

Geometric Modeling: Interoperability and New Challenges

Edited by

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Abstract

This report documents the program and the outcomes of Dagstuhl Seminar 21471 “Geometric Modeling: Interoperability and New Challenges”. This seminar was initially planned on May 2021, and was delayed due to the pandemic. The seminar took place as a hybrid version with on site and remote participants. It provided a great opportunity for exchanges which, as pointed out by participants, were very appreciated in this period where international scientific interactions have been diminished.

This report summarizes the seminar communications, first by providing the abstracts of the talks which present recent results in geometric modeling. Moreover, the scientific exchanges during the seminar provided a great basis for scientific discussions that resulted to the included five reports which highlight the new and future challenges in Geometric Modeling.

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Edited in cooperation with Konstantinos Gavriil

1 Executive Summary

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The Dagstuhl seminar, initially planned in May 2020, took place as a hybrid conference in November 2021. Eighteen participants were on site, and thirty three participated remotely out of which five from East Asia and twelve from America.

Due to the pandemic, getting together for a conference has been an important event, and an outstanding exchange time between researchers (compared to a two years pandemic context where interaction has greatly been reduced). In particular, having a significant part of the participants on site has been a real asset compared to the full online conferences. Note also that this has been particularly true for young researchers that are in the process of developing networks and developing collaborations.



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48 talks were given including 18 on site and 30 remotely. The program was organized into topics and structured to the extent possible to minimize the challenges posed by the time difference between on-site and remote participants. Speakers from East-Asia were assigned time slots in the morning and speakers from America in the afternoon. The beginning of the afternoon was a privileged time for all participants to meet. The social afternoon was canceled, as it would not have been inclusive for remote participants.

The time freed allowed us to extend the time assigned to topic focused groups sessions. This triggered, under the supervision of five on-site participants, development of topic focused reports. Two of these reports, *The Future of CAD* (group led by Tom Grandine) and *Design Optimization* (group led by Konstantinos Gavriil) address the evolution of the application fields in Geometric Modeling, closely linked to its use in Industry. Three other reports on emerging topics have also been based on the group working sessions. *Additive Manufacturing* (a group led by Sylvain Lefebvre) has been identified as a disruptive technology and has triggered the emergence of new geometric models and materials. *Isogeometric Analysis* (group led by Carla Manni) addresses how the gap between geometric modeling and simulation can be bridged by replacing the traditional shape functions of Finite Element Analysis by B-splines that cross element boundaries. It thus supplies continuous models connecting the representations of Computer Aided Design and Finite Element Analysis. *Geometric Machine Learning* (group led by Rene Hiemstra) is a fast evolving domain. Deep learning approaches have already changed the field of Computer Vision, and the contribution into Geometric Modeling is becoming more pregnant. These reports offer to the participants, and beyond, a perspective of the coming challenges in the field of Geometric Modeling.

On top of the communications done in Dagstuhl, a special issue of the journal Graphical Models, has been planned. Submission to the journal is pending.

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3 Overview of Talks

3.1 On the new class of spatial PH B-Spline curves

Gudrun Albrecht (Universidad Nacional de Colombia – Medellín, CO)

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 Gudrun Albrecht

Joint work of Gudrun Albrecht, Carolina Beccari, Lucia Romani

In this talk we present the spatial counterpart of the recently introduced class of planar Pythagorean-Hodograph (PH) B-Spline curves. Spatial Pythagorean-Hodograph B-Spline curves are odd-degree, non-uniform, parametric spatial B-Spline curves whose arc length is a B-Spline function of the curve parameter and can thus be computed explicitly without numerical quadrature. We provide the general construction of these curves using quaternion algebra and formulate the problem of point interpolation by clamped and closed PH B-Spline curves of arbitrary odd degree. In particular, we provide closed form solutions for the cubic and the quintic cases, and discuss how degree- $(2n + 1)$, C^n -continuous PH B-Spline curves can be computed by optimizing several scale-invariant fairness measures with interpolation constraints. Finally, we define Rational B-Spline Euler Rodrigues Frames (RBSERF) for regular PH B-Spline curves as well as rational tensor product B-Spline pipe surfaces. A functional is introduced to minimize the rotation of the RBSERF, and the results are illustrated on the corresponding rational pipe surface.

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<https://doi.org/10.1016/j.cagd.2017.09.001>

3.2 Exploring challenges in shape analysis, generation, and optimization with neural networks

Arturs Berzins (SINTEF – Oslo, NO)

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 Arturs Berzins

Triangular surface meshes are a widespread representation in 3D shape applications and a variety of neural network (NN) architectures have been developed in the recent years to handle them directly. However, with the advent of additive manufacturing, shapes with internal structures gain ever more significance, motivating the need for NN architectures capable of processing representations that admit disconnected boundaries. For analysis tasks, a potential solution is to extend existing NN architectures to handle tetrahedral volumetric meshes. On the other hand, generative tasks pose a greater challenge with both surface and volumetric meshes being restricted to a fixed topology. NNs representing implicit level-set functions offer greater topological flexibility but can also produce unwanted disconnected components. This talk will explore early-stage ideas on NN architectures for handling tetrahedral volumetric meshes, imposing shape connectivity on NNs representing implicit level-set functions and, finally, interoperability of NNs and PDE solvers for shape and topology optimization as a particular generative task.

3.3 Constructing planar domain parameterization with HB-splines via quasi-conformal mapping

Falai Chen (University of Science & Technology of China – Anhui, CN)

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Joint work of Falai Chen, Maodong Pan

Main reference Maodong Pan, Falai Chen, Weihua Tong: “Low-rank parameterization of planar domains for isogeometric analysis”, *Comput. Aided Geom. Des.*, Vol. 63, pp. 1–16, 2018.

URL <https://doi.org/10.1016/j.cagd.2018.04.002>

Constructing a high-quality parameterization of a computational domain is a fundamental research problem in isogeometric analysis, which has been extensively investigated so far. However, most of the current approaches employ non-uniform rational B-splines (NURBS) as the geometric representation of the physical domain. NURBS introduce redundant degrees of freedom due to their tensor-product structure. In this paper, we propose a new parameterization method for planar domains by adopting hierarchical B-splines (HB-splines) as the geometric representation that possess local refinement abilities. Starting from an initial parameterization such as a harmonic map, our method repeats the following two steps until a bijective parameterization with low distortion is achieved. First, a non-linear optimization model is proposed to compute a quasi-conformal map represented by HB-splines, and an efficient algorithm is provided to deal with this model by alternatively solving two quadratic optimization problems. Second, the parameterization is refined locally through HB-splines based on the bijectivity and conformal distortion of the parameterization. Several examples are demonstrated to verify the effectiveness and advantages of the proposed approach.

3.4 AI and Beyond in the World’s Largest 3D Capture Stage

Ilke Demir (Intel – Hermosa Beach, US)


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One picture is worth a thousand words, so what have been told with videos? What about 100 simultaneous videos to reconstruct every frame of life in a 10.000 sq. ft dome? Is it enough to reconstruct and digitize us realistically? Similar to other industries, entertainment industry is also being reshaped by AI, especially towards AR/VR consumption. Before democratization of AI and data, such immersive experiences were lacking an essential element: photorealism. As the amount of data increased, our models got deeper, and the reality became decipherable.

This talk will introduce recent deep learning advancements in 3D vision, reconstruction, and shape understanding techniques with a focus on generative models to digitize performances and scenes. Then we will shift gears with an overview of such models in 3D, and their progression on voxels, point clouds, meshes, graphs, and other 3D representations. Back to our studio, in addition to a discussion about how to process such large visual data, the challenges of scaling 10x over current capture platforms, and over 200x over state-of-the-art datasets will be presented. The talk will conclude with a sneak peek of upcoming VR/AR productions from the world’s largest volumetric capture stage at Intel Studios, as an example of real-world use cases of such AI approaches.

3.5 On the effect of scaled B-splines for different approaches to locally refined splines


Tor Dokken (SINTEF – Oslo, NO)

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Both Truncated Hierarchical B-splines and LR B-splines use scaled B-splines as part of the construction to ensure partition of unity. Certain configurations of refinements have a surprisingly big effect on the scaling factor. As the scaling factors have a direct effect on magnitude of the elements in the mass and stiffness matrices scaling consequently directly impacts the condition numbers of these matrices. The talk addressed how these effects can be observed already for bi-degree (3,3), and that the effect grows with growing polynomial degrees.

3.6 Volumetric Representations: Design, Analysis, Optimization, and Fabrication of Porous/Heterogeneous Artifacts

Gershon Elber (Technion – Haifa, IL)

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The needs of modern (additive) manufacturing technologies can be satisfied no longer by Boundary representations (B-reps), as they requires the representation and manipulation of interior (material) properties and fields. Further, while the need for a tight coupling between the design and analysis stages has been recognized as crucial almost since geometric modeling (GM) was conceived, contemporary GM systems only offer a loose link between the two, if at all.

For about half a century, (trimmed) Non Uniform Rational B-spline (NURBs) surfaces has been the B-rep of choice for virtually all the GM industry. Fundamentally, B-rep GM has evolved little during this period. In this talk, we will present a kernel of a volumetric representation (V-rep) that is based on (trimmed) trivariate NURBs and successfully confront the existing and anticipated design, analysis, and manufacturing foreseen challenges, toward porous, heterogeneous and anisotropic representation. With a V-rep kernel that supports all fundamental B-rep GM operations, such as primitive constructors and Boolean operations, we present a tight link to (Isogeometric) analysis on one hand and the full support of (heterogeneous) additive manufacturing on the other.

In this talk, we will present numerous examples that exemplify the portrayed advantages of V-reps over B-reps.

Work in collaboration with many others, including Ben Ezair, Fady Massarwi, Boris van Sosin, Jinesh Machchhar, Ramy Masalha, Q Youn Hong, Sumita Dahiya, Annalisa Buffa, Giancarlo Sangalli, Pablo Antolin, Massimiliano Martinelli, Bob Haimes and Stefanie Elgeti.

3.7 Computational Design of Cold Bent Glass Façades

Konstantinos Gavriil (SINTEF – Oslo, NO)

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Joint work of Konstantinos Gavriil, Ruslan Guseinov, Jesús Pérez, Davide Pellis, Paul Henderson, Florian Rist, Helmut Pottmann, Bernd Bickel

Main reference Konstantinos Gavriil, Ruslan Guseinov, Jesús Pérez, Davide Pellis, Paul Henderson, Florian Rist, Helmut Pottmann, Bernd Bickel: “Computational design of cold bent glass façades”, *ACM Trans. Graph.*, Vol. 39(6), pp. 208:1–208:16, 2020.

URL <https://doi.org/10.1145/3414685.3417843>

Cold bent glass is a promising and cost-efficient method for realizing doubly curved glass façades. They are produced by attaching planar glass sheets to curved frames and require keeping the occurring stress within safe limits. However, it is very challenging to navigate the design space of cold bent glass panels due to the fragility of the material, which impedes the form-finding for practically feasible and aesthetically pleasing cold bent glass façades. We propose an interactive, data-driven approach for designing cold bent glass façades that can be seamlessly integrated into a typical architectural design pipeline. Our method allows non-expert users to interactively edit a parametric surface while providing real-time feedback on the deformed shape and maximum stress of cold bent glass panels. Designs are automatically refined to minimize several fairness criteria while maximal stresses are kept within glass limits. We achieve interactive frame rates by using a differentiable Mixture Density Network trained from more than a million simulations. Given a curved boundary, our regression model is capable of handling multistable configurations and accurately predicting the equilibrium shape of the panel and its corresponding maximal stress. We show predictions are highly accurate and validate our results with a physical realization of a cold bent glass surface.

3.8 Recent advances on adaptive isogeometric methods with hierarchical spline models

Carlotta Giannelli (University of Firenze, IT)


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Joint work of Cesare Bracco, Carlotta Giannelli, Tadej Kanduč, Mario Kapl, Massimiliano Martinelli, Giancarlo Sangalli, Mattia Tani, Rafael Vázquez

The design and analysis of adaptive isogeometric methods with hierarchical spline constructions has attracted remarkable interest in the last few years. In order to increase the flexibility of the hierarchical approximation framework, while simultaneously preserving the performance of the overall adaptive scheme, particular attention is currently devoted to address the fast formation of system matrices arising from hierarchical discretization as well as to the development of effective multi-patch extensions. The talk will present recent results on these directions.

3.9 If I could do it over, I would...


Thomas A. Grandine (Seattle, US)

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I recently retired after a nearly 35 year career researching, developing, and deploying geometric modeling and processing tools for The Boeing Company. The year I've spent away from the daily demands of the job have given me an opportunity to reflect on what mathematical technologies I wish I had made more effective use of, those which I wish I had been able to push more deeply into the company's well-established bag of tricks, and those I didn't pursue at all, but wish I had. Additionally, there are things I did pursue that turned out not to be very good ideas. This talk will provide a quick summary of the lessons learned.

3.10 Geometric construction and fabrication of auxetic metamaterials

Stefanie Hahmann (INRIA Grenoble Rhône-Alpes, FR)

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Joint work of Stefanie Hahmann, Georges-Pierre Bonneau, Johana Marku

Main reference Georges-Pierre Bonneau, Stefanie Hahmann, Johana Marku: "Geometric construction of auxetic metamaterials", *Comput. Graph. Forum*, Vol. 40(2), pp. 291–304, 2021.


URL <https://doi.org/10.1111/cgf.142633>

Recent advances in digital manufacturing, where computational design, materials science and engineering meet, offer whole new perspectives for tailoring mechanical properties and fabrication of new meta-materials with applications as diverse as product design, architecture, engineering and art. A meta-material is a material whose microstructure can be controlled to achieve the desired macroscopic deformation behavior.

This presentation is devoted to a category of metamaterials called auxetic structures, or auxetic networks. Auxetic materials are characterized by a negative Poisson's ratio. They do not behave like usual materials, because when they are stretched in one direction, they expand in the perpendicular direction. Whereas regular auxetic networks are well studied, our focus is on disordered auxetic networks. In particular, we are exploring geometrical strategies to generate 2-dimensional random auxetic meta-materials. Starting from a dense irregular network, we seek to reduce the Poisson's ratio, by pruning bonds (edges) based solely on geometric criteria. To this end, we first deduce some prominent geometric features from regular auxetic networks and then introduce a strategy combining a pure geometric pruning algorithm followed by a physics-based testing phase to determine the resulting Poisson's ratio of our networks. We provide numerical results and statistical validation. We also show physical tests with both laser-cut rubber networks and 3D-printed networks showing auxetic behaviour.

3.11 Learning quadrature for implicit domains

Rene Hiemstra (Leibniz Universität Hannover, DE)

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Implicit geometry representations are becoming increasingly widespread in applications, driven by a need and interplay of complex geometry, topology and physics. In this work I develop a supervised learning approach to “learn” quadrature for implicitly defined domains by means of feed-forward artificial neural networks. Once optimized, these networks can accurately and efficiently evaluate quadrature rules for implicit domains. This greatly simplifies and accelerates numerical quadrature for fictitious domain methods, which is illustrated by several numerical benchmarks.

3.12 Geometric Regularizations and Representations for Neural 3D Synthesis


Qi-xing Huang (University of Texas – Austin, US)

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Synthesizing 3D shapes and scenes is a core problem in visual computing. Recent advances in deep generator models have pushed this field to a new ear. However, existing approaches predominately generalize machine learning algorithms developed on images to the 3D domain. They do not fully utilize geometric properties of 3D shapes, e.g., in shape deformation and 3D representations. This talk covers recent works that construct geometric regularizations and hybrid representations for 3D synthesis. Specifically, I will first discuss an as-rigid-as possible regularization loss that regularizes the tangent spaces defined by the generator for training deformable shape generators. I will then move to the domain of 3D scenes and present a recent work that combines the strengths of neural generators and traditional approaches for modeling uncertainties of geometric attributes.

3.13 Complete Classification and Efficient Determination of Arrangements Formed by Two Ellipsoids

Xiaohong Jia (Chinese Academy of Sciences, CN) and Wenping Wang (Texas A&M University – College Station, US)

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Joint work of Xiaohong Jia, Changhe Tu, Bernard Mourrain, Wenping Wang

Main reference Xiaohong Jia, Changhe Tu, Bernard Mourrain, Wenping Wang: “Complete Classification and Efficient Determination of Arrangements Formed by Two Ellipsoids”, *ACM Trans. Graph.*, Vol. 39(3), pp. 27:1–27:12, 2020.

URL <https://doi.org/10.1145/3388540>

Arrangements of geometric objects refer to the spatial partitions formed by the objects and they serve as an underlining structure of motion design, analysis and planning in CAD/CAM, robotics, molecular modeling, manufacturing and computer-assisted radio surgery. Arrangements are especially useful to collision detection, which is a key task in various applications such as computer animation, virtual reality, computer games, robotics, CAD/CAM and computational physics.

Ellipsoids are commonly used as bounding volumes in approximating complex geometric objects in collision detection. In this paper we present an in-depth study on the arrangements formed by two ellipsoids. Specifically, we present a classification of these arrangements and propose an efficient algorithm for determining the arrangement formed by any particular pair of ellipsoids. A stratification diagram is also established to show the connections among all the arrangements formed by two ellipsoids.

3.14 Numerical integration on trimmed planar domains via high-order transport theorems for implicit curves

Bert Jüttler (Johannes Kepler Universität Linz, AT)

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Joint work of Felix Scholz, Bert Jüttler

Main reference Felix Scholz, Bert Jüttler: “Using High-Order Transport Theorems for Implicitly Defined Moving Curves to Perform Quadrature on Planar Domains”, *SIAM J. Numer. Anal.*, Vol. 59(4), pp. 2138–2162, 2021.

URL <https://doi.org/10.1137/20M1341283>

We study numerical integration over a planar domain that is cut by an implicitly defined boundary curve. This important problem arises, for example, in unfitted finite element methods and in isogeometric analysis on trimmed computational domains. We present a general version of the transport theorem for moving domains defined by implicitly defined curves. This result is then used to derive an efficient and accurate quadrature rule for this class of domains. Numerical experiments are presented in order to demonstrate that the method achieves a high rate of convergence.

3.15 Supporting Expensive Physical Models With Geometric Moment Invariants to Accelerate Sensitivity Analysis for Shape Optimisation

Panagiotis Kaklis (The University of Strathclyde – Glasgow, GB)

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Joint work of Panagiotis Kaklis, Shahroz Khan, Andrea Serani, Matteo Diez

Parametric Sensitivity Analysis (PSA) investigates the sensitivity of parameters, defining the design space of a shape-optimisation problem, for tackling the challenges of the curse of dimensionality or decreasing the uncertainty in design’s performance. However, the analytical implementation of PSA can often be tricky, especially if the chosen method requires the evaluation of high-dimensional integrals or if the baseline simulation codes do not provide an analytical solution to design performance. Therefore, PSA needs to be implemented with sampling methods, such as Monte Carlo sampling, which is highly susceptible to slow convergence and necessitates a sufficiently large number of samples for stable results, especially for high-dimensional problems.

In this work, we aim to address above the mentioned challenges associated with PSA by offloading the evaluation of parametric sensitivities from physical quantities to quantities, which are relatively inexpensive but, like physical metrics, provide important clues about the form, distribution and validity of the design. It is well known that shape’s integral properties, such as geometric moments and their invariants serve as a geometric foundation for different

designs' physical analyses. In this connection, we propose a geometric moment-dependent PSA approach, that harnesses the geometric variation of designs in the design space using geometric moments as a quantity of interest (QoI) to identify parametric sensitivities. These results can serve as prior estimates of parametric sensitivities with respect to physics. The selection of geometric moments in our work is motivated by the following baseline insights:

- It is very likely that physics analysis requires the computation of such integral properties of the geometry such as the stiffness and mass matrix, and moments of a domain are sufficient to ensure accurate integration of a large class of integrands.
- Like physics, geometric moments can also act as a compact shape signature or descriptor to a specific design falling in a specific category, which facilitates various shape processing tasks.

To validate our approach and experimentally demonstrate the effectiveness of geometric moments, we used two ship hulls parameterised with 27 and 26 parameters using two different techniques based on *procedural deformation* (PD) and global modification function (GMF), respectively. In this setting, we use the *wave-resistance coefficient* (C_w) as the physical QoI, as it plays a crucial role in ship hull design. The longitudinal distribution of the hulls' geometry has a similar impact on geometric moments as C_w .

To commence, we construct the so-called shape-signature vector ($\mathcal{M}\mathcal{I}^s$), that will be used as shape descriptor and contains all the geometric moments up to s order. To align better with C_w , all moments in this vector are taken invariant with respect to translation and scaling. A Global Variance-Based Sensitivity Analyses (GVBSA) is performed for learning parametric sensitivities with respect to $\mathcal{M}\mathcal{I}^s$ and C_w . Here $\mathcal{M}\mathcal{I}^s$ is purely a vector quantity containing the moments of various orders while C_w is a scalar and computationally expensive one. Therefore, learning sensitivities to $\mathcal{M}\mathcal{I}^s$ requires implementing a multivariate extension of GVBS, such as covariance decomposition, which provides generalised sensitivity indices of design parameters to all moments in $\mathcal{M}\mathcal{I}^s$.

The results from the experiments conducted in this study show a good correlation between the sensitive parameters obtained from C_w and $\mathcal{M}\mathcal{I}^s$, specifically with the fourth-order shape-signature vector $\mathcal{M}\mathcal{I}^4$. In the case of the PD-based hull, 7 parameters sensitive to $\mathcal{M}\mathcal{I}^4$ are also among the 8 parameters sensitive to C_w . Interestingly, similar results are obtained for the GMF-based hull, where 6 out of 7 sensitive parameters to C_w are also sensitive to $\mathcal{M}\mathcal{I}^4$. Afterwards, two different design spaces are constructed for both hull models, one with sensitive parameters obtained with C_w and the other with $\mathcal{M}\mathcal{I}^4$. Shape optimisation is performed in both spaces performed with a meta-heuristic optimisation approach. Final optimisation results showed that the design generated from design space constructed with sensitive parameters of C_w and $\mathcal{M}\mathcal{I}^4$ for both types of hulls offer similar performance. These results indicate that PSA performed with moments can reasonably estimate parameters' sensitivity to the design's physics with considerably reduced computational cost.

3.16 Efficient Multimodal Belief Propagation for Robust SLAM Using Clustering Based Reparameterization

Tae-wan Kim (Seoul National University, KR)

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Joint work of Seungwon Choi, Tae-Wan Kim

Main reference Seungwon Choi, Taewan Kim: “Efficient Multimodal Belief Propagation for Robust SLAM Using Clustering Based Reparameterization”, in Proc. of the IEEE/RSJ International Conference on Intelligent Robots and Systems, IROS 2021, Prague, Czech Republic, September 27 – Oct. 1, 2021, pp. 3354–3360, IEEE, 2021.

URL <https://doi.org/10.1109/IROS51168.2021.9636040>

Due to the presence of ambiguities caused by sensor noise and structural similarity, simultaneous localization and mapping (SLAM) observation models are typically multimodal. The multimodal inference process can be directly dealt with by belief propagation (BP) using weighted Gaussian mixture messages, but for efficiency, a combinatorial explosion of the complexity must be suitably relaxed. In this study, we present an effective multimodal BP SLAM for robust inference with ambiguities. Using Gaussian bandwidth mean shift and cluster-based reparameterization, we reduce the number of Gaussian components in each message due to the BP nature. The proposed algorithm reduces the number of components of the product by summarizing indistinguishable modes in weighted Gaussian mixtures and keeping only the significant modes, making BP computationally efficient.

3.17 On Triangular Splines: CAD and Quadrature

Jiri Kosinka (University of Groningen, NL)

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Joint work of Gerben Jan Hettinga, Michael Barton, Jiri Kosinka

The standard representation of CAD (computer aided design) models is based on the boundary representation (B-reps) with trimmed and (topologically) stitched tensor-product NURBS patches. Due to trimming, this leads to gaps and overlaps in the models. While these can be made arbitrarily small for visualisation and manufacturing purposes, they still pose problems in downstream applications such as (isogeometric) analysis and 3D printing.

It is therefore worthwhile to investigate conversion methods which (necessarily approximately) convert these models into water-tight or even smooth representations. After briefly surveying existing conversion methods, we will focus on techniques that convert CAD models into triangular spline surfaces of various levels of continuity. In the second part, we will investigate efficient quadrature rules for triangular spline spaces.

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<https://doi.org/10.1016/j.cam.2018.10.036>

3.18 Cyclidic splines and kinematic interpretation of quaternionic curves/surfaces

Rimvydas Krasauskas (Vilnius University, LT)

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Joint work of Rimvydas Krasauskas, Jean Michel Menjanahary

Regular circular quad meshes produce smooth cyclidic splines composed of principal patches of Dupin cyclides with simply computable offsets. This property is crucial in CAD and 3D printing applications. We increase flexibility of such splines by extending the variety of blended patches: now they can be bounded not only by principal circles but also by diagonals of principal patches, i.e. quartic curves in general. Our methods are based on kinematic interpretation of quaternionic-Bezier formulas and Moebius invariant constructions. In the case of cubic cyclidic splines possibility of foldings and branchings of the Gaussian map is demonstrated. Topological restrictions are detected for general cyclidic splines without spherical or planar patches.

3.19 Generating oriented structures and trajectories within part volumes

Sylvain Lefebvre (LORIA & INRIA – Nancy, FR)

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Joint work of Sylvain Lefebvre, Jonàs Martinez, Cédric Zanni, Thibault Tricard, Samuel Hornus, Jimmy Etienne, Adrien Bedel, Yoann Coudert-Osmont, Rahnuma Islam Nishat, Sue Whitesides, Vincent Tavernier, Fabrice Neyret, Pierre-Alexandre Hugron, Tim Kuipers

Generating trajectories for Additive Manufacturing processes is typically performed under conflicting objectives. In particular, it is often desirable for the trajectories to follow specific directions within the part volume, aligning with shape features or following a user-specified control field. This directionality may for instance result in controlled anisotropic properties (elasticity, specularity), which could not be easily obtained with traditional manufacturing processes.

However, such an objective conflicts with that of producing equally spaced trajectories – avoiding porosities or excess material curing/deposition – and process constraints such as solidification radii bounds, admissible overhangs or continuity of deposition.

In this presentation I will discuss some of our latest research in controlling deposition orientation within part volumes – as well as their potential applications – for both sparse and dense infills.

3.20 Deep Implicit Moving Least-Squares Functions for 3D Reconstruction

Yang Liu (Microsoft Research – Beijing, CN)

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Point set is a flexible and lightweight representation widely used for 3D deep learning. However, their discrete nature prevents them from representing continuous and fine geometry, posing a major issue for learning-based shape generation. In this work, we turn the discrete

point sets into smooth surfaces by introducing the well-known implicit moving least-squares (IMLS) surface formulation, which naturally defines locally implicit functions on point sets. We incorporate IMLS surface generation into deep neural networks for inheriting both the flexibility of point sets and the high quality of implicit surfaces. I do see that there are many opportunities to bridge classic and well-defined shape representation and machine learning for improving the interoperability of shape learning and synthesis and making classic methods more robust and applicable.

3.21 Outlier-free isogeometric discretizations

Carla Manni (University of Rome “Tor Vergata”, IT)

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Joint work of Carla Manni, Espen Sande, Hendrik Speleers

Main reference Carla Manni, Espen Sande, Hendrik Speleers: “Application of optimal spline subspaces for the removal of spurious outliers in isogeometric discretizations”, *Computer Methods in Applied Mechanics and Engineering*, Vol. 389, p. 114260, 2022.

URL <https://doi.org/10.1016/j.cma.2021.114260>

Spectral analysis can be used to study the error in each eigenvalue and eigenfunction of a numerical discretization of an eigenvalue problem. For a large class of boundary and initial-value problems the total discretization error on a given mesh can be recovered from its spectral error. This is of primary interest in engineering applications.

The isogeometric approach for eigenvalue problems has been widely investigated in the literature. Maximally smooth spline spaces on uniform grids are an excellent choice for addressing eigenvalue problems. Yet, they still present a flaw: a very small portion of the eigenvalues are poorly approximated and the corresponding computed values are much larger than the exact ones. These spurious values are usually referred to as outliers. The number of outliers increases with the degree p . However, for fixed p , it is independent of the degrees of freedom for univariate problems, while a thin layer of outliers is observed in the multivariate setting.

Outlier-free discretizations are appealing, not only for their superior description of the spectrum of the continuous operator, but also for their beneficial effects in various contexts, such as an efficient selection of time-steps in (explicit) dynamics and robust treatment of wave propagation. For a fixed degree, the challenge is to remove outliers without loss of accuracy in the approximation of all eigenfunctions.

In this talk we discuss isogeometric Galerkin discretizations of eigenvalue problems related to the Laplace operator subject to any standard type of homogeneous boundary conditions conditions in certain optimal spline subspaces. Roughly speaking, these optimal subspaces are obtained from the full spline space defined on specific uniform knot sequences by imposing specific additional boundary conditions. The spline subspaces of interest have been introduced in the literature some years ago when proving their optimality with respect to Kolmogorov n -widths. For a fixed number of degrees of freedom, all the eigenfunctions and the corresponding eigenvalues are well approximated, without loss of accuracy in the whole spectrum when compared to the full spline space. Moreover, there are no spurious values in the approximated spectrum. In other words, the considered subspaces provide accurate outlier-free discretizations in the univariate and in the multivariate tensor-product case.

The role of such spaces as accurate discretization spaces for addressing general problems is discussed as well.

3.22 Scale-Space for Machine Learning on 3D point clouds

Nicolas Mellado (CNRS – Toulouse, FR)

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Applying Machine Learning algorithms to acquired point clouds with hundreds of millions of points remains a challenging task. First, networks have to handle the size of the point cloud, which is out of reach of most approaches found in the literature, only demonstrated on point clouds with a few thousands points. Second, the methods need to handle the complexity of the represented shapes (e.g., millimeter-scale acquisition of entire buildings), while being robust to acquisition artifacts (noise, sampling, holes). In this talk we introduce a new approach where point samples are used to compute implicit surface representation at multiple scales using state of the art algorithms, known to be robust, fast and stable. A neural network is then used to analyze the differential properties of the reconstructed surfaces, and perform a given task (here illustrated on pointwise edge classification). Instead of trying to learn how to be robust to acquisition defects, we propose to hide the complexity of the acquired data using surface reconstruction, and to define small, and fast networks requiring very small amounts of training data. We demonstrate the benefit of our approach on very large point clouds (e.g., buildings with dozens of millions of points) and also on collections of CAD geometry with thousands of objects (ABC dataset). We also show that low processing time and low data requirements unlock the definition of interactive learning applications, where the user can interactively show localized classification examples, train the network in seconds, and classify the entire dataset in seconds.

3.23 Tubular parametric volume objects

Géraldine Morin (IRIT – University of Toulouse, FR)

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Joint work of Samuel Peltier, Géraldine Morin, Damien Aholou

Main reference Samuel Peltier, Géraldine Morin, Damien Aholou: “Tubular parametric volume objects: Thickening a piecewise smooth 3D stick figure”, *Comput. Aided Geom. Des.*, Vol. 85, p. 101981, 2021.

URL <https://doi.org/10.1016/j.cagd.2021.101981>

A volume parametric model is computed from a piecewise smooth skeleton. Generating a volume model from a stick figure S defined in 3D is an intuitive process: given S whose topology is a pseudo-graph and whose edges are embedded as Bézier curves in \mathbb{R}^3 , we propose a method for creating a thick volume parametric model “around” S . The volume model we generate is based on semi-simploidal sets, which guarantees a proper topology and provides a 3D parametric domain for Bézier spaces. This volume is a continuous piecewise Bézier representation which boundary corresponds to a B-Rep made of tensor product Bézier patches.

3.24 nTopology: A Design System Based on Implicit Modeling

Suraj R. Musuvathy (nTopology – New York, US)

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URL <https://ntopology.com>

Additive manufacturing enables the design and manufacturing of objects with unprecedented complexity and customizability. Advances in generative design exploration methods such as topology optimization, multi-disciplinary optimization, and AI have enabled rapid exploration of large design spaces. Most, if not all, major CAD software systems today are built on Boundary Representations (B-Reps). In our view B-Reps have reached their limits on addressing the design opportunities available today due to limitations in scalability and reliability. B-Reps require explicit representations of geometry and topology, thereby falling short on the ability to model complex structures that are manufacturable today by several orders of magnitude. B-Rep based modeling algorithms (Booleans, offsets, blends, etc.) are fragile thereby limiting automation required for generative techniques and mass customization applications. nTopology has developed a design system based on procedural implicit modeling that addresses these limitations. Solid geometry is represented as an implicit scalar-valued expression consisting of standard mathematical operators (arithmetic, logic, trigonometric, etc.) and custom operators. The custom operators enable interfacing any kind of data, including other representations of geometric data, with the solid modeling system by implementing a set of queries including computing scalar-field values, and optionally gradients and intervals. For example, a custom operator can be built for querying physics simulation analysis results in order to drive solid model geometry directly. The most common modeling algorithms are simple mathematical expressions (e.g., Booleans can be defined with min/max functions or other R-function variants), and are therefore robust and computationally fast. Procedural implicit functions can represent geometry of arbitrary complexity, and fundamental geometry processing algorithms can be easily parallelized thereby enabling effective use of modern multi-core CPUs and GPUs. There have been advances in visualization, physics simulation, topology optimization, and machine learning approaches that work directly with implicits. As these applications mature, an implicit representation approach holds great promise in delivering design engineering applications required for product development with unprecedented capabilities.

3.25 Polyhedral net spline modeling

Jörg Peters (University of Florida – Gainesville, US)

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Joint work of Jörg Peters, Kestutis Karčiauskas, Kyle Lo
URL <https://uf-cise-surflab.github.io/blender-polyhedral-splines-web/>

Piecewise polynomial splines with polyhedral control nets allow for merging parameter directions and transitioning between coarse and fine meshes in a unified fashion. This talk summarizes recent work and available software for interpreting quad-dominant polyhedral control nets as control nets of smooth polyhedral splines of degree at most bi-3.

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<https://doi.org/10.1016/j.cagd.2020.101934>

3.26 Topology Optimization for Additive Manufacturing

Xiaoping Qian (University of Wisconsin – Madison, US)

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Topology optimization (TO) and additive manufacturing (AM) are twin-technologies that can be synergistically integrated to exploit shape flexibility in part design and fabrication. AM processes can fabricate parts of complex geometric shapes. However they also pose geometric constraints for part design. Some of these constraints such as overhang angle and support volume depend on part build orientation, and are not differentiable to build orientation. In topology optimization where a large number of optimization variables, often on the orders of millions, are used, gradient based optimization is preferred. How to formulate differentiable AM constraints for TO has been a challenge.

In this talk, I will present several formulations of AM constraints in density-based TO that are differentiable with respect to both density variables and build orientation. These differentiable formulations have explicit geometric meanings including projected undercut perimeter, overhang angle for self-support constraint, and support volume. These formulations thus enable simultaneous topology and build orientation optimization, yielding designs that meet AM constraints. Two essential elements of such differential formulations are implicit treatment of density representation, and the use of advection-diffusion equations for discerning accessibility and occlusion. Numerical examples will be given to demonstrate the efficacy of the proposed formulations.

3.27 Interoperability of Geometric Models and Numerical Analysis by Immersed Boundary Methods

Ernst Rank (TU München, DE)

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Joint work of Ernst Rank, Davide d'Angella, Stefan Kollmannsberger, Nina Korshunova, László Kudela, Beatrice Wassermann
URL <https://www.cms.bgu.tum.de/en/team/rank>

Immersed Boundary Methods (IBM) like the Finite Cell or the CutFEM method have gained large interest in the mathematical as well as in the engineering community. A domain of computation is embedded in a larger, typically simply shaped fictitious domain, which is meshed e.g. in a simple Cartesian grid. The exact shape of the original domain is

only observed on the level of element matrices by using a point membership test (PMT), which can be specifically designed for a given geometric model. By construction, Immersed Boundary Methods do NOT need any generation of body fitted meshes and thus relieve from one of the major practical obstacles of true geometry-analysis interoperability. This advantage comes yet with significant challenges, like precise numerical integration of cut cells, adequate imposition of boundary conditions, (pre)-conditioning of the arising algebraic systems or local refinement of the approximation. Successful solutions for these problems have recently been obtained, without compromising the accuracy or computational efficiency of the corresponding Finite Element or Isogeometric Element approximations. This presentation will focus on the principles of IBM and then show examples with various types of geometric models. Among these examples are (flawed) BRep- and Constructive Solid Geometry models, VReps, Computer Tomograms and Point Cloud models. Also evolving domains relevant in process simulation for additive manufacturing profit from the non-boundary conforming discretization of IBMs.

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<https://doi.org/10.1016/j.matdes.2021.109693>

3.28 ABC-Surfaces

Ulrich Reif (TU Darmstadt, DE)

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Joint work of Florian Martin, Ulrich Reif

Main reference Florian Martin, Ulrich Reif: “Trimmed Spline Surfaces with Accurate Boundary Control”. In: C. Manni and H. Speleers (eds.) *Geometric Challenges in Isogeometric Analysis*, Springer INdAM Series, to appear.

Composite trimmed NURBS surfaces are a standard tool in industrial free form modeling. However, they are typical discontinuous along boundaries of neighboring patches. In this talk, we present a solution of the problem, called ABC-surfaces. It is based on an appropriate blend of a given surfaces patch, representing the overall shape, and so-called ribbons, representing the shape near the segments of the boundary. Using ABC-surfaces, it is possible to model composite spline surfaces of arbitrary smoothness. Another important feature is the fact that all building blocks and also the resulting surfaces can be represented in terms of standard NURBS elements, what is crucial for a potential integration in commercial CAD systems.

ABC-surfaces can also be used for single-patch parametrizations of planar domains bounded by spline curves. These parametrizations are close to the identity and can be constructed in a systematic way, avoiding the notorious problems of meshing. Thus, ABC-surfaces are a promising new tool for the simulation of boundary value problems. A generalization to the 3D case is possible.

3.29 3D printed metamaterials in industry

Elissa Ross (Metafold 3D – Toronto, CA)

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Additive manufacturing has opened doors to the physical realization of geometry that cannot be fabricated by traditional methods. Examples include 3D lattice structures, which may have elements composed of either beams or surfaces, and may be arbitrarily complex or have extremely high surface area. By varying the lattice geometry together with the 3D printing medium, it is possible to achieve a vast spectrum of material behaviour, ranging from fully flexible forms to completely stiff examples with high strength. This range of material expression makes lattice geometry extremely promising for industrial applications, yet there remain numerous obstacles to their adoption. In this talk I will discuss recent work to address this through the development of 3D printing software and hardware specifically to print lattices, microstructures, metamaterials, and procedurally generated geometry.

3.30 CAD Model Details via Curved Knot Lines and Truncated Powers

Malcolm A. Sabin (Cambridge, GB)

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Joint work of Malcolm A. Sabin, Chris Fellows, Jiří Kosinka

Main reference Malcolm A. Sabin, Chris Fellows, Jiří Kosinka: “CAD Model Details via Curved Knot Lines and Truncated Powers”, *Comput. Aided Des.*, Vol. 143, p. 103137, 2022.

URL <https://doi.org/10.1016/j.cad.2021.103137>

This presentation describes the background of and concepts underlying the work in [1].

In particular it covered the requirements for automotive body shell design and how they can be met better than by the current conventions and workflow practises. Other talks in this meeting which address this issue are those by Ulrich Reif (Talk 3.28) and by Tamás Várady (Talk 3.36).

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3.31 Geometric interpolation of Euler-Rodrigues frames with G^2 Pythagorean-hodograph curves of degree 7

Maria Lucia Sampoli (University of Siena, IT)

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Joint work of Marjeta Knez, Maria Lucia Sampoli

Main reference Marjeta Knez, Maria Lucia Sampoli: “Geometric interpolation of ER frames with G^2 Pythagorean-hodograph curves of degree 7”, *Comput. Aided Geom. Des.*, Vol. 88, p. 102001, 2021.


URL <https://doi.org/10.1016/j.cagd.2021.102001>

In this talk a novel construction of spatial curves interpolating assigned positions and boundary frames is presented. The proposed construction results in Pythagorean-Hodograph (PH) curve segments of degree 7 with G^2 continuity and having the associated Euler-Rodrigues

frame G^1 continuous. Therefore it can be used to form a spline curve whose frame is varying continuously, which is a feature very useful in motion design applications. Exploiting the relation between rotational matrices and quaternions on the unit sphere, geometric continuity conditions on the frames are expressed through conditions on the corresponding quaternion polynomials. This leads to a nonlinear system of equations whose solvability is investigated, and asymptotic analysis of the solutions in the case of data sampled from a smooth parametric curve and its general adapted frame is derived. It is shown that there exist PH interpolants with optimal approximation order 6, except for the case of the Frenet frame, where the approximation order is at most 4. Several numerical examples are presented, which confirm the theoretical results.

3.32 Explicit error estimates for isogeometric discretizations of partial differential equations

Espen Sande (EPFL – Lausanne, CH)

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Joint work of Espen Sande, Carla Manni, Hendrik Speleers

Main reference Espen Sande, Carla Manni, Hendrik Speleers: “Explicit error estimates for spline approximation of arbitrary smoothness in isogeometric analysis”, *Numerische Mathematik*, Vol. 144(4), pp. 889–929, 2020.


URL <https://doi.org/10.1007/s00211-019-01097-9>

In this talk we discuss techniques to obtain error estimates with explicit constants for Ritz-type projections onto spline spaces of arbitrary smoothness defined on arbitrary grids. The presented error estimates indicate that smoother spline spaces exhibit better approximation per degree of freedom, even for low regularity of the function to be approximated. This is in complete agreement with the numerical evidence found in the literature.

The extension of these error estimates to the case of mapped geometries (both single-patch and multi-patch) will also be mentioned.

3.33 C^1 isogeometric spaces

Giancarlo Sangalli (University of Pavia, IT)

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Joint work of Giancarlo Sangalli, Andrea Benvenuti, Annabelle Collin, Gabriele Loli, Mario Kapl, Thomas Takacs

Main reference Mario Kapl, Giancarlo Sangalli, Thomas Takacs: “A family of C^1 quadrilateral finite elements”, *Adv. Comput. Math.*, Vol. 47(6), p. 82, 2021.

URL <https://doi.org/10.1007/s10444-021-09878-3>

In this talk I have presented results (from papers in collaboration) about the construction of C^1 isogeometric quadrilateral elements that could be seen as extensions of the the classical Argyris triangular element. The structure is different (triangular and quadrilateral elements are structurally different) but the d.o.f.s and space constraints have some similarities. When the quadrilateral is a spline patch, the optimal order of approximation requires some constraints of the parametrization that needs to be “analysis-suitable G^1 ”. An alternative is to enforce the C^1 interelement continuity in a weak sense, e.g. by the mortar method.

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3.34 Smooth polar spline representations suited for design and analysis

Hendrik Speleers (University of Rome “Tor Vergata”, IT)

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Joint work of Hendrik Speleers, Deepesh Toshniwal

Main reference Hendrik Speleers, Deepesh Toshniwal: “A General Class of C^1 Smooth Rational Splines: Application to Construction of Exact Ellipses and Ellipsoids”, *Comput. Aided Des.*, Vol. 132, p. 102982, 2021.

URL <https://doi.org/10.1016/j.cad.2020.102982>

One of the upshots of CAD representations of arbitrary genus surfaces with finite number of polynomial patches is the introduction of holes surrounded by periodic configurations. Such holes can then be filled by means of polar spline surfaces, where the basic idea is to use periodic spline patches with one collapsed boundary (polar singularity).

In this talk, keeping in mind applications to design as well as analysis, we focus on C^k polar spline surfaces. We present a simple, geometric construction of basis functions over such polar configurations possessing interesting properties as nonnegativity and partition of unity. The polar basis functions are assembled by transforming sets of B-splines/NURBS via compatible extraction matrices. To increase flexibility, one could also start from different sets of B-splines/NURBS that are allowed to have different polynomial degrees and weight functions.

The polar spline representations are suited for geometric modeling of geometries with one or more polar singularities, and in particular allow for compact, smooth, low degree descriptions of ellipsoids. Moreover, the constructed splines show optimal approximation behavior, even at the polar singularity. These properties make them also attractive for isogeometric analysis. Thanks to their construction in terms of B-splines/NURBS, they can be readily implemented and used in CAD or CAE software.

3.35 Segmentation of X-Ray CT Volume of Binned Parts by Constructing Morse Skeleton Graph of Distance Transform

Hiromasa Suzuki (University of Tokyo, JP)

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Joint work of Hiromasa Suzuki, Tatsuya Yatagawa, Yutaka Ohtake

Industrial X-ray CT scanners have delivered non-destructive evaluation of industrial products with its capability of inspecting even inside the body of products. This paper introduces a new approach to accelerate inspection of a large number of the same mechanical parts by scanning their heap in a bin at once. The scanning result is a CT volumetric image containing all of these parts out of which each part is segmented for inspection. This segmentation is a kind of template matching problem. However, random postures and dense contacts of the binned parts prohibit extracting the parts one-by-one using a traditional template matching due to its high computational complexity. To reduce the computational complexity, we convert both the scanned volumetric images of the template and the binned parts to simpler graph structures, and then, we solve well-studied graph matching problem to distinguish each part. We convert a discrete volume data to a distance field by the distance transform, and then, construct a graph consisting of nodes at extremum points of the distance field based on the Morse theory. The experimental evaluation demonstrates that our method without manual arrangement of the target parts works even for the scan of a heap of 50 binned parts in CT volumes of about 800^3 voxels, and an average processing time is as short as 30 minutes.

3.36 Multi-sided surface patches over curved, multi-connected domains

Tamás Várady (Budapest University of Technology and Economics, HU)

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Joint work of Márton Vaitkus, Tamás Várady, Péter Salvi, Ágoston Sipos

Main reference Márton Vaitkus, Tamás Várady, Péter Salvi, Ágoston Sipos: “Multi-sided B-spline surfaces over curved, multi-connected domains”, *Comput. Aided Geom. Des.*, Vol. 89, p. 102019, 2021.

URL <https://doi.org/10.1016/j.cagd.2021.102019>

A new control point based parametric surface representation is presented, that interpolates a collection of surface ribbons, i.e. boundary curves and cross-derivatives, given in Bézier or B-spline form. A single surface equation can describe complex, multi-connected free-from surfaces, that are compatible with tensor-product surfaces. The scheme is defined over a planar domain with curved boundaries that mimic the shape of the 3D boundary curves, and it is capable to handle strongly concave boundaries and periodic hole loops in the interior.

We discuss (i) an algorithm for curved domain generation, (ii) the methods of defining local parameterizations using harmonic functions, (iii) the blending functions associated with the control points of the ribbons, (iv) the composition of the surface equation and (v) options to edit the interior of the patch.

The main area of application is curve network based design, hole filling (vertex blending) and general lofting, in particular when watertight connections are important. The strength of the scheme is its flexibility to define complex shapes; its main weakness is that it cannot be given in standard form. Several examples will be given to compare the difficulties of classical surfacing approaches and the benefits of the new multi-sided scheme.

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3.37 On Modeling Neural Implicit Surfaces with Detailed Features

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The neural implicit representation has recently emerged as a compact, powerful means for shape representation. A main challenge in this direction of research is to enable neural networks to accurately represent important shape characteristics, e.g. sharp edges or fine-scale details. Sinusoidal positional encoding (PE) has been proposed in network training to better represent high-frequency details in images or shapes. However, naively applying sinusoidal PE often results in unwanted wavy artifacts on surfaces or even failure of the learned implicit to converge to the target shape. We study how the interplay between the point sample density and the dimension of PE used for network training would affect the expressiveness of a neural implicit representation model. Our finding is that while increasing the dimension of PE is beneficial to modeling fine geometric details, it is critical to also increase the point sample density accordingly in order to avoid unwanted artifact. Specifically, we derive empirical results on the optimal coupling of the point sampling and the dimension of PE. Extensive experiments show that our new training strategy outperforms the other competing SOTA methods for neural implicit surface modeling, in terms of approximation accuracy, shape feature preservation, and training efficiency.

3.38 A Deep Learning Approach for Non-rigid Registration

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Joint work of Juyong Zhang, Wanquan Feng

Main reference Wanquan Feng, Juyong Zhang, Hongrui Cai, Haofei Xu, Junhui Hou, Hujun Bao: “Recurrent Multi-view Alignment Network for Unsupervised Surface Registration”, *CoRR*, Vol. abs/2011.12104, 2020.

URL <https://arxiv.org/abs/2011.12104>

Learning non-rigid registration in an end-to-end manner is challenging due to the inherent high degrees of freedom and the lack of labeled training data. In the first work, we resolve these two challenges simultaneously. First, we propose to represent the non-rigid transformation with a point-wise combination of several rigid transformations. This representation not only makes the solution space well-constrained but also enables our method to be solved iteratively

with a recurrent framework, which reduces the difficulty of learning. Second, we introduce a differentiable loss function that measures the 3D shape similarity on the projected multi-view 2D depth images so that our full framework can be trained end-to-end without ground truth supervision. In the second work, we propose the differentiable deformation graph based neural non-rigid registration method. Specifically, we design a neural network to predict the correspondence and its reliability confidence rather than the strategies like nearest neighbor search and pair rejection. The model is trained in a self-supervised manner, and thus can be used for arbitrary datasets without ground-truth.

3.39 An Isogeometric Analysis Based Topology Optimization Framework for Additive Manufacturing of 2D Cross-Flow Heat Exchangers

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Joint work of Xinghua Liang, Angran Li, Anthony D. Rollett, Yongjie Jessica Zhang
Main reference Xinghua Liang, Angran Li, Anthony D. Rollett, Yongjie Jessica Zhang: “An isogeometric analysis based topology optimization framework for additive manufacturing of 2D cross-flow heat exchangers”. *Engineering with Computers*, under review, 2021

Heat exchangers (HXs) have gained increasing attention due to the intensive demand of performance improving and energy saving for various equipment and machines. As a natural application, topology optimization has been involved in the structural design of HXs aiming at improving heat exchange performance (HXP) and meanwhile controlling pressure drop (PD). In this paper, a novel multiphysics based topology optimization framework is developed to maximize the HXP between two fluids with different temperatures for 2D cross-flow HXs, and concurrently minimize the PD between the fluid inlet and outlet. In particular, an isogeometric analysis (IGA) solver is developed to solve the coupled steady-state Navier-Stokes and heat convection-diffusion equations. Non-body-fitted control mesh is adopted instead of dynamically remeshing the design domain during the evolution of the two-fluid boundary interface. The method of moving morphable voids (MMVs) is employed to represent and track boundary interface between these two different fluids. In addition, various constraints are incorporated to guarantee proper manufacturability of the optimized structures with respect to practical manufacturing process such as additive manufacturing. To implement the iterative optimization process, the method of moving asymptotes (MMA) is employed. Numerical examples show that the HXP of the optimized structure is greatly improved compared with its corresponding initial design, and the PD between the fluid inlet and outlet is minimized concurrently. Moreover, smooth boundary interface between two fluids and improved manufacturability are also obtained for the optimized structures.

4 Working groups

4.1 The Future of CAD

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4.1.1 Robustness of solid modeling operations

Introduced in the 1970's, boundary representations (B-reps) of solids are today's standard for CAD and engineering applications used in product development including physics simulation and manufacturing. Despite improvements over the past four decades B-rep modeling algorithms (Booleans, offsets, blends, etc.) are still fragile. This is due to the fact that they are built on a fundamentally flawed representation of trimmed surfaces. A B-rep containing several faces will contain many surface-surface intersections, and failure in the computation in any one makes the entire model invalid. Modeling failures usually require tedious manual intervention and rework by experienced CAD users. Therefore design exploration techniques (MDO) and applications like mass customization that require automation of engineering workflows driving parametric solid models are severely limited. New shape synthesis algorithms such as topology optimization create complex organic shapes that challenge B-rep modeling algorithms. It is time to reconsider solid modeling representations and algorithms from a fundamental perspective.

4.1.2 Additive manufacturing induced scalability issues

Additive manufacturing enables fabrication of shapes and structures of unprecedented complexity including for example lattices, geometric surface textures, and organic shapes generated by topology optimization. B-reps require explicit representation of geometry and topology. Consider a hierarchical lattice containing $100 \times 100 \times 100$ beams and each beam being a smaller scale lattice consisting of a 1000 primitives. A B-rep for such a structure requires billions of faces just to represent it. Performance of mainstream commercial CAD systems degrades with objects having more than a hundred thousand faces, leaving them short of designing such complex structures by several orders of magnitude. A fundamentally different approach for representing and performing modeling operations is required in order to leverage the capabilities of additive manufacturing. Other related engineering applications including physics simulation, manufacturing, design exploration, interop standards, etc. will also need to work with new modeling representations in order to support complete product engineering workflows.

4.1.3 Augmentable engineering rich models, variable materials

Modern engineering relies on robust digital models and simulations across separate disciplines to design, produce, maintain, and support products. A key component in integrating disciplines is the creation of a digital thread, a communications framework connecting authoritative sources of information in standard formats throughout the product lifecycle. Current CAD models typically lack sufficient engineering data, e.g. material or structural properties, for downstream models and simulations, e.g. electromagnetic or aerodynamic analysis. In order to support a digital thread, CAD models must incorporate the information required for discipline-specific models and simulations. A promising idea for delivering this information is the extension of geometry models past two or three dependent variables, allowing structural or material data to be delivered with design information.

4.1.4 Adaptive models for digital twins

A digital twin is a virtual representation of a physical system that captures system performance and maintains synchronization with that system through its operational life. The connection between a digital twin and its physical system occurs through sensors gathering data on real-time operations, maintenance and repair reports, etc. The geometric representation of a digital twin differs from traditional design in that the representation must serve an entire engineering process instead of an individual component in the process. In particular, the representation must be adaptable to changes that occur throughout the operational life of its physical counterpart and integrated with multiphysics models that enable accurate predictions of system performance.

4.1.5 V-Rep geometry

The geometric CAD world is employing B-reps or boundary-representations for over half a century, B-reps that are B-spline surfaces based. This representation is no longer sufficient consider the need for representing complex interior geometries (i.e. micro-structures) as well as functionally graded properties. Future fabricated artifacts will be porous as well as heterogeneous, two new degrees of freedom that are enabled by AM. AM not only allows one to create highly complex (porous) geometries but also deposit different materials in different places. Such printers are already out there and yet there is a complete lack of support of such abilities in contemporary CAD software. One possible remedy can be found in an emerging representation that is trivariate based V-reps or volumetric-representation. V-reps fully encompass the geometry as in B-reps but also allows the tight representation of boundary-compatible internal scalar, vector and tensor fields alongside the geometry. The V-reps not only seamlessly support micro-structure representations but also allows one to have multiresolution microstructures, allowing for nanostructures inside microstructures, picostructures in nanostructures, etc. Further, the V-rep representation is fully compatible with IGA and hence makes the connection between design and analysis/optimization much tighter (then in B-reps), as it should be. Finally, V-reps already support 3D printing of heterogeneous (and porous) geometries.

4.1.6 Implicit modeling

Implicit function representations of solids present several benefits. Primitive shapes commonly used in design as well as complex structures like lattices and textures can be represented easily by analytical expressions (e.g., conics, triply periodic minimal surfaces) or procedural

formulations (e.g., the modulo function). Modeling operations such as Booleans are simple math expressions (min/max or other R-function variants) irrespective of the geometric and topological complexity of the objects. Therefore modeling operations are robust and computationally fast. Implicit representations naturally lend themselves to parallelizable algorithms and so modern multi-core CPU and GPU architectures can be effectively leveraged. There have been advances in procedural modeling, visualization, physics simulation, topology optimization, and machine learning approaches that work directly with implicits. The theoretical foundations of implicit modeling have been introduced in the literature more than two decades ago, and as implicit function based applications mature, it holds much promise in addressing robustness and scalability challenges of B-rep based design systems. However, several challenges exist in adopting implicit modeling based approaches for engineering product design. Signed distance functions (SDFs) are especially useful for modeling but most implicit functions are not SDFs and the result of modeling operations on SDFs are no longer SDFs. So computing SDFs from arbitrary implicits efficiently remains an open challenge. Given that B-reps are the standard for mainstream product development today, effective and automated interop solutions with B-reps are necessary until entire product engineering workflows can be performed with implicits. Automated construction of a B-rep from an implicit remains an open challenge, especially for objects with sharp features and high genus. It may be desirable to develop other engineering applications such as NC machining directly based on implicits. New interop standards for implicits will also need to be developed.

4.1.7 Topology optimization

The long-standing challenge of topology optimization in the context of CAD is that its outcome is based on the finite element discretization and the piecewise constant representation of geometry. The recent emergence of the level set topology optimization approach has decoupled the geometry update of the optimization operation to the analysis and the implicit level set design representation opens up a new path that can enable a closer integration with CAD and a wider range of computational mechanics methods. This is particularly relevant for complex systems for coupling multiple scales and disciplines, and presents exciting new challenges in interoperable multifidelity mechanics models for topology optimization. The recent trends in topology optimization for complex coupled systems are timely with the rising interests of the digital twin and CAD interoperability. The research is not only from the mathematical and engineering mechanics operations, but also needs to consider the overall design workflow architecture and software modularization, i.e. the geometry is a core element of analysis software interoperability that follows and record the specific physical and mathematical assumptions. There are realistic pathways and the associated challenges now to enable a deployment of topology optimization within CAD to solve complex hierarchical problems and integrate back into the overall systems design.

4.1.8 Local refinement of tensor product spline spaces

There are three current approaches to local refinement of tensor product spline spaces:

- Specification of regions to be refined. Truncated Hierarchical B-splines (THB)
- Refinement by adding new meshline segments: Locally Refine B-splines (LRB)
- Refinement by adding new vertices in the control mesh: Standard T-splines (STS)

The spline spaces of LRB and STS are spanned by B-splines. In the general case the B-splines spanning the space will not form a partition of unity. However, partition of unity is imposed by scaling the B-splines with positive scaling factors of value less than or equal to

1. For THB partition of unity is achieved by truncating B-splines from a rougher level with B-splines from the finer levels. However, for all approach there is a risk that the scaling or truncation of some B-splines is so extreme that it has a direct effect on condition numbers for stiffness and mass matrices. A proposed new direction is to combine the requirement for minimal support B-splines from LRB and truncation from THB to significantly improve these condition numbers. There is also a need to better understand the richness and structure of B-splines of the different approaches and how they distribute the B-splines over the domain. An unwanted spatial distribution can directly influence the result of analysis and other computations.

4.1.9 Other topics

Other topics mentioned during the working group discussion but not developed further are listed here:

- Watertight models
- Integrating analysis results back into CAD
- Additive manufacturing induced scalability issues
- Robustness of solid modeling operations
- Global and sufficiently regular parametrization of CAD models
- CAD interoperability, including proper handling of proprietary data
- Parametric families of non-constant topology models
- Representing geometry to leverage AI techniques
- Rational offset surfaces
- Non-constant geometry models (time-variant, deformable, robotic, etc.)
- New representations (e.g. macro elements, polar splines)
- AI techniques for CAD
- Quantum computing
- Less primitive primitives

4.2 Design Optimization

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4.2.1 Explainable optimization

A black-box approach or a fully automated optimization process is not always desired. The input and interpretation of an expert designer can lead the optimization process to more desirable results, not possible through rigid automated processes. To facilitate this designer-in-the-loop option, the explainability of the optimization is essential. This can be achieved by several key improvements and features. Clear communication of the design space insights to the designer would eliminate the ambiguity inherent in black-box approaches. Treating the designer's personal preference as a latent optimization objective would set in place a system that leads the solution to the designer's intention. Providing better visualization of the analysis and optimization results will also make the design interaction easier. The possibility

of multiple solutions is also a possibility that explainable optimization should be able to handle. This is a more general issue where the compatibility of the problem formulation and the solution methodology is critical and will lead to a better definition of the engineering problem. We find this an important challenge that needs to be addressed by the community.

4.2.2 Exploratory design optimization

We identify several potential future challenges in exploratory design optimization. These are the handling of multiple design optimization solutions during exploration, improved communication and feedback on quantities of interest, and the enhancement of the relation between exploratory design and the digital twin.

Elaborating on the latter part, the relation between design exploration and the digital twin should be bidirectional. The design model should be not only sufficiently flexible to represent the geometry and performance alterations during the product's life cycle, but also be able to incorporate the data collected through the digital twins in a manner that improves design optimization and guides design exploration. This incorporation is an inverse design problem and could lead to augmented simulation, supported by real-life usage data across different scenarios or circumstances, allowing for further adaptation of the design to specific usage needs.

4.2.3 Sensitivities in design optimization

The reliability of the optimization solution is critically dependent on the reliability of the forward solver. The forward solver analyzes the response of the design and provides the critical sensitivity information to the optimizer to search for improving a design or configuration. Therefore, the robustness of the solver convergence is a key enabler. Many forward solvers are sensitive to numerical parameter settings and discretization, which may not converge to an accurate enough solution as the design/configuration changes. As the design changes, the solver or governing equations or assumptions can change and the analysis results are meaningless. As an optimizer searches a wide range of design space going through significant design changes, there remains challenges in ensuring that the forward solvers can guarantee to provide reliable solutions. In addition, the optimization search is critically dependent on the sensitivity therefore, the accuracy, continuity and numerical errors can fundamentally influence the resulting design. The current state of the art solvers are not usually well-equipped to provide reliable sensitivity and have limited understanding of their errors' influence on optimization. There is a need for research in computing reliable sensitivity (which is not necessarily the same as the traditional computational mechanics of predicting a specific response).

4.2.4 Multifidelity and uncertainty management propagation in design optimization

One prominent emerging concept across all engineering disciplines is digital engineering via digital twin. A digital twin is defined as “a virtual representation of a connected asset”¹, with an aim to predict the physical asset's behavior via computational models. Modern engineering systems however, are complex in nature, in which there are many components across a range of scales and their behavior is intrinsically unknown due to the interdependencies and

¹ Digital Twin: Definition and Value, AIAA and AIA position paper, Dec 2020, <https://www.aiaa-aerospace.org/report/digital-twin-paper/>

nonlinear interactions. The computational capabilities today are developed to model a specific behavior at one or two scales and the available computational resources are far from being able to model all complex behavior with emergence and nonlinearity across all scales and all governing physics. Indeed, there are many responses and behaviors we still do not understand and are unable to model. In order to construct and utilize a digital twin to predict unintended consequences, therefore, it is imperative that we have multifidelity models that can integrate and propagate the high order effects and uncertainties across disciplinary and scale boundaries. In the context of design optimization, an accurate prediction of unintended consequences and failure mechanisms is a critical requirement of a digital twin.

4.2.5 Design optimization methods

One fundamental challenge in design optimization arises from design parameterization/representation which defines the design variables. The design variables and their relationship to the governing equations and functional objective/constraints define whether the design space is continuous or discontinuous, convex, multi-modal, ill-posed and whether the existing optimization methods can find an optimum solution. Therefore, research is needed to formulate the geometry and design representation, and to efficiently explore and research the associated design spaces. Today's typical engineering systems are almost always ill-defined and highly complex thus, hence it goes without saying that high performance computing, efficient data structure and parallel algorithms are underlying enablers for design optimization. It is also important that the parameterization and data-structures from design, analysis, manufacturing to operation can be uniquely mapped such that the analyzed and designed and manufactured designs remain consistent. It should be noted that research in efficient design optimization methods would be hugely limited without the simultaneous research in the computational sciences and mechanics research. We recognize that design optimization is not aimed at automating design and taking people out of the design process: Rather, the true purpose is to aid an engineer's design activities. The focus of the design optimization methods research therefore, needs to be on informing an engineer to manage internal requirement conflicts and balance the short- and long-term consequences, offering a tool for investigating the complex design space and the "what-if" scenarios, and providing the necessary data to support engineers' creativity.

4.2.6 Parametric Modelers (PM) in the shape-optimisation loop

Concerning parametric modelers (PM) in the shape optimization loop, we list several topics of interest or desirable features for future research and consideration.

- The capability of a PM to incorporate local and global geometric quantities.
- Parent instances and their impact on the quality of the PM.
- The robustness efficiency of a PM, and specifically estimating the probability of producing non geometrically valid objects.
- The geometric properties of the design space and their influence on its exploration.
- Achieving dimensionality reduction and accelerating Parametric Sensitivity Analysis (PSA) via physics-informed geometric functionals.
- The smooth embeddability and integration of PMs to CFD/FEA solvers.
- Automatic differentiation of QoI (Quantities of Interest) with respect to design parameters.

4.3 Additive Manufacturing

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The following list contains talks that took place at the Dagstuhl seminar and relate to the Additive Manufacturing working group (in order of presentation):

1. Stefanie Hahmann. *Geometric construction and fabrication of auxetic metamaterials.*
2. Sylvain Lefebvre. *Generating oriented structures and trajectories within part volumes.*
3. Gershon Elber. *Volumetric Representations: Design, Analysis, Optimization, and Fabrication of Porous/Heterogeneous Artifacts.*
4. Xiaoping Qian. *Topology Optimization for Additive Manufacturing.*
5. Elissa Ross. *3D printed metamaterials in industry.*
6. Yongjie Jessica Zhang. *An Isogeometric Analysis Based Topology Optimization Framework for Additive Manufacturing of 2D Cross-Flow Heat Exchangers.*
7. Ernst Rank. *Interoperability of Geometric Models and Numerical Analysis by Immersed Boundary Methods.*
8. Suraj R. Musuvathy. *Implicit Modeling : Driving A CAD Renaissance.*
9. Géraldine Morin. *Tubular parametric volume objects.*

4.3.1 New opportunities and challenges in AM: overview

AM enables fabrication of shapes of unprecedented complexity, and in particular enables internal structuring of a part interior. This paves the way to the fabrication of volumes embedding microstructures, where small scale geometries directly impact the macro scale physical properties of the part. As 3D printing resolution increases, and as the size of the fabricable objects increases, the micro-structures are becoming akin to a material [3.29], that can be specifically tailored to the object and its future function, including gradients of properties [3.10,3.19,3.6].

This raises novel challenges regarding representation of these geometries [3.6,3.24,3.23] and calls for novel methodologies to analyze and simulate designed parts [3.6,3.26,3.39,3.27]. In particular, design and simulation are merging into a single integrated process, where simulation drives the design to automatically optimize the final parts [3.26,3.39,3.27].

4.3.2 Multiscale modeling, micro-structures as materials

A unique possibility opened by fine scale structuring of a part interior is to enable gradients of internal properties, varying the geometric details such that macro-scale properties change in different locations within the part. Designing such micro-structures requires solving for multiple challenges: the generation techniques have to produce micro-structures triggering the desired behaviors (e.g. anisotropy [3.19], auxeticity [3.10]), have to scale to large volumes, enforce geometric constraints of the target fabrication processes, and offer some degree of control to the designers. Several approaches are considered, such as repeating representative elements, possibly at multiple scales, supported by accurate and efficient volumetric

representations [3.6,3.23], that allows, for example, nanostructures inside microstructures, picostructures in nanostructures, etc., limited only by memory and computation abilities. Other techniques rely on implicit definitions to capture highly detailed, unstructured content [3.19,3.24]. A key future challenge is to allow for the efficient simulation of such models, which are diverging from the traditional representations (tetrahedral and hexahedral meshes) used by current state of the art simulation frameworks. Promising directions emerge towards this objective, with simulation approaches that avoid conversions and can work on transient representations of the data [3.27]. Generally, transient representations are created on-the-fly, when needed for display, simulation and production, at the exact resolution they are required. More research is called for at the interaction of these topics, in order to unlock the full potential of these emerging methodologies and develop a complete, novel ecosystem for AM.

4.3.3 Designing and optimizing for final physical properties

Designing with the full potential of AM requires novel workflows supported by computational design. In particular, topology optimization approaches allow optimizing a shape in ways that would be extremely difficult to achieve for a human designer. Such optimization techniques, however, have to be constrained in such a way that they enforce manufacturing constraints, and take them into account to produce parts that are not only optimal for a given function, but also optimal in terms of their fabricability on a target process [3.26,3.39]. Further research is required to further integrate the process in existing topology optimization frameworks, and to make topology optimization amenable to shape representations that are better suited to fabrication and analysis [3.39].

4.3.4 Novel geometric representations and interoperability

As novel representations are developed, based on V-reps [3.6,3.23], implicit functions especially signed distance fields [3.29,3.24] (SDF), or random porous geometries [3.10,3.19], novel challenges appear to allow their interoperability with existing workflows. For instance, conversions from and between such representations often leads to open questions: how to obtain precise SDFs from B-reps or arbitrary implicit formulations and vice-versa, how to obtain quad meshes and surface representations from SDFs, how to obtain volumes from lattice structures [3.23]?

Another question is how to redefine the design engineering processing pipeline of AM (including but not limited to physics simulation and hybrid AM with machining) from these novel representations, or transient representations, avoiding uncontrolled approximations due to conversions. Ultimately, novel industrial standards will have to emerge to support these evolutions.

A major aspect of future fabrication, in addition to porosity, is heterogeneity. AM not only allows one to create highly complex (porous) geometries but also deposit different materials in different places, aka functionally graded materials. Such printers are already out there and yet there is a complete lack of support of such abilities in contemporary CAD software. One possible emerging representation is trivariate based V-reps, that fully encompass the geometry as in B-reps but also allows the tight representation of scalar vector and tensor fields alongside the geometry. Further, this volumetric representation is fully compatible with IGA and hence makes the connection between design and analysis/optimization much tighter, as it should be. Finally, V-reps already support 3D printing of heterogeneous (and porous) geometries. There is also a need for new analysis methods able to deal with graded materials and solve inverse modeling problems.

4.4 Isogeometric Analysis

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In a discussion session on the current status of isogeometric analysis (IGA) and on the interaction between IGA and computer-aided geometric design, we identified future challenges and main areas of interest. This report briefly summarizes this discussion; it is also based on an extended comment by Malcolm Sabin.

At more than 15 years from its inception, IGA is a well-established technology. The field is very active, but it is facing some very difficult challenges and only few industrial inroads have been made.

The original idea of IGA was that the boundary representation (B-rep) of models held in CAD systems could use the basis functions of the NURBS surfaces as the basis for analysis, thus avoiding the need for meshing and remeshing steps along the whole analysis process.

The IGA approach puts B-splines as foundation (basis) for finite element analysis. As a consequence, the accuracy as a function of mesh density is optimal. Moreover, if a model is built primarily for analysis using B-spline elements it will be easy to export to a CAD system for subsequent addition of all the little tweaks which are needed for completion of the design and other downstream reasons.

However, there are some theoretical and practical issues that still need to be pointed out.

- There is a technology gap between 2-variate CAD and 3-variate analysis. Volumetric IGA needs elements fitted to the boundary, which is utterly non-trivial (although there are approaches capable of almost always constructing well-formed hex meshes in a typical B-rep shape). CAD must move to mathematical volumes to properly support 3D IGA. The legacy of existing CAD-models is blocking a move as well.
- In current CAD-systems, representations of real shapes hold rather badly fragmented B-reps. There are a lot more “faces” than the graphics representations on the screen indicate, and they are split in ways which do not really reflect the way that a mesh should flow for good analysis results. Moreover, the mathematics is hidden from the user. This makes bridging analysis and geometry sometimes easier without CAD.
- Finally, and regardless of the aforementioned improvements that should be made to CAD (e.g., 3-variate analysis, tighter integration between mesh ↔ geometry ↔ analysis), another important research direction is the development of IGA approaches for performing analysis on the many existing legacy-CAD-based geometries. These include approaches for watertight reconstructions (i.e., untrimming) as well as IGA in the presence of gaps and overlaps.

As of 2021 the IGA field shows some appreciable progress over the last 4 years.

- There are relevant practical applications where IGA has now proved to be useful as shell modelling, turbulent Navier Stokes or Maxwell’s equations (while this was not thought be possible some years ago).
- The IGA approach is embracing more technologies as immersed/embedded methods.

- There is mature software that is publicly available to both the academic and user community. Spline elements are getting into FEM-code (example: LS-DYNA) and there is progress on improving the STEP ISO 10303 standard.

Finally, we report that the wide scientific community is changing its mind about IGA, becoming less skeptical and more positive. In this perspective it is also worth to mention that there are now more (yet still few) joint projects related to IGA funded by industry. Also, in the last 10 years there have been a lot of projects (especially in Europe) training the young generation in IGA before they start working in industry (examples: MSCA ITN networks ARCADES, GRAPES and several ERC projects).

As for future directions we can identify the following items, with the first four issues situate in a closer future while the remaining ones seem to belong to a more distant horizon:

- Many interesting and new spline constructions are available, but it is not yet clear that they would enter the CAD system and help solve the interoperability issue.
- Volume representations (V-reps) still require a lot of investigations and are surely “work in progress”.
- Additive manufacturing is a unique opportunity for IGA: a posteriori error estimates can be used in practice to drive refinement and coarsening.
- Address “killer applications” including higher co-dimension contouring, level set methods for topology optimization, simultaneous material/shape optimization, etc.
- Implicit models and embedded IGA have a future but are far away from standards.
- Interaction with machine learning can be profitable: challenges in IGA could be shared with the machine learning community.
- Augmented reality could be a good application of IGA gathering the same basis functions for geometry and analysis.
- The forefront of PDEs on networks could be an area of application for IGA.

Summarizing, all the participants in the focus group agree that IGA can contribute positively to interoperability issues. Besides the need of promotion outside academia, communication of results is critical for interoperability also within academia (between engineers and mathematicians).

4.5 Geometric Machine Learning

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4.5.1 Summary

Machine learning is expected to have a significant impact on the fields of computer aided design, engineering analysis and manufacturing, and the interoperability between these disciplines. In recent years deep structured learning techniques have been wildly successful in several computer vision tasks, speech recognition, and natural language processing, to name a

few. Advances in deep learning now progress slowly towards other application fields. Besides enabling new applications within the scope of the product development process, machine learning techniques may augment existing processes, yielding improved interoperability of geometry modeling, analysis, and manufacturing, thereby enabling more efficient design optimization and product development.

Several key challenges are to be resolved in coming years. Application of soft and, in particular, hard constraints into neural network architectures remains a challenging aspect that requires further study. Development of deep learning tools for different geometry representations, including hybrid representations remains an active area of research. The main challenge, however, is to develop one unified theory that encompasses different geometric representations. General and complete theories of geometric machine learning should be developed. Finally, applications where machine learning can boost efficiency and efficacy of the product development process need to be identified. This way more machine learning experts from other fields could start contributing within these areas.

4.5.2 Status of geometric machine learning in 2021

Much progress has been made on deep neural networks, for a range of geometry representations. Explicit representations, including point-clouds and parametric representations such as simplicial meshes, spline surfaces and subdivision surfaces have been considered. Implicit representations, including algebraic surfaces and level-set methods have been investigated. Some of the advantages of explicit and implicit representations have been combined in hybrid representations. Hybrid representations exist in many CAD software tools, addressing limitations of geometric modeling under one representation.

Enforcement of geometric constraints is another area of active research. Soft constraints are well understood and lead to deep learning models with regularization constraints. Imposing hard constraints in current network architectures remains an active area for further research. Examples include equivariant and invariant neural networks. A unified theory that encompasses different geometric representations is still lacking. General and complete theories of geometric machine learning should be developed.

4.5.3 How can machine learning improve the interoperability between geometric modeling, simulation, manufacturing?

Machine learning may enhance geometric modeling, numerical simulation and manufacturing, providing automated procedures that optimize for different end-goals, such as efficiency, accuracy, and durability. An important goal of machine learning is to learn representations from data. With sufficient data machine learning may be used to automate certain manual labor intensive tasks, including geometry clean-up, meshing for engineering analysis, transfer of analysis results back to the geometric modeling process.

Deep learning techniques provide new ways to link classical disciplines, which is hard to achieve using conventional approaches. An example is generation of image descriptions using natural language processing. In the context of geometric modeling, simulation, and manufacturing, deep learning has the potential to establish new links that were previously beyond reach. One example is the use of numerical simulation to generate training data for supervised geometric neural networks. A second example is the development of neural networks that integrate complex user-constraints, e.g. manufacturability constraints, into the geometric modeling process.

We summarize a set of applications where machine learning could be used to augment / improve geometry modeling / isogeometric analysis / additive manufacturing, including the interoperability between these fields:

- Shape registration and analysis
- Reverse engineering and 3D shape generation / scene reconstruction
- Feature learning on surfaces
- Topology optimization
- Generation of quadrature rules for fictitious domain methods
- Learning multiscale models for microstructures.
- Optimization of global quadrilateral parameterizations / meshes
- Deep learning in reduced order modeling
- Learning “cleaning / fixing” of CAD models
- Driving refinement / coarsening of FEA / IGA spaces, domain decomposition
- Machine learning to augment preconditioners and solvers

4.5.4 Challenges in the short-, mid-, and long-term

There are a number of challenges that require attention in the short and mid-term. The goal of machine learning is to learn representations or models from data. Data is application dependent and may be challenging to acquire depending on the application. Availability of open source datasets will benefit the research community. Development of deep learning tools for different geometry representations, including hybrid representations remains an active area of research. For example, recently there has been a lot of progress on neural implicit representations. Some of the new works go beyond traditional geometric modeling tools. The main challenge in the mid- to long-term, however, will be to develop a unified theory of geometric machine learning that encompasses a wide range of geometry representations. Establishing such general theoretical foundations for geometric deep learning, will involve aspects from approximation theory, geometry, topology, optimization, and statistical machine learning.

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