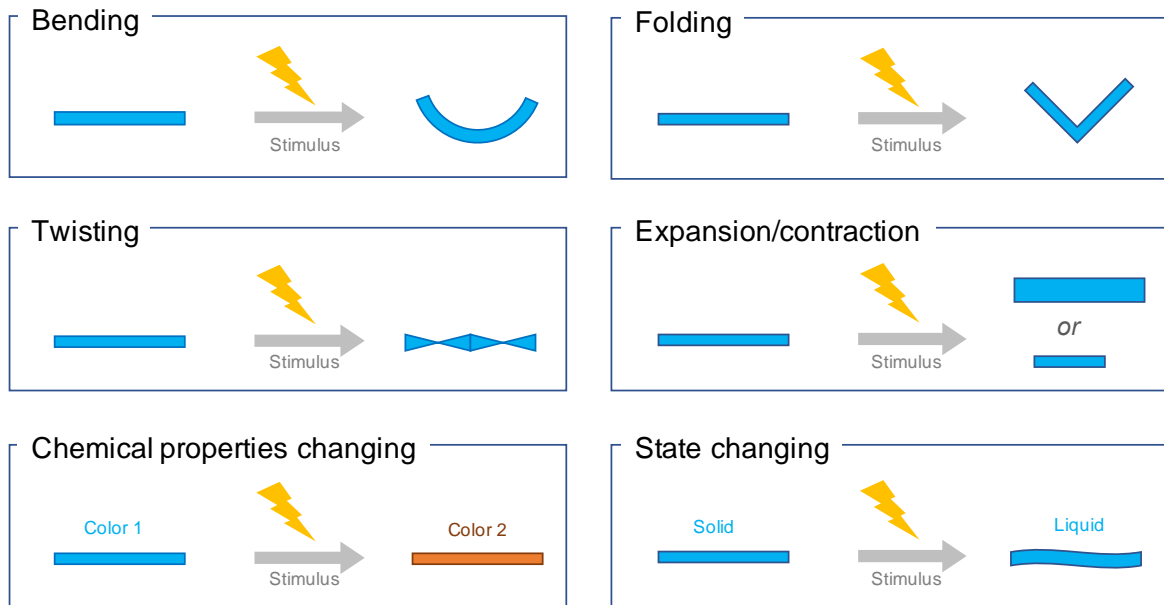


Fig. 11. Transformation functions

Here, one can specify Transformation_function with Dimension and Effect classes in order 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 Fig. 12. *One_way* is the change of an original shape/property to a permanent shape/property after being triggered. As for *Reversible* and *Repeatable*, objects will be able to switch between two states in a single cycle or several ones respectively.

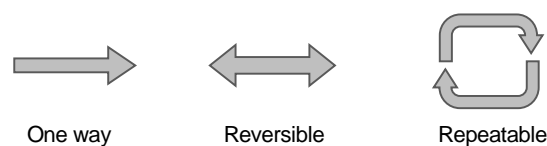


Fig. 12. Transformation effects in 4D printing

In this view, a Transformation_function can be fulfilled by Transformation_process (as a Process class in BFO) that is composed of a set of transformation steps (among Training, Stimulation and Actuation classes) structured and temporally distributed via a Transformation_sequence which is under Temporal_region. Transformation_step is presented as Process class in BFO. The latter class introduces a temporal logic order that is

required to build the targeted shape, property or functionality changes. The Training step is limited to Constrained-Thermo-Mechanics mechanism, in which the trigger is done in a sequential manner. As an example, such step is about heating to the highest critical temperature of the material, application of a strain to the structure, cooling while keeping the strain, the desired shape is hence obtained and to retrieve the initial form/shape the structure should be reheated. Stimulation step consists in applying one or several stimuli (as a subclass of Occurrent in BFO). Exposing smart material to a specific stimulus will require the support of the transformation sequence – ensuring the allocation of appropriate physical property(ies) at the right value at the right place and at the right time with a specific duration – in order to achieve the actuation towards the targeted shape. The stimulus is selected according to the requirements of the application, which will also determine the kind of **SMs** used in the 4D printed structure. Particularly, the Stimulus class in this view is semantically associated **with** the material and design and engineering views as schematised in Fig.13 below.

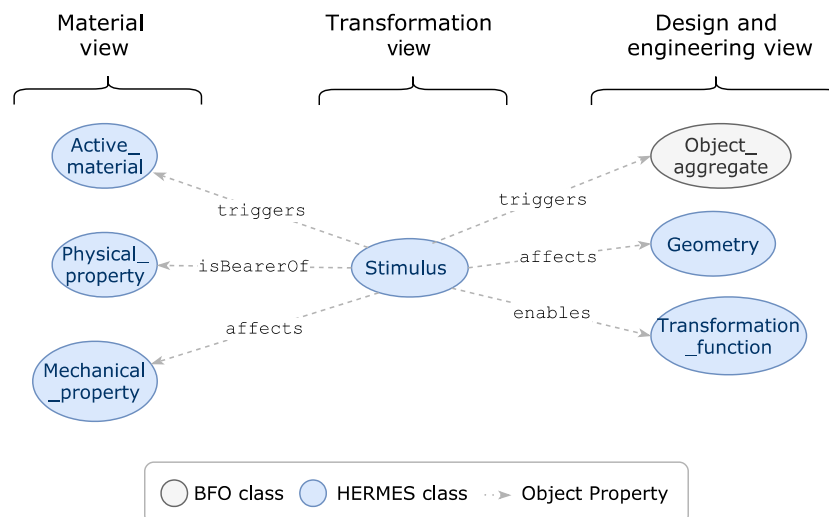


Fig. 13. Semantic relationships between Transformation, material and design and engineering views

4.5 DL rules for classes restriction

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 indeed important to support inference reasoning mechanisms; for instance, consistency checking, subsumption, realization and retrieving. Consistency checking assures the coherence of the presented ontological model with respect to this language. It provides the possibility to reason over it with the appropriate algorithms. In this context, Table 1 highlights relevant DL rules that have been implemented in HERMES ontology. The application of DL rules is useful to structure and classify knowledge, and also to provide a comprehensive machine language which can be further interpretable.

Table 1. DL rules for HERMES class restrictions

Class name	Rule type	DL rule
Product	Min cardinality	Product \sqsubseteq Object_aggregate Product \sqsubseteq (\forall isComposedOf.Hybrid_part \sqcap \exists isComposedOf.Homogeneous_part \sqcap \exists isComposedOf.Embedded_part)
Homogeneous_part	Min cardinality	Homogeneous_part \sqsubseteq Object_aggregate Homogeneous_part \sqsubseteq (\forall isComposedOf.Voxel \sqcap \forall hasSpatialRelation.Hybrid_part)
Hybrid_part	Min cardinality	Hybrid_part \sqsubseteq Object_aggregate Hybrid_part \sqsubseteq (\forall isComposedOf.Voxel \sqcap \exists hasSpatialRelation.Embedded_part)
Voxel	Cardinality	Voxel \sqsubseteq Object Voxel \sqsubseteq (isArrangedIn = 1 Voxel_grid \sqcap has = 1 Position \sqcap has = 1 Color)
Object	Min cardinality	Object \sqsubseteq Material_entity Object \sqsubseteq (\forall has.Geometry \sqcap \forall has.Transformation_function \sqcap \forall has.Material.Material \sqcap isManufacturedBy = 1 Machine \sqcap \forall isProcessedBy.Additive_manufacturing_process)
Transformation_function	Min cardinality	Transformation_function \sqsubseteq Function Transformation_function \sqsubseteq (\forall isComposedOf.Technical_function \sqcap hasTransformationDimension = 1 Transformation_dimension \sqcap hasTransformationEffect = 1 Transformation_effect \sqcap \forall isFulfilledBy.Transformation_process)
Bending	Cardinality	Bending \sqsubseteq Transformation_function Bending \sqsubseteq (has = 1 Bending_torque \sqcap has = 1 Bending_radius)
Twisting	Cardinality	Twisting \sqsubseteq Transformation_function Twisting \sqsubseteq (has = 1 Twisting_angle)
Folding	Cardinality	Folding \sqsubseteq Transformation_function Folding \sqsubseteq (has = 1 Folding_torque \sqcap has = 1 Folding_angle)
Transformation_process	Cardinality	Transformation_process \sqsubseteq isComposedOf = 1 Transformation_step
Stimulation	Cardinality	Stimulation \sqsubseteq Transformation_step Stimulation \sqsubseteq (uses = 1 Stimulus)
Stimulus	Min cardinality	Stimulus \sqsubseteq Occurent Stimulus \sqsubseteq (\forall triggers.Object_aggregate \sqcap \forall affects.Geometry \sqcap enables = 1 Transformation_process \sqcap \forall triggers.Material \sqcap \forall isBearerOf.Physical_property \sqcap \forall affects.Mechanical_property)
Material	Min cardinality	Material \sqsubseteq Material_entity Material \sqsubseteq (\forall fulfils.Technical_function \sqcap \forall hasMechanicalProperty.Mechanical_property \sqcap hasMaterialDistribution = 1 Material_distribution \sqcap isTriggeredBy = 1 Physical_property)
Machine	Min cardinality	Machine \sqsubseteq Material_entity Machine \sqsubseteq (\forall has.Process_condition \sqcap applies = 1 Additive_manufacturing_process \sqcap \forall manufactures.Object)

Process_condition	Cardinality	Process_condition \sqsubseteq Quality Process_condition \sqsubseteq (inheresIn = 1 Additive_manufacturing_process)
Additive_manufacturing_process	Cardinality	Additive_manufacturing_process \sqsubseteq Process Additive_manufacturing_process \sqsubseteq (isAppliedWith=1 Machine $\sqcap \forall$ creates.Object)

5. Illustrative cases

To demonstrate the applicability of the developed HERMES ontology, an implementation has been made in Protégé software and two use cases **are** introduced. The consistency of the ontology **is** checked by using Hermit reasoner and DL rules for classes restrictions have been set up. It is about describing the folding function realised by an origami cube **case** from (Ge *et al.*, 2014) and also a multi-bending actuator similar to the case presented in (Westbrook and Qi, 2008), therefore showing 2D-to-3D and 3D-to-3D transformation dimensions respectively.

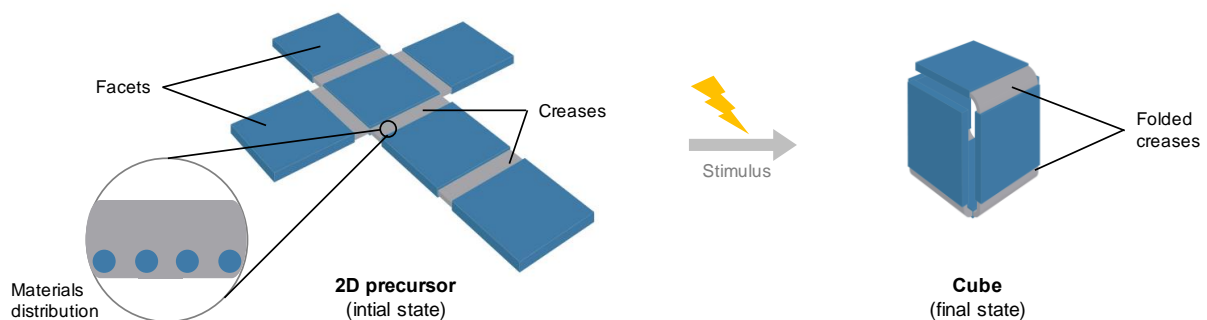


Fig. 14. Active origami cube as case study

The **objective here** is to capture relevant 4D printing knowledge ensuring the transformation from a 2D origami precursor to cube **as illustrated in Fig. 14**. In its actual shape, the HERMES ontology has then been manually populated by the ontology specialist, leading to an instance graph represented in Fig. 15. For the sake of clarity, few features have been selected to show how HERMES ontology represents knowledge on a logical and functional points of view. For instance, voxels and geometry have not been considered here but some common classes in the design and transformation views are illustrated to demonstrate the suitability of the ontology in preliminary design phases. Information about **the 2D_precursor** composition is fully covered by the property *isComposedOf* in order 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 mereotopology 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 view as well as the material view have also been built in order to have a comprehensive knowledge description from conceptual design stage.

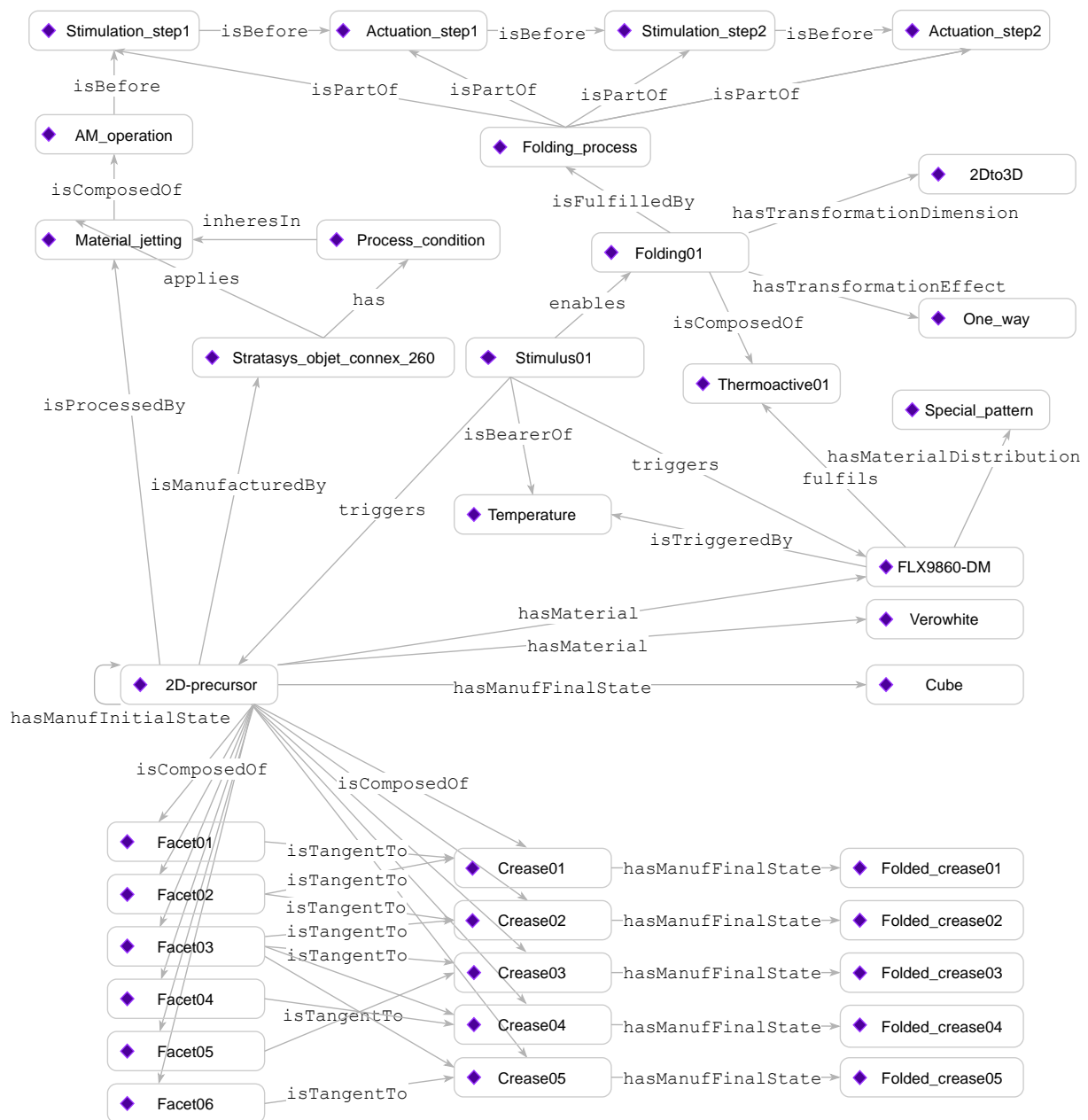


Fig. 15. Instance graph of the active origami cube implemented in Protégé

In the present case study, a *2D_precursor* has two different materials: the active digital material *FLX9860* and the passive *VeroWhite* ones. It exhibits a thermoactive function via a special patterned materials distribution. This multi-material 2D precursor is printed through an appropriate AM machine respecting the main conditions and following a set of universal and agreed operations. These AM operations are 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 Fig. 15).

In addition, a beam is considered as a second illustrative case to realise a bending resulting from multiple contractions. This beam – which actually plays the role of actuator – is represented in various ways in Fig. 16. Starting from a geometric definition, the 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, a Grasshopper plugin within Rhinoceros3D environment (Sossou et al., 2019a, 2019b).

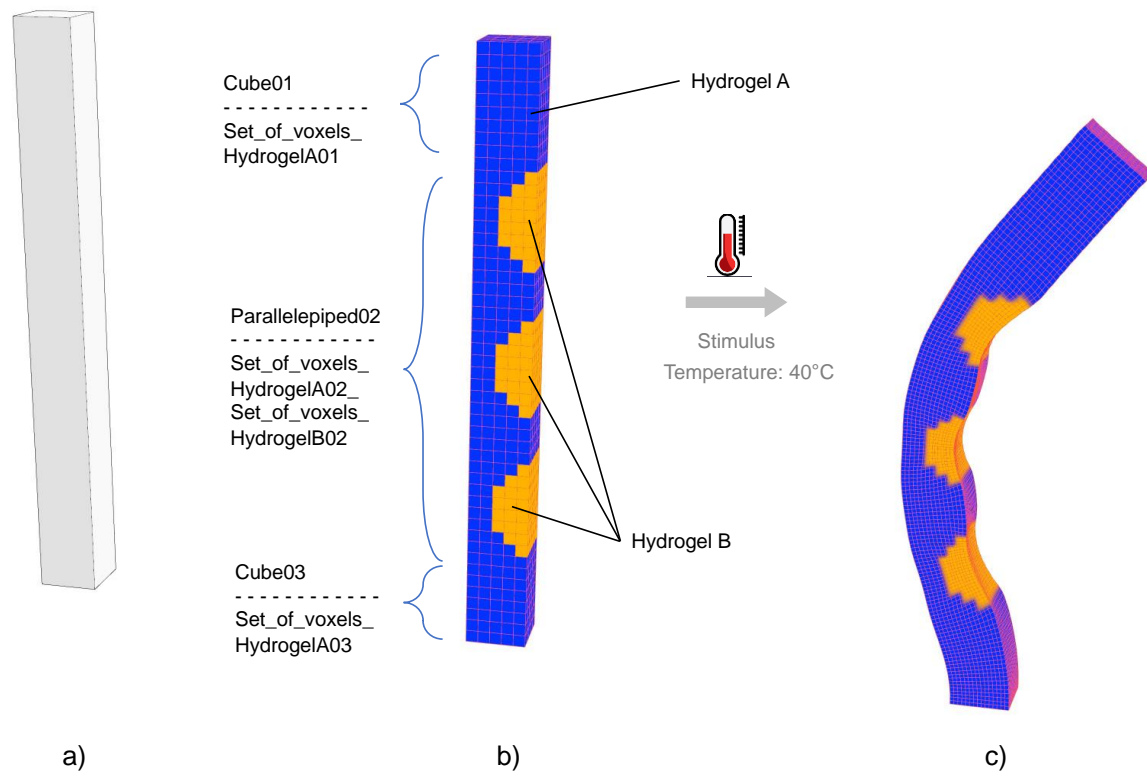


Fig. 16. Actuator as second illustrative case through its (a) 3D representation, (b) voxel-based representation and (c) simulated representation of the transformation through VoxSmart application

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. Among the three identified pieces of the actuator, both extremum sides can be considered as homogeneous parts composed of an hydrogel A (with the following parameters: Young modulus $E=30$ MPa, shear modulus $G= 10$ MPa, relative swollen ratio limit $\nu_{min}=0.01$ and relative collapsed ratio limit $\nu_{max}= 0.4$) and the internal zone refers to the hybrid part with a special pattern distribution of two different materials hydrogels A and B. The latter has similar characteristics but exhibits different swelling ratio such as $\nu_{min}=0.4$ and $\nu_{max}=0.8$. While triggered by its appropriate stimulus (i.e. Lower Critical Solution Temperature (LCST) around 40°C), the thermoactive hydrogel B shrinks in volume; hence the multi-contracted sections created will enable the bending of the whole structure. It is mainly about having different transformation functions via a single triggering. This use case goes beyond the preliminary design phase and illustrates a physical point of view with some mereotopological relations. For instance, on one side, the cubes 01 and 03 are composed of hydrogel A voxels. 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 internal part of*' mereotopological connection. In a same way, cubes 01 and 03 are tangent to 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 Fig. 17), the first defines the contraction steps and the second is for the bending function. Its starts as usual by the AM operations then a stimulation step and ends by an actuation step. As a result, the multi-contraction actuation leads to a bending actuation; they are two steps in parallel. Both use cases are demonstrating how the HERMES ontology is perceiving interlinked concepts and formalising **scattered** knowledge of the 4D printing domain.

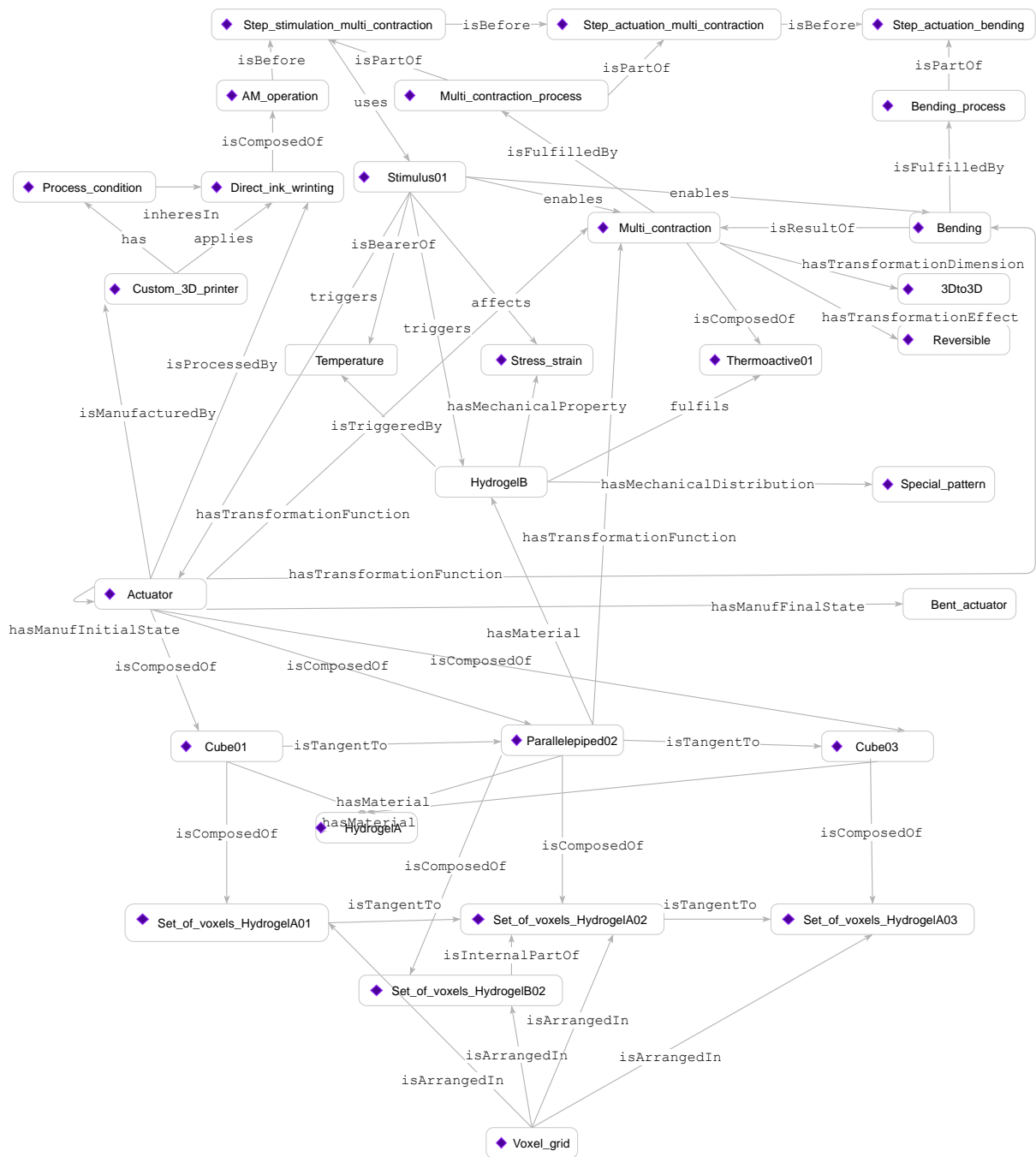


Fig. 17. Instance graph of the actuator case implemented in Protégé

6. Discussions

The proposed research work has highlighted the usefulness of an ontology to federate the scattered knowledge related to the emerging 4D printing technology. It therefore represents a pioneer effort towards knowledge formalisation and representation for multiple purposes (as

introduced in Fig. 2). 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 to 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 aim of capturing 4D printing related knowledge that is aligned with a preliminary design phase. As such, mechanical design is structured in several phases (i.e. preliminary design, embodiment design and detailed design) and steps in order to address different abstraction levels (i.e. functional, logical, physical, etc.). In our opinion, presenting the second case study with further formalisations comparing 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.

However, 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 abundant research advances of this emerging research field, in such a context one may assume that underlying body of knowledge will evolve accordingly. Except for obvious 4D cases, 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. 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 be the consideration of a closed-loop system for ontology implementation which can assure a continue data collection. On the other hand, having a complete understanding of the overall conceptualization provided by such an ontology is often illusory and delicate. It is therefore essential to provide to the involved

stakeholders (i.e. product architect, product designer, material expert, process planner) a custom access to a portion of the corresponding ontology based on their own assumptions. **Such a performance could not only be produced by the proposed views as reported in previous sections; but also by considering a stakeholders based views respecting their different design needs.** At this stage, the investigation has been limited the product/part design for 4D printing. 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.

7. Conclusion and Future Work

The paper underlines a pioneer effort dedicated to the formalisation and representation of 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 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 as a domain ontology, the HERMES ontology has been built upon BFO upper ontology and therefore provide a significant contribution of IOF community regarding 4D printing knowledge. 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, future work will study alignment and interoperability issues between HERMES and EMMO ontology in order to tackle material design aspect. To increase its operational level, several APIs and reasoning-based requests – dedicated to specific purposes like transformation sequence planning, smart material selection and distribution, AM process planning – will be developed. This will ensure the capture and

reuse of appropriate knowledge with appropriate semantic to the right person at the right time. This will particularly be critical for product architects and designers to make right decision during the design process of alive and transformations products/objects. In such a way, special attention will be paid to the integration of HERMES ontology with VoxSmart application in order to combine its inherent symbolic artificial intelligence with machine learning techniques related to voxel-based modelling and computing with smart materials but not limited to.

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