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Abstract The classical material-by-design approach has been extensively perfected by materials scientists, while engineers have been optimising structures geometrically for centuries. The purpose of architected materials is to build bridges across the microscale of materials and the macroscale of engineering structures, to put some geometry in the microstructure. This is a paradigm shift. Materials cannot be considered monolithic anymore. Any set of materials functions, even antagonistic ones, can be envisaged in the future. In this paper, we intend to demonstrate the pertinence of computation for developing architected materials, and the not-so-incidental outcome which led us to developing large-scale additive manufacturing for architectural applications.

Introduction

Materials are ubiquitous in nature and man-made applications, from electronics to transportation or energy, but also biomedical, defence, architecture or construction. Materials have such a predominance in human existence that prehistoric periods were named after materials use (Hummel 2004). Technological progress and its impact on everyday's life are intimately linked with our capacity to control matter in the form of industrialised materials. The classical material-by-design approach has been extensively perfected by materials scientists, while civil engineers and architects have been optimising structures geometrically for centuries. The purpose of architected materials is to build bridges across the microscale of materials and the macroscale of engineering structures, to introduce some geometry within the microstructure. This is a paradigm shift in the sense that materials cannot be considered as monolithic artefacts anymore. Any set of material functions, even antagonistic ones (Steeves et al.

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2007), can be envisaged in the future. The development of architected materials is intrinsically transdisciplinary, on the fringes of physics, chemistry, and mechanical engineering, but also biology, computer science, architecture, design, etc. In this work, we intend to demonstrate the pertinence of a computational approach for developing architected materials, and the not-so-incidental outcome which led us to developing large-scale additive manufacturing for architectural applications. This paper is an extended version of a preliminary conference abstract submitted for the Next Generation Building workshop held at TU Delft in 2016 (Dirrenberger 2017).

The chapter is organised as follows: an introduction to architected materials is given in Sect. 4.2. An overview of the computational tools relevant for the development of such materials is presented in Sect. 4.3. The translation of architected materials concepts to the architectural scale corresponds to Sect. 4.4. Finally, conclusions and perspectives are postponed to Sect. 4.5.

Architected Materials

Many industrial applications require new materials with enhanced specific properties, i.e. performance per unit of mass; this is especially true for the transportation and biomedical sectors. For instance, the automotive industry, with its ever increasing requirements regarding passenger safety and fuel consumption, is an edifying example: nowadays, classical steel-based material solutions are being challenged by new lightweight aluminium alloys and advanced composites. A response from steel manufacturers was the development of advanced high-strength steels (AHSS) for yield strength designed parts in order to reduce both thickness and mass. AHSS with very high strength (1000 MPa and more) commonly exhibit poor sheet formability hence limiting the mass reduction attainable. This is especially true for martensite-based AHSS such as dual-phase (DP), complex phase (CP) and martensitic (MS) steels, depending on their martensite content. The higher the martensite content, the lower the thin-sheet formability. In order to mitigate failure and tearing of thin-sheets during deformation-based forming (stamping, blanking, etc.), a possible solution is to rely on the concept of localised heat treatment in order to soften the material where needed by locally annealing martensite, hence changing the local yield strength/ductility trade-off. Introducing such geometrical discontinuities in terms of material behaviour is characteristic of architected materials.

Architected materials are a rising class of materials that bring new possibilities in terms of functional properties, filling the gaps and pushing the limits of Ashby's materials performance maps (Ashby and Bréchet 2003). The term architected materials encompasses any microstructure designed in a thoughtful fashion, such that some of its materials properties, e.g. yield strength/density, have been improved in comparison to those of its constituents, due to both structure and composite effects, which depend on the multiphase morphology, i.e. the relative topological arrangement between each phase (Ashby and Bréchet 2003; Bouaziz et al. 2008; Bréchet and Embury 2013). Localised material processing methods, such as additive

manufacturing, or localised laser heat treatment in the case of AHSS, appear as natural candidates for developing architected materials.

There are many examples: particulate and fibrous composites, foams, sandwich structures, woven materials, lattice structures, etc. with different objectives. For instance, developing architected porous materials for structural, acoustic and insulation properties (Coty et al. 2008; Fallet et al. 2008), entangled monofilament of perlitic steel (Courtois et al. 2012), sandwich composite structures (Kolopp et al. 2013), segmented interlocking structures (Djumas et al. 2016), woven and non-woven textile composites (Mezeix et al. 2009; Lewandowski et al. 2012; Dirrenberger et al. 2014), crumpled metallic foils (Bouaziz et al. 2013), etc. Architected materials have been an exciting research topic in recent years, especially regarding the processing of architected metallic foams (Brothers and Dunand 2006; Erk et al. 2008), multi-scale architected ceramics (Mirkhalaf et al. 2014), or architected metallic sheets (Embury and Bouaziz 2010; Chéhab et al. 2009). Apart from processing, most efforts have been focused on the modelling of architected materials. In particular, the pioneering works done on truss-structures (Deshpande et al. 2001) and metallic foams (Deshpande and Fleck 2000) led to useful results for the modelling of architected materials (Fleck et al. 2010). The mechanical modelling of bio-inspired architected materials has been pursued successfully, yielding results for multi-layered materials that could be used for modelling architected metallic sheets (Turcaud et al. 2011; Stoychev et al. 2012). Other works demonstrated the interest for designing recursive or nested material architectures to achieve enhanced specific mechanical properties (Ajdari et al. 2012; Rayneau-Kirkhope et al. 2012); finally, elastic instabilities have been considered for shape-generation of architected materials (Bertoldi et al. 2010; Shim et al. 2013).

One can play on many parameters in order to obtain architected materials, but all of them are related either to the microstructure or the geometry. Parameters related to the microstructure can be optimised for specific needs using a materials-by-design approach, which has been thoroughly developed by chemists, materials scientists and metallurgists. Properties improvements related to microstructural design are intrinsically linked to the synthesis and processing of materials and are therefore due to micro and nanoscale phenomena, taking place at a scale ranging from 1 nm to 10 μm . This scale is below the scope of the present chapter, in terms of topology optimisation, but has been extensively studied in the literature (Embury and Bouaziz 2010; Olson 2001; Freeman 2012).

Until now, most architected materials in the literature have been obtained empirically. By capitalising on the concept of localised processing of thin structures, our efforts at the PIMM laboratory¹ have been focused on developing systematic tools to determine materials architecturation patterns, for a given set of requirements. For instance, these patterns come as an output from a computational shape-optimisation loop developed around a heuristic generative geometry module, based on cellular automata (CA), and a cost function evaluation module, based on the finite element (FE) method. This cost function has to be minimised for given constraints (Bendsøe

and Sigmund 2004). In the case of linear elastic problems, the cost function can be related to the elastic energy density computed by numerical homogenisation at the scale of the structure (Allaire 2002). The cost function value is then used as a feedback, and an optimised shape is generated accordingly following a specific evolution algorithm. The spatial resolution associated with the shape-optimisation can be chosen to be relevant for localised laser treatment, i.e. 1 mm, corresponding to a representative scale of the underlying microstructure (Bironeau et al. 2016); this allows us to use homogenised behaviour for each grid-cell in the simulation (Dirrenberger 2012).

From a macroscopic viewpoint, parameters related to the geometry have mainly been the responsibility of structural and civil engineers for centuries: to efficiently distribute materials within structures. An obvious example would be the many different strategies available for building bridges. At the millimetre scale, materials can be considered as structures, i.e. one can enhance the bending stiffness of a component by modifying its geometry while keeping the lineic mass (for beams) or surfacic mass (for plates) unchanged (Weaver and Ashby 1996). On the other hand, one might need a lower flexural strength for specific applications, with the same lineic and/or surfacic masses. This can be achieved with strand structures, i.e. by creating topological interfaces in the material. Processing remains the key technological issue for further development of architected materials, and progress is made every day in this direction at the lab scale, as it was done in (Schaedler et al. 2011) by using a sequence of several processing techniques in order to fabricate ultralight metallic microlattice materials (Schaedler and Carter 2016). There is still a long way to go for the industry to actually apply architected materials in product manufacturing.

Architected materials lie between the microscale and the macroscale. This class of materials involves geometrically engineered distributions of microstructural phases at a scale comparable to the scale of the component (Ashby and Bréchet 2003; Bouaziz et al. 2008; Bréchet and Embury 2013), thus calling for enriched models of continuum mechanics in order to determine the effective properties of materials (Geers and Yvonnet 2016; Matouš et al. 2017), e.g. generalised continua theories, in order to describe the behaviour of architected materials, such as strain-gradient elasticity (Auffray et al. 2015), and strain-gradient plasticity. This topic has been especially fruitful these last few years in the mechanics of materials community (Lebée and Sab 2012; Trinh et al. 2012; Chen et al. 2014; Auffray et al. 2015; Placidi and El Dhaba 2015; Rosi and Auffray 2016; Andreus et al. 2016; Placidi et al. 2017; dell'Isola et al. 2017); this results in the availability of versatile models able to describe the various situations encountered with architected materials. Given mature processing techniques, architected materials are promised to a bright future in industrial applications due to their enticing customisable specific properties and the opportunity of multifunctionality.

When considering actual applications, one engineering challenge is to predict the effective properties of such materials; computational homogenisation using finite element analysis is a powerful tool to do so. Homogenised behaviour of architected materials can thus be used in large structural computations, hence enabling the dissemination of architected materials in the industry. Furthermore, computational

homogenisation is the basis for computational topology optimisation (Allaire 2002; Bendsøe and Sigmund 2004; Guest and Prévost 2006; Challis et al. 2008; Xu et al. 2016; Vicente et al. 2016; Xu et al. 2016; Salonitis et al. 2017; Asadpoure et al. 2017; Khakalo and Niiranen 2017; Wang et al. 2017) which will give rise to the next generation of architected materials as it can already be seen in the works of (Laszczyk et al. 2009; Andreassen et al. 2014; Körner and Liebold-Ribeiro 2015; Hopkins et al. 2016; Kotani and Ikeda 2016; Ghaedizadeh et al. 2016; Ren et al. 2016; Liu et al. 2016; Dalaq et al. 2016).

Materials science comes from the following fact: microstructural heterogeneities play a critical role in the macroscopic behaviour of a material (Besson et al. 2010; Bornert et al. 2001; Jeulin and Ostoja-Starzewski 2001; François et al. 2012; Torquato 2001; Ostoja-Starzewski 2008). Constitutive modelling, thanks to an interaction between experiments and simulation, is usually able to describe the response of most materials in use. Such phenomenological models, including little to no information about the microstructure, cannot necessarily account for local fluctuation of properties. In that case, the material is considered as a homogeneous medium. Studying the behaviour of heterogeneous materials involves developing enriched models including morphological information about the microstructure (Smith and Torquato 1988; Yeong and Torquato 1998; Torquato et al. 1998; Decker et al. 1998; Jeulin 2000; Kanit et al. 2006; Peyrega et al. 2011; Jean et al. 2011; Escoda et al. 2015). These models should be robust enough to predict effective properties depending on statistical data (volume fraction, n -point correlation function, etc.) and the physical nature of each phase or constituent. As a matter of fact, advanced models are often restricted to a limited variety of materials. Although isotropic and anisotropic polycrystalline metals, for instance, have been extensively studied by the means of both analytical and computational tools (Cailletaud et al. 2003; Kanit et al. 2003; Madi et al. 2007; Berdin et al. 2013; Fritzen et al. 2013; Hor et al. 2014; Kowalski et al. 2016; Amodeo et al. 2016; Schindler et al. 2017), architected materials bring up new challenges regarding the determination of effective properties.

The development of architected materials is related to the availability of appropriate computational tools for both design and modelling, but also for computerised manufacturing as for the various additive manufacturing techniques considered to produce architected materials.

Computation for Design, Modelling, and Manufacturing

The merit of additive manufacturing is often summarised as its ability to produce shapes that result from a topology optimisation process. Topology optimisation aims at attaining the most efficient structure for a given set of requirements. It is a long-standing topic of research and development for engineers that can be traced back to the seminal work of (Michell 1904) on frame structures one century ago, or even 30

years earlier with (Lévy 1874), who gave the first proof for determinacy in statics for single-load trusses. The topic of optimisation has been active ever since. Nowadays, optimality in terms of industrial design is becoming more and more critical due to scarcity of material resources and the need for lightweight structures.

This technique has become well-established in the field of structural mechanics, especially when associated with FE simulation. Classical methods (Bendsøe and Kikuchi 1988; Rozvany 1995; Duysinx and Bendsøe 1998), such as SIMP (Bendsøe and Sigmund 2004) (Solid Isotropic Material with Penalisation) rely on node-based values to evaluate and optimise the geometry, i.e. the number of design variables is equal to the number of elements available in the model at initialisation. Then, the optimisation procedure consists in determining at each element if it should either stay a material element or become a void element, i.e. be removed. This technique has been applied to different scales: for instance with regards to the design of efficient building structures (Cui et al. 2003), or as a tool for designing micro- and nano-architected materials (Zhou and Li 2008).

Most computational approaches for topology optimisation used in engineering are gradient-based, they are also known as local approaches. In recent years, so-called global approaches emerged, and are currently subject to epistemological controversy in the optimisation community due to the lack of proof for global convergence, as well as inefficiency in comparison with classical gradient methods (Sigmund 2011; Le Riche and Haftka 2012). Although the fact that being based on heuristics has been held against global approaches in structural mechanics, heuristics itself should not be considered a shortcoming but rather an epistemological hypothesis.

The computational framework being developed at PIMM rely on a global topology-optimisation approach making use of cellular automata, as well as FE for evaluating of the cost function, which has to be minimised for given constraints (Bendsøe and Sigmund 2004). This evaluation step is straightforward since it consists in performing a FE computation on the generated model using predefined local constitutive behaviours, and averaging the response of the structure, to a given set of boundary conditions and applied loads, by the computational homogenisation method (Dirrenberger et al. 2011, 2012, 2013, 2014). The topology optimisation step is somewhat more difficult as choices have to be made with regards to the many approaches available and the type of problem being dealt with. Several reviews are available on this topic, see for instance (Bendsøe and Sigmund 2004; Rozvany 2009; Eschenauer and Olhoff 2001). Most developments in topology optimisation dealt with the efficiency of structures, i.e. minimising the mass of materials while optimising the elastic stiffness of a structure under a given load, which means choosing between void and matter for any given point in the design space, either continuous (Allaire 2002) or discrete (Bendsøe and Sigmund 2004).

Architecturation patterns can be either continuous, discrete, periodic or random, therefore cellular automata (CA) seem like natural candidates for generating them. CA correspond to an evolving structure based on a regular lattice, they are characterised by 5 properties: lattice geometry and dimensionality, cellular neighbourhood, cell state, local rule of transition, and boundary conditions. CA have already been used for topological optimisation, but not for solving pattern-type problems (Hajela

and Kim 2001; Missoum et al. 2005; Hopman and Leamy 2010). An alternative method, the hybrid cellular automata (HCA) method, was proposed by (Tovar et al. 2004) by taking the best of both CA and SIMP. This method has been developed thoroughly for structural optimisation (Tovar et al. 2007). A critical improvement to the CA approach was the implementation of multigrid methods in order to accelerate the convergence during optimisation (Kim et al. 2004; Zakhama et al. 2009). The development of genetic algorithms in structural optimisation is known as evolutionary structural optimisation (ESO). It was first proposed by (Xie and Steven 1993; Chu et al. 1996) in the early 1990s, but suffered from various drawbacks (lack of convergence, mesh-dependency) which were partially overcome by the bi-directional evolutionary structural optimisation (BESO) approach developed by the same team a decade later (Huang and Xie 2007). Other developments have been undertaken regarding genetic algorithms, e.g. in terms of multi-criterion optimisation (Canyurt and Hajela 2010).

Therefore, a framework based on CA with a local rule of transition using the BESO approach, along with multigrid implementation appears like an appropriate option to design architected materials, especially by the ability of such framework to deal with multiple scales of topology optimisation. In order to be fully efficient, the multiscale optimisation scheme must comply with optimising multiple anisotropic materials with nonlinear elastoplastic behaviour, which will yield nonlinearities in structural response of the architected materials for various sets of requirements/cases of application, in terms of ductile fracture or fatigue properties (Torabian et al. 2016a, b, 2017a, b).

Generating and modelling shapes for additive manufacturing follows specific rules, coming from both processing constraints, e.g. layer thickness, product dimensions, etc., and the functional properties of the produced part, e.g. mechanical strength, thermal conductivity, etc. An usual and straightforward method for generating an additive manufacturing building path is to use a 3D-to-2D slicing software. It consists in slicing the 3D shape, i.e. computer-aided design (CAD) file, of an object into flat thin layers of constant thickness which can be layered one up onto the other, i.e. computer-aided manufacturing (CAM) file. This results in a cantilever-method strategy. Each layer is then made of a contour line, as well as a filling pattern such as a honeycomb structure or a space-filling curve (Peano curve, Hilbert curve, etc.); the filling density can be adjusted for given requirements. This method is well-established for small-scale additive manufacturing.

Development of the Large-Scale Additive Manufacturing

The industrial applications of small-scale additive manufacturing in production (in opposition to prototyping) concern either geometrically complex products in high value-adding sectors (biomedical, sports, aerospace) and/or parts made of costly materials, typically alloys which include Titanium, Nickel and/or Chrome in their

composition. This type of additive manufacturing is usually powder-based, which is intrinsically costly, but enables very good spatial accuracy and microstructural control. Technologies such as direct metal laser sintering (DMLS), selective laser sintering (SLS), electron beam melting (EBM) or direct metal deposition (DMD) are taking off in high-end industries due to its cost-saving possibilities both in terms of reducing the number manufacturing steps and the amount of materials used (Gutowski et al. 2009; Allwood et al. 2011; Yoon et al. 2014; Baumann et al. 2016; Ford and Despeisse 2016).

The DEMOCRITE project (2014–2015, funded by HESAM Université) aimed at transposing such possibilities within an architectural context, i.e. developing large-scale additive manufacturing with the same level of material performance than conventional processing methods and comparable accuracy as DMLS, i.e. a spatial resolution circa 0.1% of the building size, about 1 mm for a metre-wide printer. Our group at the PIMM lab explored the potential applications of large-scale additive manufacturing techniques to civil engineering structures. Thanks to this large-scale processing technique, one could apply the concept of architected materials within an architectural context; multifunctional properties can be achieved for structural elements, by optimising geometry and material composition, as it was done in Gosselin et al. (2016), for an enhanced thermal insulation case study regarding a structural wall element produced by large-scale additive manufacturing. An example of topology optimisation based on the SIMP approach, performed during the DEMOCRITE project is given in Fig. 4.1. The initial optimisation results (Fig. 4.1a) were adapted and refined in order to fit the additive manufacturing constraints as well as the architectural scenario. The rendering shown on Fig. 4.1b actually includes the visible layers of printed concrete resulting from the building process.

Based upon an understanding of the limitations identified in previous projects present in the literature, the DEMOCRITE project dealt with the large-scale additive

Fig. 4.1 An example of implementation of topology optimisation in the DEMOCRITE project: **a** Boundary conditions and results for the structural optimisation problem; **b** Rendering of the actual multifunctional wall including both the structural and thermal insulation parts

manufacturing of selective deposition for ultra-high performance concrete (UHPC) (Duballet et al. 2015). The 3D printing process involved is based on a Fused Deposition Modelling-like technique, in the sense that a material is deposited layer-by-layer through an extrusion printhead. The project also explored the possibilities offered by CAD and optimisation, and their integration within the product design process in the case of large-scale additive manufacturing. Thus, the introduced technology succeeded in solving many of the problems that could be found in the literature. Most notably, the process enabled the production of 3D large-scale complex geometries, without the use of temporary supports, as opposed to 2.5D examples found in the literature for concrete 3D printing (Khoshnevis 2004; Buswell et al. 2007; Cesaretti et al. 2014).

According to Gosselin et al. (2016), the concept of freeform commonly used in the literature is not adequate nor sufficient for describing concrete 3D printing. For a given printing process and automation complexity, one can attain specific types of topologies within a given time-frame and performance criterion for the material and/or structure to be built. Design conditions for large-scale additive manufacturing depend on many other parameters than just the properties of extruded cementitious materials; parameters such as the printing spatial resolution, overall size of parts to be printed, the environment, the presence of assembling steps, etc. A tentative classification of such relationships between geometrical complexity, processing, and design is proposed in Duballet et al. (2017). The cantilever strategy, which is characteristic of small-scale additive manufacturing, is not appropriate for large-scale printing since it does not take into account the processing constraints and their impact on the performance of the printed structure. The building path should be adapted and optimized based on simulation results in order to take into account constraints and to exhibit more robustness for complex geometries.

The processing constraints depend mostly on the fresh material properties in its viscous state, as well as early-age behaviour, in interaction with the building strategy and the stiffness of the structure being built. On the other hand, functional requirements will depend on the properties of the hardened material, its durability (Lecampion et al. 2011), as well as the structural geometry for effective stiffness, and other functional properties such as thermal and sound insulation. See Gosselin et al. (2016) for a geometrically induced thermal insulation case study. Both types of constraints have to be considered at the design stage.

Printing path generation is a critical step during the design phase. There are two main approaches to tool-path generation in the context of 3D printing: (1) 3D-to-2D slicing, which is by far the most common method adopted, yields planar layers of equal thickness built on top of each other. This approach is not optimal from a design and structural viewpoint as it will induce cantilevers when two consecutive layers have different sizes and limit the attainable geometries; (2) the tangential continuity method, which has been introduced in Gosselin et al. (2016) in order to optimise the structure being built by creating layers of varying thickness. These layers exhibit a maximised surface area of contact between each other, hence stabilising the overall structure. Moreover, this method is actually exploiting the possibilities

Fig. 4.2 The stand-alone concrete additive manufacturing process developed during the DEMOCRITE project, currently being implemented commercially by XtreeE

of the process in terms of printing speed and flow for generating variations in the layer thickness. Capitalising on the relative success of the DEMOCRITE project, a spin-off company, XtreeE,² was created in order to develop and commercialise the 3D printing technology introduced. The large-scale robotic additive manufacturing process for concrete presented in Fig. 4.2 was developed during the DEMOCRITE project before being applied within the construction industry by XtreeE.

Figure 4.3 shows a 3D-printed 4 metre-high post supporting the playground roof of a school in Aix-en-Provence, France, produced by XtreeE. The structure was made of two parts: the 3D-printed envelope, used as a lost formwork, and the core, made of conventional cast concrete. The total printing time was 15 h and 30 min.

A driving force for additive manufacturing is its ability to produce more complex 3D shapes in comparison to casting or subtractive processes. This complexity allows to design optimal structures based on topology optimisation techniques. One of the main current challenges is to modify optimisation algorithms in order to account for the additive manufacturing constraints, especially with regards to the processing parameters and structural stability while printing. A possible answer to these challenges would be to consider the multiphysics phenomenon aspect of 3D printing, which involves the elastic stability of the overall structure being built, the kinetics

Fig. 4.3 Close-up view of a 4 metre-high post in Aix-en-Provence, France. Source www.xtreee.com

of hydration, the evolving viscoplasticity of fresh cement, the evolution of temperature within the printing environment, etc. As a matter of fact, all these physical problems, with multiple time and space scales, can be modelled on their own, but coupling them generates complexity and uncertainty regarding the process of 3D printing. Therefore, efforts should be concentrated on understanding and modelling the printing process in its multiple physical aspects, only then optimisation will be fully integrated with the processing, which would virtually change the way 3D printed structures are conceived today. An attempt at multi-objective optimisation for thermal, mechanical and economical criteria, in the context of a hybrid large-scale concrete 3D printing and assembling process, was proposed by Duballet et al. (2018). It consists in fabricating insulating blocks, which would be assembled by robots in order to form a layer of printing support for the mortar to be extruded; at the end, tie columns and ring beams will ensure the masonry confinement. This approach is rather new in comparison with most examples of large-scale concrete 3D printing available (Labonnote et al. 2016; Duballet et al. 2017). Indeed, the future of large-scale additive manufacturing in architecture and construction might reside in smarter, more parsimonious use of 3D printing on specific parts of the printed object, where it is the most pertinent in order to take advantage of both the material properties and morphology of the structure being built.

Conclusions and Perspectives

An overview was given regarding the concept of architected materials in general, i.e. highlighting the importance of geometry at multiple scales, as well as the computational tools associated with their development. In fact, this development is made possible by the computerisation of both the designing step, and robotisation of the manufacturing step. This automation of the process theoretically allows for a higher accuracy and infinite customisation of materials and structures according to a given set of requirements. In this context, the top-down approach of architected materials, i.e. going from the application down to the design of materials, becomes generalisable, hence yielding new opportunities for the built environment sector, e.g. in architectural design, structural engineers' calculations, or the logistics of a construction site, if building information modelling (BIM) is integrated. From an application viewpoint, one of the most critical point is indeed to be able to incorporate robotic actions within the BIM model.

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