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Opinion

The new frontiers in computational modeling of material structures

William Regli[a,1], Jarek Rossignac[b], Vadim Shapiro[c,*], Vijay Srinivasan[d]

[a] College of Computing and Informatics, Drexel University, United States
[b] College of Computing, Georgia Institute of Technology, United States
[c] University of Wisconsin at Madison, United States
[d] National Institute of Standards and Technology, United States

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ABSTRACT

We are witnessing the emergence of a new paradigm in the modeling of *material structures*. It stems from the digitization of manufacturing and is fueled by advances in additive manufacturing and material science. This paper strives to provide a critical examination of this new paradigm in a historical and technological context and to show that it requires non-trivial extensions and generalizations of the classical theoretical foundation and algorithmic solutions originally developed for solid modeling. Specifically, it requires new models and data-intensive representations for materials, physical behavior, and manufacturing processes across multiple scales. In particular, we argue that most computational tasks that support traditional and emerging manufacturing may be formulated systematically and addressed in terms of relations (*conversions*, *synthesis*, *change propagation updates*, *verification*, and other *harmonization* activities) among four views (manifestations) of an engineered artifact: *Functional*, which captures the design constraints and tolerances on shape, properties, and behavior; *Designed*, which represents a toleranced design that satisfies these constraints; *Planned*, which defines a manufacturing process plan; *Simulated*, which models the expected outcome of the process plan; and a *Real* sample set of physical artifacts produced by executing the process plan on a particular manufacturing technology. Based on this formulation, we outline important directions for a research agenda aimed at enabling, driving, and amplifying further advances in digital design and manufacturing.

1. Introduction

Sutherland's Sketchpad [1] is often cited as an example of the early CAD systems. Support of 3D rendering, and other early developments in CAD have been driven largely by design and manufacturing applications: Bezier's curves and surfaces were developed for modeling stamping dies in automotive manufacturing, wireframes were used for modeling aerospace parts, and solid models were originally intended for representing NC-machined parts and mechanical assemblies [2].

With the advent of solid modeling, fundamentally new mathematical theories and representations emerged. They made it possible to capture the complete geometry and topology of manufactured artifacts, as well as some physical properties. They opened the door to a transition from purely visual depiction to computational models of physical artifacts. Over the last four decades, solid modeling has developed into a mature discipline that is based on rigorous foundations [3–5], supported by a vibrant research community [6], and is at the core of virtually all computer-aided design and manufacturing activities—these, in turn, support over $10 trillion in global engineering, manufacturing and commerce annually [7]. Solid modeling and computer graphics were tightly intertwined till the early 1990s, at which time computer animated movies and video gaming hardware suddenly consumed the attention of the mainstream graphics community. Modeling in support of commercial computer-aided design focused on improved robustness and performance, more powerful design tools, more useful tolerancing, faster and more accurate analysis, and supporting product data and product life cycle management (PDM/PLM).

Presently, we are witnessing the emergence of the need for new modeling paradigms that go beyond solid modeling. It is largely fueled by the Third Industrial Revolution, which is based on the digitization of manufacturing [8]. Advances in materials science and additive manufacturing make it possible to manufacture

* Corresponding author.
E-mail addresses: vadim.shapiro@gmail.com, vshapiro@wisc.edu (V. Shapiro).

[1] Currently serving as the Deputy Director, Defense Sciences Office, DARPA, United States.

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artifacts with a complex material structure that for example makes them extremely light and strong (Fig. 1). Supporting such models require that we go beyond representing discrete homogeneous parts, sheet metal, and assemblies (as used in the aerospace and automotive industry) or surface and polygonal mesh models (as used in animation and gaming). Although several researchers have proposed theoretical foundations and practical implementations of non-manifold structures (see examples of proposals and surveys in [9–13]) that extend the representational capabilities of solid modeling, these early attempts do not suffice, by themselves, to address the novel challenges discussed here.

These challenges require the capabilities of modeling embedded microstructures, internal geometry architectures, multi-scale behaviors, and composite multi-material objects, because such artifacts are now physically realizable and widely used. Further, it is now commonly possible to vary internal material properties throughout the artifact, either by using graded microstructures (e.g., lattices) or via fabrication processes that can alter the crystalline structures of metals as they are deposited using 3D printing. The palettes of physical realizations that are now possible are unmatched by the relatively primitive design and modeling capabilities intended to support the mass production systems of the last century.

This paper attempts to describe key aspects of the next frontier for modeling, with a particular focus on the opportunities (and challenges) emerging from additive manufacturing and the revolution in materials science. Additive manufacturing technologies promise to radically alter production and manufacturing. Elimination of industrial waste, part-count reduction, new forms of multi-functional products and vastly lower material and energy costs are benefits that – at least in principle – will flow from the rapid adoption of additive processes. We examine the set of representational challenges that must be solved in order to support advances in production processes and materials. We also hope that the issues identified in this paper will guide the agenda for research and technology development in CAD, modeling, graphics, and visualization for the coming decade and beyond. In doing so, we follow the spirit of some of the early pioneers in solid modeling [14–17] and provide a brief context of current technology needs with respect to existing work in geometric and solid modeling.

2. Historical context

2.1. Geometry-based representations in design and manufacturing

The ability to represent and communicate information about the design and manufacturing of artifacts is at the heart of the modern manufacturing enterprise. Detailed geometric drawings specifying construction of buildings were already in use in ancient Greece [18]. Without the ability to describe and communicate the shape of interchangeable components, manufacturing was largely confined to low-volume and inaccessible artisan activity [19]. The need to describe and communicate the shape of interchangeable mechanical components in assemblies, tooling, and fixtures, as well as the methods of their manufacturing, has led to the wide adaption of standard engineering drawing practices in support of mass production [20].

In spite of enhanced computerization and automation, traditional manufacturing processes, such as CNC machining, casting or forging, have remained largely unchanged for over 50 years. Computer-Aided Design (CAD) emerged as a means of automating mechanical drafting, and Computer-Aided Manufacturing (CAM) relied on the CAD models to directly drive machine tools, to automate tool paths and to facilitate the direct exchange of digital models.

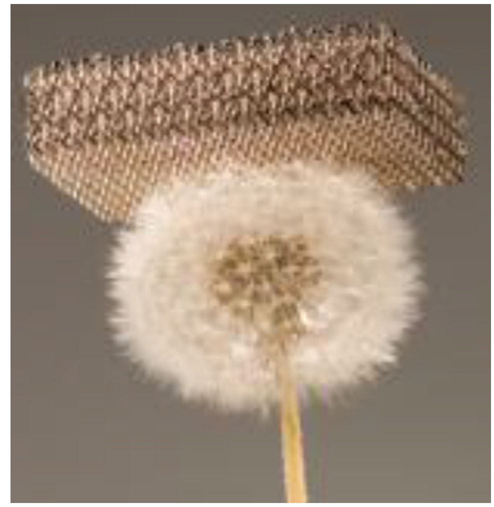

Fig. 1. An example of a 3D lattice structure, designed and fabricated by Hughes Research Labs (HRL), representing the new frontiers for materials and design. 99.99% of this metallic truss structure is air. The remaining 0.01% is made of very thin (nanometer, micron and millimeter scale) features.

During the 1970s and 1980s, in a major technological paradigm shift, solid modeling emerged in the attempt to create an informationally complete model of a *manufactured shape* that could be used throughout the manufacturing enterprise and support engineering activities throughout the product life cycle. The pioneers of solid modeling also recognized that the notion of informational completeness is not absolute, but is relative to assumed or postulated mathematical models. The latter, in turn, are based on target class of physical artifacts and processes. The instantiation of these techniques in data structures, algorithm and interfaces was a triumph of software industry during this time. Many practical issues related to the underlying representations (constructive solid geometry, non-uniform rational b-splines, winged edge and half edge data structures) and mathematical limits of digital computing (floating point accuracy, error stack up, robustness) were, for most practical purposes, overcome and the resulting companies constitute a $10B/year industry [21].

The currently accepted mathematical notion of a rigid, internally homogeneous solid was deemed adequate for supporting most (but not all) engineering activities in traditional manufacturing of mass-produced mechanical assemblies and is the basis for all modern commercial CAD systems. Early geometric and solid modeling systems were aimed to support NC machining, sheet metal forming, design and planning of mechanisms and assemblies, tolerance analysis, as well as simulation via finite element analysis. Later geometric and solid modeling tools evolved to represent geometry (shapes and operations) associated with most unit[2] manufacturing processes [22] and became the backbone of the modern PLM (Product Life-cycle Management) systems.

While PLM systems provide "geometry-based" representations of mechanical systems, they aspire to represent a complete virtual product model, including materials, physics (simulated or experimental), and intended behavior (usually in a form of performance specification and testing procedures). Of course, this virtual product model is never truly complete, but is sufficient to effectively support the paper-based and human-centric processes that have been used in most organizations. Many of these processes have evolved over decades and represent best practices, as well as

2 Informally, unit processes are individual steps in a manufacturing process that transform the raw material into a finished product [22].