Report from Dagstuhl Seminar 19151

# Visual Computing in Materials Sciences

**Edited by**

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## Abstract

Visual computing has become highly attractive for boosting research endeavors in the materials science domain [1]. Using visual computing, a multitude of different phenomena may now be studied, at various scales, dimensions, or using different modalities. This was simply impossible before. Visual computing techniques generate novel insights to understand, discover, design, and use complex material systems of interest. Its huge potential for retrieving and visualizing (new) information on materials, their characteristics and interrelations as well as on simulating the material's behavior in its target application environment is of core relevance to material scientists. This Dagstuhl seminar on Visual Computing in Materials Sciences thus focuses on the intersection of both domains to guide research endeavors in this field. It targets to provide answers regarding the following four challenges, which are of imminent need:

- **The Integrated Visual Analysis Challenge** identifies standard visualization tools as insufficient for exploring materials science data in detail. What is required are integrated visual analysis tools, which are tailored to a specific application area and guide users in their investigations. Using linked views and other interaction concepts, these tools are required to combine all data domains using meaningful and easy to understand visualization techniques. Especially for the analysis of spatial and temporal data in dynamic processes (e.g., materials tested under load or in different environmental conditions) or multimodal, multiscale data, these tools and techniques are highly anticipated. Only integrated analysis concepts allow to make the most out of all the data available.
- **The Quantitative Data Visualization Challenge** centers around the design and implementation of tailored visual analysis systems for extracting and analyzing derived data (e.g., computed from extracted features over spatial, temporal or even higher dimensional domains). Therefore, feature extraction and quantification techniques, segmentation techniques, or clustering techniques, are required as prerequisites for the targeted visual analysis. As the quantification may easily end up in 25 or more properties to be computed per feature, clustering techniques allow to distinguish features of interest into feature classes. These feature classes may then be statistically evaluated to visualize the properties of the individual features as well as the properties of the different classes. Information visualization techniques will be of special interest for solving this challenge.
- **The Visual Debugger Challenge** is an idea which uses visual analysis to remove errors in the parametrization of a simulation or a data acquisition process. Similarly, to a debugger in computer programming, identifying errors in the code and providing hints to improve, a visual debugger in the domain of visual computing for materials science should show the following characteristics: It should indicate errors and identify wrongly used algorithms in the data analysis. Such a tool should also identify incorrect parameters, which either show no or very limited benefit or even provide erroneous results. Furthermore, it should give directions on how to improve a targeted analysis and suggest suitable algorithms or pipelines for specific tasks.


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- **The Interactive Steering Challenge** uses visual analysis tools to control a running simulation or an ongoing data acquisition process. Respective tools monitor costly processes and give directions to improve results regarding the respective targets. For example, in the material analysis domain, this could be a system which provides settings for improved data acquisition based on the current image quality achieved: If the image quality does no more fulfill the target requirements, the system influences all degrees of freedom in the data acquisition to enhance image quality. The same holds for the materials simulation domain. Visual analysis can help to steer target material properties in a specific application environment by predicting tendencies of costly simulation runs, e.g., using cheaper surrogate models.

**References**

1 Heinzl, C. and Stappen, S. (2017), STAR: Visual Computing in Materials Science. Computer Graphics Forum, 36: 647-666. doi:10.1111/cgf.13214

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## 1 Executive Summary

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In this Dagstuhl workshop, we brought together computer and computational scientists interested in building tools for use in visual computing with material scientists with expressed interest in using such tools. As would be anticipated when one brings together two distinct fields, the initial challenge we encountered was that of language. Although both groups came together having experiences with visual computing tools – some as developers and some as users – although they often used the same terms, they semantically meant different things. We found that the Dagstuhl philosophy of "immersion" was most helpful to this issue as having several days together helped break down these barriers. Over the course of the week, we interspersed talks by computational scientists and material scientists. The talks by computational scientists often presented their current understanding of what kinds of tools are needed, demonstrations of current tools they have developed in collaboration with domain-specific experts, and success stories of applications they have currently impacted. The talks by the material scientists often presented a description of the tools they currently use, the positive points and deficiencies of current tools, the types of features that they would like to see in future tools, and examples of current challenge problems and how they might be impacted by the next generation of tools.

**Fundamental Results:**

1. The systems that are desired by many material scientists will be used both for exploration and for interactive steering. When used for exploration, material scientists want tools that not only present the data with its corresponding reliability (uncertainty) bounds, but which also give predictive capabilities such as where next to sample.
2. There is a general acknowledgement that both automation and interactivity are needed. Automation of tasks and procedures through AI and Machine Learning can be used to help deal with the volumes of data being produced – helping scientists sift through the field of possibilities to isolate those places for which they should expend human effort. At the same time, there are many current practices that continue to require "the human in the loop" to make decisions. In such cases, tools are needed that have smart defaults but yet allow the user to explore, navigate and possibly refine data.
3. Although many current tools used for material science applications leverage previous visualization and interaction technologies, there is still much to be done. Many material science applications require specialization of currently existing algorithms and techniques, especially in cases of real-time systems. Furthermore, many techniques originally designed for batch or manual processing need to be re-engineered to allow for the interactive procedures required by current and future material science application scientists.
4. With regards to visualization scientists, there is a need for both data and tasks. Many researchers requested data on which they can try their methods. In addition to the data itself, descriptors of the data are necessary so that it can be interpreted properly. Once read into their system, the visualization scientists then requested a collection of tasks (driven by the material science domain experts) which would help drive their tool development and evaluation.

### Final Comments

Due to the ever-increasing interest in this topic, we foresee that future review articles and/or special issues of journals driven by multilateral research cooperations between seminars' participants will be an outcome of this workshop. To ensure and stimulate further cooperation in this field, a list of specific follow up activities has been elaborated and discussed with the participants. All in all, a fruitful discussion was stimulated across the two domains throughout the complete week of this Dagstuhl workshop which will become more obvious in joint research efforts of all kinds.

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**Working groups**

# 3 Overview of Talks

## 3.1 Intuition-based Visual Analysis of Microstructures

*Amal Aboulhassan (Material Solved – Alexandria, EG)*



In our ongoing research, we propose a new direction of analyzing microstructures based on an intuitive visual analysis paradigm. We enable the researchers to predict the structure-function relationships even if modelling techniques or experimental data are limited due to various reasons (multi-scale and multiphysics phenomena occurring during the process, or limited access to the measurements). Our paradigm aims to include the human intuition into the analysis process naturally. It is achieved through an instantaneous update of the properties due to the edits in the microstructure. For example, the user immersed in the microstructure finds a small potential defect or bottleneck, removes it manually and gets an instant update on the properties. To enable such instant feedback the online analysis of the existing information is needed. In an ideal case scenario, the optimal update is also suggested. To handle the latter situation the inverse problem needs to be solved. Both these scenarios rely on two critical elements: (i) enabling the user to alter parts of the data and (ii) quantifying how these edits influence the overall performance. Editing the microstructures on the fly and link it with the properties is a challenging problem since this type of data is complex and big in many cases. Visual analysis and exploration is one strong potential solution in this case. Finally, once the ideal update to the structure is identified, the question remains – how to modify the manufacturing process to realize this editing? – which is an open problem in materials science.

## 3.2 Inline inspection and dynamic angle acquisition

*Jan De Beenhouwer (Universiteit Antwerpen – Wilrijk, BE)*


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In conventional X-ray-CT inspection of objects generated from a computer-aided design (CAD) model, a 3D CT reconstruction of the object is compared with the reference CAD model. This is a cost inefficient and tedious procedure, unsuitable for inline inspection. Alternatively, X-ray radiography based inspection is fast but fails to provide full 3D inspection. Here, we propose an inspection scheme based on a limited set of radiographs, which are dynamically selected during the scanning procedure. An efficient framework is described to determine the optimal view angle acquisition from a given CAD model and to automatically estimate the object pose in 3D with a fast, iterative algorithm that dynamically steers the acquisition geometry to acquire the set of chosen projections.

## 3.3 Tomography and the challenges in visualization

*Gursoy Doga (Argonne National Laboratory – Lemont, US)*



X-ray tomography is a nondestructive imaging technique that provides the internal structure of samples and its implementations at synchrotrons is heavily used by materials scientists. However, as the applications are pushed further into the nanoscale, the radiation dose limited conditions become more apparent, leading to challenges in achieving high resolution reconstructions. In this talk I will introduce a set of new computational imaging techniques that can yield superior reconstructions for high-speed or photon-limited imaging conditions when implemented as an integral part of the imaging setup. This approach requires re-design of both hardware and software components of a tomography system such that the overall performance is optimized rather than optimizing individual components. I will highlight some of the main challenges in visualization and other parts of this system compared to conventional systems.

## 3.4 Droplets, Bubbles and other Material Structures

*Thomas Ertl (Universität Stuttgart, DE)*



Visualization research at the University of Stuttgart contributes to material science in several large interdisciplinary projects primarily in the context of simulation-based research. The SFB 716 focused on particle simulation for which we developed MegaMol, a visualization framework providing advanced interactive visualization techniques for large particle datasets. The presented examples cover space-time clustering of atoms in laser ablation, extracting stacking faults, debugging clustering criteria in nucleation simulations, or discovering flexoelectricity effects in cracking metal oxides. The SFB/TRR 75 deals with droplet behavior under extreme conditions. By direct multi-phase flow simulation, breakup and coalescence of droplets are studied which pose many visualization challenges like coupling the spatial representation with space-time diagrams showing the topological evolution or tracking droplet dynamics over time. In the new SFB 1313 on interfaces in porous media we study the relation of CO2 bubbles and its porous surrounding geometry in saturated sandstone. The distribution of these bubbles does influence seismic properties of the material which will influence measuring leakage in CO2 sequestration. We present an analysis pipeline which groups extracted bubbles and surrounding structures according to their similarity and clusters them, allowing visual comparison after registration. By investigating bubble size and shape distribution, effects on phase velocity dispersion could be demonstrated.

### 3.5 The visualization challenge of tensor-valued strain data from loading experiments to predict mechanical failure

*Christian Gollwitzer (BAM – Berlin, DE)*



Concrete bars were subjected to mechanical load in different configurations (uniaxial pressure, double punch test and reinforcement bar pullout) until the samples were broken. During the loading, the samples were observed using X-ray computed tomography. Digital Volume Correlation (DVC) was then used to measure the deformation field in the sample between the unloaded state and the individual load steps. It would be valuable to predict the failure of the sample from the small deformations inside the sample. Classic failure criteria for concrete (Drucker-Prager, von Mises) were tested to evaluate the correlation between the location of the final cracks and the locations indicated by the failure criteria. Due to the derivative of the measured deformation fields for the failure criteria, the data is very noisy which makes the predicted locations of failure hard to see. On the other hand, displaying the projection of the deformation field across the crack direction indicates, that the information of the crack location is contained in the data. The challenge was formulated to derive a good visualization indicating only the failure location without computing noise-prone numerical derivatives.

### 3.6 Reformation and Sparse Interaction in Visualization

*Eduard Gröller (TU Wien, AT)*



Data visualization provides computer-supported interaction with visual representations of (abstract) data to amplify cognition. The increasing complexity of data requires interaction support and simplification of visual representations, also in light of investigating ensembles of data. Motivated by historical examples, typical case scenarios from various domains are discussed. These include: curved planar reformations, myocardium unfolding to bull's-eye plots, knowledge-based navigation, molecular dynamics exploration, defects analysis in industrial XCT data, and comparisons of large sets of volumetric data.

### 3.7 MESHFREE: CFD-simulation with interactive/computational steering

*Hans Hagen (TU Kaiserslautern, DE)*



MESHFREE is an innovative, gridfree simulation tool in fluid and continuum mechanics, developed by Fraunhofer ITWM. The numerical modelling is based on a cloud of points carrying all relevant physical information. Due to the meshfree character, it almost naturally mimics applications with free surfaces, moving geometries, and fluid structure interaction

(FSI). The gridfree setting of the method allows local/global refinement of the pointcloud (adaption of numerical resolution) as well as immediate response of the simulation towards changes in the geometry (adaption to form changes). Both types of adaptions may be subject to interactive steering, to be performed while the simulation is running. On-the-fly adaption of parameters of a running simulation is highly efficient, saving a lot of computation time as well as man-power in optimizing simulation results, especially in industrial design cycles. Only gridfree simulation methods provide the full potential to interactive steering. Based on a body inside of a flow, we will show how to: (1) interactively adapt the (local) refinement of the numerical pointcloud in order to gain a requested quality of the computed result (let us say the resistance force), and (2) interactively perform a simple shape optimization of the body towards some optimization constraint (let us say the minimization of resistance force).

## 3.8 Tomviz: An open source integrated tool for analysis, visualization, and debugging

*Marcus Hanwell (Kitware – Clifton Park, US)*



The Tomviz project has been funded by the US Department of Energy SBIR program, and offers a permissively licensed open source tool for tomography. It uses JSON to describe its pipeline, including all processing steps, and visualization parameters. This is coupled with a Python-centric data processing pipeline, and wrapped C++ taking advantage of parallelism and GPUs for visualization. Recently "live updates" were added to aid in the development of and debugging of reconstruction parameters in challenging atomic/high resolution scanning transmission electron microscopy tomography. The live updates of the pipeline as data is acquired on a microscope will also be described as it pertains to aiding in data acquisition. More generally at Kitware we develop a number of open source libraries, and open source tools for scientific data including VTK, ParaView, ITK, CMake, and others. There is a new project with a national lab to extend Tomviz to help their beamline tomography users, and a new project with another national lab to process 4D STEM data using HPC resources for very high data rate acquisitions. A recent Phase I SBIR seeks to develop a general framework for high data rate 4D STEM microscopy, offering a Python/C++ library for processing, web-based data management platform, and web application visualizing/previewing data. At the core the development of open source platforms as collaborative research and development platforms offers viable business models that can help drive open, reproducible science workflows forward.

## 3.9 Visually assisted reconstruction of geometric objects in microscopic data

*Hans-Christian Hege (Konrad-Zuse-Zentrum – Berlin, DE)*



The reconstruction of geometric objects from voxel data is a very common task in many fields, including almost all natural, materials, engineering, environmental and life sciences, as well as other fields such as archaeology. Research in image and geometry processing over the past decades has provided solutions for image denoising, image registration, image segmentation, surface and volume mesh creation that enable us nowadays to build up a generic geometry reconstruction pipeline in which at each stage a particular algorithm can be plugged in, selected from a small set of field-proven algorithms. This results in a fully automated reconstruction. The only phase for which considerable progress is still required is image segmentation. Here we should continue to strive for a smaller set of general applicable approaches that meet the needs of a wide range of applications with rather different needs (in terms of image properties, prior knowledge and segmentation objectives). Machine learning methods are particularly promising here.

Focusing on the situation, where the generic reconstruction pipeline needs to be extended or modified by some complex operation, the following strategy has proven to be successful: First, try to bridge the difficult/complex parts of the geometry reconstruction pipeline with manual, interactive, visually supported operations. Second, apply the resulting pipeline to real-world data sets, thereby creating (hopefully) ground truth results and getting more insight into the problem while solving it manually. Finally, utilize the gained insight and the established ground truth results to algorithmize the remaining manual portion. Do this gradually, until (ideally) no manual interaction is left. This approach has proven to be successful in many applications where a pure computer-vision approach, trying to solve the entire problem algorithmically from the beginning, would have failed. The strategy is illustrated on the example of two problems: (a) the reconstruction and quantification of dislocation substructures from stereo-TEM and (b) the reconstruction and unrolling of ancient papyri from $\mu$CT.

## 3.10 Imaging and Tracking Dynamic Phenomena in Materials Research

*Wolfgang Heidrich (KAUST – Thuwal, SA)*



Many applications in Material Science require imaging of time-varying data as well as an analysis of the motion fields between different configurations. In this talk I will focus on joint 4D (space+time) geometry and motion analysis using new tomographic reconstruction methods. These methods are applicable in any scenario where either a) a time-varying phenomenon is investigated with tomographic methods (X-ray, EM etc), and the time scale of the motion is comparable the frame rate of projections in the imaging system, or b) whenever the sample undergoes uncontrolled deformation during the scanning process (e.g. drift, heat expansion, or sample degradation). I will illustrate the methods using examples from composite material analysis and material porosity analysis among others. I will also highlight the relationship of these methods to recent fluid imaging methods.

## 3.11 Quantitative X-ray computed tomography for materials sciences

*Johann Kastner (FH Oberösterreich – Wels, AT)*


**URL** http://www.3dct.at

X-ray computed tomography (XCT) currently transforms from a qualitative diagnostic tool to a quantitative characterization method. Quantitative XCT is the combination of XCT with quantitative 3D image analysis. Only through preprocessing and data enhancement, segmentation, feature extraction and quantification, rendering of the results, in-depth insights into XCT data a sample may be facilitated. In the beginning of industrial XCT, XCT images were generated mainly for visual inspection. The most important application of quantitative XCT is metrology Additionally, quantitative XCT is increasingly used for extracting a large variety of characteristics of materials and samples:

- Characterization of pores metallic and polymeric foams
- Porosity evaluation of metals and polymers
- Determination of fiber orientation, diameter and length of fiber-reinforced polymers as well as their distributions
- Fiber bundle extraction and characterization of technical textiles
- Quantitative data concerning the 3D structure of inhomogeneous metals or other materials (e.g., interconnectivity, sphericity, etc.)
- 3D characterization of isolated discontinuities such as cracks, voids, inclusions, delamination, etc.
- Phase identification and characterization
- Physical and mechanical properties (physical density, crack growth, wear) and, to a certain extent, chemical composition (alloy and phase identification, impurities)

## 3.12 Uncertainty Quantification and Its Role in Materials By Design

*Robert Michael Kirby (University of Utah – Salt Lake City, US)*



When computational methods or predictive simulations are used to model complex phenomena such as the response of physical systems to a range of conditions or configurations, researchers, analysts and decision-makers are not only interested in understanding the data but are also interested in understanding the uncertainty present in the data as well. Quantification, communication and interpretation of uncertainty are necessary for the understand and control of the impact of variability; these three – quantification, communication and interpretation of uncertainty – help add both understanding and robustness to the design process. In this talk, we present an overview of the multiscale modeling and uncertainty quantification efforts accomplished as part of the Center for Multiscale Modeling of Electronic Materials (MSME), a collaborative partnership between academia and the Army Research Laboratory. In particular, we will focus on our successes in cross-cutting areas – bringing uncertainty quantification techniques originally developed within a particular discipline to a broader class of materials by design problems. We will also attempt to address the question of "why now?" – what current factors and trends explain the recent rise in uncertainty quantification efforts, and what we can learn from these trends.

## 3.13 Advanced impact damage characterisation of composite laminates by X-ray Computed Tomography

*Fabien Leonard (BAM – Berlin, DE)*



One of the great strengths of X-ray computed tomography over conventional inspection methods (ultrasound, thermography, radiography) is that it can image damage in 3D. However for curved or deformed composite panels, it can be difficult to automatically ascribe the damage to specific plies or inter-ply interfaces. An X-ray computed tomography (CT) data processing methodology is developed to extract the through-thickness distribution of damage in curved or deformed composite panels. The method is applied to [(0°/90°)2]s carbon fibre reinforced polymer (CFRP) panels subjected low velocity impact damage (5 J up to 20 J) providing 3D ply-by-ply damage visualisation and analysis. Our distance transform approach allows slices to be taken that approximately follow the composite curvature allowing the impact damage to be separated, visualised and quantified in 3D on a ply-by-ply basis. In this way the interply delaminations have been mapped, showing characteristic peanut shaped delaminations with the major axis oriented with the fibres in the ply below the interface. This registry to the profile of the panel constitutes a significant improvement in our ability to characterise impact damage in composite laminates and extract relevant measurements from X-ray CT datasets.

## 3.14 Through the micro-CT and what we found there? Quantifying images of fibrous materials

*Stepan V. Lomov (KU Leuven, BE)*



Description of a textile composite microstructure involved, identification of individual yarns/fibrous plies in the textile reinforcement. definition of local parameters of fibrous geometry: local fibre directions, local fibre volume fraction and description of the amount and (especially in the case the textile is a reinforcement of an impregnated composite) morphology of voids. The advanced method for acquiring such a description is micro-computed (micro-CT) tomography, which is a powerful tool for imaging of the internal structure of materials. The result of a micro-CT imaging is a 3D array of values ("grey scale"), which characterise the X-ray attenuation in the corresponding locations in the material. The challenge of the textile materials characterisation using micro-CT images is quantification of the image, identifying the parameters of the microstructure by analysis of the grey scale array. Such a quantification can be partially done by image thresholding and binarisation, which is the most common way of the 3D image processing. However, direction-related features are not easily determined using the binarisation. The paper describes methods and the software (VoxTex), which analyse the grey scale array to produce the description of the textile microstructure as an array of volume elements (voxels), each of element carrying information of the fibre directions and fibre volume fraction in it. Apart from that, the void contents and the voids morphology in textile composites are characterised. The methods are based on a two-parameters analysis of the image: local grey scale value and anisotropy, defined via the structure tensor of the grey scale field [1]. The paper presents validation of the VoxTex quantification of fibre directions and voidage measured with independent methods and overviews application of the methods to different problems related to details of the fibrous microstructure of textiles.

#### References

1 Straumit, I., S. V. Lomov and M. Wevers, "Quantification of the internal structure and automatic generation of voxel models of textile composites from X-ray computed tomography data", *Composites Part A*, 69: 150-158 (2015)

## 3.15 Experiences with synchrotron users working in material science and some of their challenges in the domain of 'The integrated Visual Analysis'

*Lucia Mancini (Elettra – Sincrotrone Trieste S.C.p.A. – Trieste, IT)*



Imaging techniques based on the use of hard X-rays play an important role in several research fields and industrial applications. Many topics in medicine, biology, material science, geosciences and cultural heritage studies can be afforded thanks to the high potential and large applicability of hard X-ray imaging techniques. In the last twenty years a great effort has been devoted to the development of X-ray computed microtomography (micro-CT) techniques, both employing microfocus and synchrotron radiation sources. Nowadays, these techniques allows to produce 3D or 4D (dynamic) micro-CT images of the internal structure of objects at the micron- and submicron- scale. Investigations performed directly in the 3D domain overcome the limitations of stereological methods usually applied to microscopy-based analyses and a non-destructive method is more suitable for further complementary analyses and for precious or unique samples (fossils and archeological finds, in-vivo imaging, etc ...). In the field of materials science, an intriguing challenge is to extract directly from 3D and 4D images some parameters allowing to characterize structural, chemical and physical properties of the studied materials. However, accurate image processing, analysis and visualization methods for an effective assessment of these parameters are still an open issue especially in the case of time-resolved and multi-scale and multi-modal CT experiments. In this talk, thanks to the experience gained working in collaboration with several users of the SYRMEP beamline of the Elettra synchrotron facility or working as user in different laboratories and synchrotron facilities, several scientific applications of advanced hard X-ray imaging techniques will be presented trying to critically expose the progress, limitations and open problems in the different fields.

## 3.16 Why do we need visual and automatised data reduction schemes in X-ray experiments?

*Rajmund Mokso (Lund University, SE)*



Tomographic measurements at synchrotron and laboratory X-ray sources are today fast and come with a large data sizes. Visualisation is important at various stages of these studies and we may distinguish between three types of visualisation tools as a function of time counted from the start of an X-ray imaging experiment. First we aim to follow the acquisition process itself but visualising the streams of data. At this stage we would need to employ robust and simple visualisation tools which will enable quick decision making during the acquisition. The second stage is just after the data is acquired. The tomographic reconstruction is fast and in the majority of cases we rely on visualising a gray scale image of one slice as quality control. Here we would welcome the visualisation of the features of interest in 3D instead of the gray scale slice. In the third stage for the final quantification of the volumes, the challenge is in decomposing the found quantities (e.g. particle shapes, orientations or curvatures) into as simply as possible arrays to characterise the material in 3D and often in a time resolved manner. Owners of imaging data are most often not experts in image analysis or visualisation, accordingly the tools must be well documented and as simple to work with as possible. The actual computing time and performance in terms of speed is only important for the first group of these tools used during the acquisition. The remaining two groups must focus on user friendly operation and the capability to deal with volumes of at least 2k x 2k x 2k pixels.

## 3.17 The DQS Advisor: A Visual Interface to Recognize Tradeoffs in Dose, Quality, and Reconstruction Speed and ColorMapND: A Data-Driven Tool for Mapping Multivariate Data to Color

*Klaus Mueller (Stony Brook University, US)*



**The DQS Advisor:** Achieving high-quality CT reconstructions from the limited projection data collected at reduced x-ray radiation is challenging, and iterative algorithms have been shown to perform much better than conventional analytical schemes in these cases. A problem with iterative methods in general is that they require users to set many parameters, and if set incorrectly high reconstruction time and/or low image quality are likely consequences. Since the interactions among parameters can be complex and thus effective settings can be difficult to identify for a given scanning scenario, these choices are often left to a highly-experienced human expert. The DQS Advisor is a computer-based assistant that allows users to balance the three most important CT metrics – dose (D), quality (Q), and reconstruction speed (S) – by ways of an intuitive visual interface. Using a known gold-standard, the system uses an evolutionary optimization algorithm to generate and learn the most effective parameter settings for a comprehensive set of DQS configurations. A visual interface then presents the numerical outcome of this optimization, while a matrix display allows users to compare the corresponding images. The interface allows users to intuitively trade-off GPU-enabled reconstruction speed with quality and dose, while the system picks the associated parameter settings automatically. Once this knowledge has been generated, it can be used to correctly set the parameters for any new CT scan taken at similar scenarios.

**ColorMapND:** In volume visualization transfer functions are widely used for mapping voxel properties to color and opacity. Typically, volume density data are scalars which require simple 1D transfer functions to achieve this mapping. If the volume densities are vectors of three channels, one can straightforwardly map each channel to RGB which requires a trivial extension of the 1D transfer function editor. We devise a new method that applies to volume data with more than three channels. These types of data often arise in scientific scanning applications, where the data are separated into spectral bands. Our method expands on prior work in which a multivariate information display was fused with a perceptual color map in order to visualize multi-band 2D images. In this current work we extend this joint interface to blended volume rendering. We design a set of functionalities and lenses that allow users to interactively control the mapping of the multivariate volume data to color and opacities. The latter enables users to isolate or emphasize volumetric structures with desired multivariate properties that can be identified in the joint interface. We also show that our method enables more insightful displays even for RGB data. We demonstrate our method with three datasets obtained from spectral electron microscopy and high energy X-ray.

## 3.18 Topology-driven approaches for analysis and visualization of material structures

*Vijay Natarajan (Indian Institute of Science – Bangalore, IN)*


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Data resulting from high fidelity computational simulations and high resolution imaging devices is becoming increasingly complex in terms of the number of features. Topological structures such as the contour tree, mapper, Reeb graph, and Morse-Smale complex provide abstract representations of features in the data that are succinct and amenable to visual analysis. Topological Data Analysis (TDA) refers to the study of such abstract representations for data analysis. These structures support feature detection, extraction, comparison, and tracking and hence enable methods for effective visualization and exploration of feature-rich data sets. In this talk, I will first give an introduction to TDA with a focus on scientific data. Next, I will introduce the problem of symmetry and similarity detection in scientific data and describe its role in the design of feature-directed visualization methods. I will present algorithms to detect symmetry and discuss applications to visualization, interactive exploration, and visual analysis of time-varying and multivariate data.

## 3.19 Next Generation NDT – An Enabling Technology for the Industry of the Future

*Ahmad Osman (HTW – Saarbrücken, DE)*


**Joint work of** Ahmad Osman, Bernd Valeske

The digital transformation has high influence on our society and a clear impact on almost every industrial segment. This essentially includes the technologies and tools for the factory of the future, medical and health care systems as well as materials development and processing. In order to continue serving as an enabling technology in industrial sectors (automotive, railway, infrastructure etc.), Nondestructive Testing (NDT) has to raise to a next level, the so called NDT 4.0 or Next Generation NDT. In modern NDT, sensors are considered not only as data providers but data processing is expected to be sensor integrated and to guide the data acquisition strategy. Modern sensor systems will be capable of transferring the big data into smart data with information that helps monitoring and optimizing production processes and products throughout their complete life cycles. Such cognitive systems will be able to autonomously specify the optimal settings for data acquisition: how, where and which data are required to assess a scene. NDT sensor systems with embedded intelligence, i.e. AI-algorithms for real time data processing and evaluation, will be part of IoT. These smart devices produce data and decisions which are saved into a digital product memory that describes the history and changes in the product properties. This upcoming evolution of sensor systems requires a radical transformation on several levels such as the qualification courses of NDT personnel, on human-machine interaction modes etc. The sensor systems should be able to guide the human in his inspection task, thereby reducing the complexity of his work, accelerating the evaluation through on-site visualization and feedback to the operator. In this work, we present features and algorithms for smart NDT inspection system which can be used for ultrasound probes, eddy current probes or micro-magnetic sensor systems. For the ultrasound probes, the sensor position is tracked using commercial webcams. The operator is not expected to follow specific trajectories in scanning the surface of a structure. The camera system tracks the probe position and acquired A-scans per position are simultaneously transferred to parallel processes. The quality of these raw signals is autonomously verified according to several criteria. Feedback is given to the operator in case where settings deviations occur or unsatisfactory data are generated. The operator can then repeat the scan to cover the indicated area. Qualified A-scans are then reconstructed into a three dimensional volume. The volumetric data are visualized in real time via various ways of augmented reality, for example on AR-lenses. The data reconstruction is done in 3D using online capable method, referred to as progressive Synthetic Aperture Focusing Technique (SAFT). The presented system is an enabler for a more flexible, faster and unconventional qualification of personnel. It eases the task of appropriate data interpretation and guarantees optimized scanning settings, repeatable and reliable quality control results for onsite inspection tasks. The system can be easily integrated into digital surrounding for data communication. As the system can be used to cover large surfaces, aspects related to big data handling, data reduction, sparse data representation, inline data processing and visualization are challenges that are currently being addressed in ongoing research and development activities at Fraunhofer Institute for Nondestructive Testing.

## 3.20 Quantitative analysis of CT data using Machine Learning

*Sidnei Paciorník (BAM – Berlin, DE)*


**Joint work of** Sidnei Paciornik, Renata Lorenzoni, Sergei Evsevleev, Giovanni Bruno

One of the most difficult steps in image analysis for Materials Science is segmentation. Traditionally, objects would be discriminated by their intensity, contour or texture. However, there are many situations in which none of these approaches work and, importantly, it is difficult to extrapolate from one problem to another. Moreover, there is no analytical or general way to decide the best segmentation method. It is always a trial and error situation. Deep Learning (DL) Convolutional Neural Networks (CNN) bring a new perspective to this problem. Using as input data the individual pixel/voxel intensities, the CNN automatically extracts discriminating features and can converge to a set of classes/objects given a reasonable training set. The training, which also serves as ground truth, is typically defined as regions of each object/class manually outlined by the user. This is the most work intensive step. However, once the network produces a reliable segmentation, in principle it can be directly applied to similar images with no further effort. This approach was used to segment two challenging sample types: a 3-phase Strain Hardening Composite Cement (SHCC) imaged by lab-scale microCT and a 5-phase Metal Matrix Composite (MMC) imaged by synchrotron microCT. In both cases morphological features included elongated fibers and more equiaxial objects. Initial results using the same network architecture – the so-called U-Net [1, 2] were very promising. Fibers and other phases were automatically segmented with good agreement with the ground truth. Different training strategies involving data augmentation were tested. Transfer learning between different samples was also successful by adding a small amount of training data to a previously trained network. These initial results raise several questions about the best strategy for using DL CNN's in image segmentation. Is there an ideal CNN architecture? How large must the training set be? Which parameters should be included in the data augmentation procedure? How should we proceed from 2D to 3D training set creation? What is required in terms of network architecture and GPU capabilities to obtain true 3D segmentation?

### References

1 Ronneberger, O. et al. Medical Image Computing and Computer-Assisted Intervention (MICCAI), Springer, LNCS, Vol. 9351: 234–241, 2015.

2 Falk, T. et al. U-Net: deep learning for cell counting, detection, and morphometry, Nature Methods. Vol. 16, 67–70, 2019. DOI: 10.1038/s41592-018-0261-2

## 3.21 Application of Machine Learning tools for quantitative 3D-4D materials science

*Guillermo Requena (DLR – Köln, DE) and Federico Sket (IMDEA Materiales – Madrid, ES)*



Neural networks (NN) have become a state of the art tools for the analysis of imaging data and the prediction of process behaviour in several fields such as medicine, earth observation and climate research. In the present contribution we explore the use of machine learning tools based on neural networks to solve current 3D and 4D material issues that can hardly be approached using classical methods. Two examples are given: (1) Segmentation of 3D imaging data using convolutional neural networks: the separation of microstructural constituents in multiphase materials can be a tedious task that requires several hundreds of hours of human work to obtain trustable 3D or 4D data for subsequent analysis. We implemented a U-net-based CNN architecture that is able to achieve at least 94% accuracy in the segmentation of absorption plus phase contrast tomography images in Al-Si alloys. Open challenges to further advance in the segmentation of 3D-4D data were also presented. (2) Understanding and prediction of mechanical properties of materials: as an example of the use of NN for the prediction of material behaviour, a framework combining design of experiment (DoE), computational micromechanical modelling, and Neural network is presented. An analytical surrogate model including some material properties was obtained and the possibility to extend it by incorporating more material properties and other simulated failure modes across relevant length scales discussed. Finally, two examples on which NN could assess the production process of materials were presented, one for in-situ curing of composite materials and other for selective laser melting manufacturing. In combination with in-line sensoring of the production process the challenge of collect data from the process as it occurs, training a machine learning algorithm to analyse them, and predict or decide in-line improvements and/or corrections was presented.

## 3.22 Multivariate Data Analysis using Fiber Surfaces for Material Science

*Gerik Scheuermann (Universität Leipzig, DE)*



Application like structural mechanics of composite materials or geomechanics of nuclear waste deposits require the analysis of multiple scalar fields at the same time. An example is provided by all invariants of tensors. A more complicated example are variables from different models in coupled simulations where structural mechanics, hydrology, and thermodynamics are simulated at the same time, all creating multiple variables to study. In this talk, I present three case studies in material science where we used tailored visualization techniques like effective combination of tensor fields to show potential failure, fiber surfaces of the stress tensor invariant space, and exploration of three scalar attributes at the same time. The studied materials are short glass fiber reinforced polymers, a hybrid metal-carbon fiber reinforced polymer component, and a combination of different rock layers in geomechanics.

## 3.23 Image modelling and computational materials science

*Katja Schladitz (Fraunhofer ITWM – Kaiserslautern, DE)*



Material versatility is ever-increasing, accompanied by need for more complex and precise structures and properties. The rise in complexity requires continued development of scalable and dedicated analysis tools, which again enable further optimization and research. Fraunhofer

ITWM and TU Kaiserslautern (departments of Computer Science and Mathematics), having decades of joint experience, form a group of leading experts in complex analysis tool development. We are working to bring new algorithms and methods for visualization, inspection, modelling and simulation of material structures and properties to the market. In order to precisely model the structural properties, material representations must first be deduced from measurements, e.g. image data of various dimensions and types/modalities. Deduction of complex materials micro-structures such as fiber reinforced composites, as well as complex surfaces calls for custom developed algorithms, which further need to be verified and validated. Validation requires the ground truth representation, which is unfortunately often unavailable due to the fact that there is no other measurement method or the phenomenon to be captured is extremely rare. Only way out, when the ground truth is unavailable, is modelling of the surface, material or structure and simulation of the imaging method. Moreover, stochastic geometry models for complex materials micro-structures are the key ingredient for so-called virtual materials design. Not only the right trade-off between the truth and physical or geometric model has to be found, models have to be visually convincing too. Atop of the correctness of the model, results of geometric analysis (curvatures, orientations) and of simulations (stress, strain, temperature...) must be visualized in a way which allows intuitive analysis and evaluation. This task is challenging, considering that we are dealing with local results on complex micro-structure as well as the embedded micro-structural information in a multi-scale simulation. However, we have developed many significant contributions to modelling, simulation and visualization and are continuously working on new ones, thanks to wide variety of collaborations with mechanical, process and civil engineers.

## 3.24 Visual Comparison of Ensemble Datasets

*Johanna Schmidt (AIT – Austrian Institute of Technology – Wien, AT)*



Comparative visualization refers to the process of using visualization techniques to understand how different datasets are similar or different, and to be able to interactively explore these differences. Comparison is getting an increasingly important task in data analysis, as it can be very cumbersome in case many data items, or complex data items have to be compared. Visualization systems successively have to move from representing one phenomenon to allowing users to analyze several datasets at once. Large data collections that contain a lot of individual, but related, datasets with slightly different characteristics can also be called ensembles. In the course of this talk a technique for the comparative visualization of 2D image datasets and for the comparison of 3D shapes are introduced. Both techniques focus on the scalable analysis to support ensemble analysis. When comparing 2D images, we propose to not only outline the differences in the data, but also to use clustering and interactive widgets to further understand the structure of the differences – how many images are affected by the difference, and how to they look like. For analyzing 3D shapes we went one step further, since here we are not only able to study individual differences, but it is also possible to understand relations between differences, e.g., if differences are always caused by the same ensemble item. We achieve this by aligning regions of interest on a reference shape as axes in a parallel coordinate plot, and then draw polylines for all ensemble items according to its error rate in the specific regions. This way the error rate of ensemble items over several regions of interests can be studied. In the course of material sciences, comparative visualization can be targeted towards the comparison of different segmentation results, either in 2D images or as 3D shapes. According to the challenge "The Visual Debugger", comparative visualization can support users to understand and analyze differences in the data being introduced when running certain feature extraction mechanisms (e.g., segmentation) with different parameters. Comparative visualization can also be seen as an extension for parameter space analysis.

## 3.25 Features of tensor fields (latent model) extracted from Kalman filter tracking data

*Jeff Simmons (AFRL – Wright Patterson, US)*



Traditional homogenization approaches produce mesoscale representations by developing a Representative Volume Element (RVE) whose properties are, with acceptable scatter, independent of position in the material. This is accomplished by biasing the analysis with an Independent and Identically Distributed (iid) assumption on the microstructural elements. That is, in order to reduce the variance to the point that the volume element is representative, it is necessary to invoke an iid assumption, which is inconsistent with the existence of an anomalous condition. Such occurrences are simply treated as outliers and "averaged away" in the process. We propose an alternative approach of applying a model-based bias, specifically, that the fibers behave as streamers in a laminar flowing fluid. With this model, the fiber orientation becomes the basis for the mesoscale representation. By analogy with fluid dynamics and the tracking discipline, we refer to this orientation as the 'velocity.' Following successful approaches in fluid dynamics analysis, we can extract a 'velocity gradient' from the data. The velocity may be extended to be a continuum field by the hypotheses that (1) the velocity field is smooth and (2) that it matches the computed velocity values at the fiber detection points. With these assumptions, the velocity field may be expanded into a Taylor's series about a detection point and the velocity gradient appears naturally as the second order coefficient. This is evaluated from a set of detection points in the neighborhood of the target point by the pseudoinverse of the matrix of distances of the neighboring detection points on the computed changes in velocity from the target point and the neighboring points. Local homogeneous strains produced in the neighborhood of fibers, as the reference frame is translated down the fiber axes, can then be computed from the symmetric part of the velocity gradient. The rotation produced by this motion, the chirality, may be computed from the anti-symmetric component. Non-uniformities can then be computed by performing an anomaly test on the fiber velocities by classifying velocities having a likelihood below a threshold as being anomalous. A consistency check, in which the anomalous classification persists through multiple successive layers is used to differentiate a true anomaly from one resulting from detection noise. It is suggested that this approach may be used to coarse grain many other microstructures by s suitable choice of biasing model. Additional image processing steps needed to extract the fiber detection positions are also described.

## 3.26 Machine Learning for Material Sciences: Computer Vision at Scientific Facilities

*Daniela Ushizima (Lawrence Berkeley National Laboratory, US)*


URL http://bit.ly/idealdatascience

Advances in imaging for the design and investigation of materials have been remarkable: the growth of X-ray brilliance and extremely quick snapshots have enabled the description of dynamic systems at the atomic scale; micro CT has focussed on capturing shape and structural properties of new compounds to measure the function and resilience of new materials. Our recent efforts in machine learning applied to image representation and structural fingerprints have streamlined sample sorting and ranking including the identification of special material configurations from million size datasets.

### References

1 Araujo, Silva, Ushizima, Parkinson, Hexemer, Carneiro, Medeiros, "Reverse Image Search for Scientific Data within and beyond the Visible Spectrum", Expert Systems and Applications 2018 .
2 Liu, Melton, Venkatakrishnam, Pandolfi, Freychet, Kumar, Tang, Hexemer, Ushizima, "Convolutional Neural Networks for Grazing Incidence X-ray Scattering Patterns: Thin Film Structure Identification", Materials Research Society – Special Issue on Artificial Intelligence (published), 2019.
3 MacNeil, Ushizima, Panerai, Mansour, Barnard, Parkinson, "Interactive Volumetric Segmentation for Textile Microtomography Data using Wavelets and Non-local means", Journal of Statistical Analysis and Mining, Sep 2019.
4 Araújo, Silva, Resende, Ushizima, Medeiros, Carneiro, Bianchi, "Deep Learning for Cell Image Segmentation and Ranking", Computerized Medical Imaging and Graphics, Mar 2019.
5 Ke, Brewster, Yu, Yang, Ushizima, Sauter, "A Convolutional Neural Network-Based Screening Tool for X-ray Serial Crystallography", Journal of Synchrotron Radiation 2018.

## 3.27 Visual Debugging in Particle-Based Simulation

*Daniel Weiskopf (Universität Stuttgart, DE)*



Visualization can play an important role for debugging because it allows us to potentially identify problems in a dataset that might be connected to issues earlier in the data production pipeline. Here, I focus on particle-based simulation as the source of data, leading to multivariate data sets in which particles are associated with multiple attributes (such as pressure, forces, etc.). The specific use case is smoothed particle hydrodynamics (SPH). I report on our experiences with a visualization system that combines spatial representations of the particles with non-spatial views such as scatterplots and parallel coordinates plots that show multivariate attributes. With such a system, we were able to identify problems with a software implementation, but we were also able to identify the impact of different models and parameters on the simulation results. Finally, I discuss the role of debugging in the larger setting of visual data analysis as well as challenges specific to visual debugging in materials sciences.

## 3.28 Visualization of Quantitative Data Derived from Volumetric Imaging

*Thomas Wischgoll (Wright State University – Dayton, US)*



This presentation discusses techniques and issues with obtaining quantitative data from imaging technology at high levels of accuracy. Current techniques are capable of deriving quantitative data from volumetric images at sub-voxel levels. However, there are limitations stemming from the fact that there are issues with different artifacts, such as noise, partial volume effects, etc., that lead to uncertainties inherently encoded within the data. Awareness of that fact can help improve the segmentation of the data and as a result the quantitative information extracted. The quantitative data can then be used for additional modelling and further analysis.

# 4 Working groups

## 4.1 Working Group Discussion Summary: Ensembles, uncertainty and parameter space analysis, multi objective / multi parameter optimization

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The following topics were discussed:

- UQ: not much data available, many phantoms but no specific phantom available, uncertainty on grey values not available by CT device manufacturers or detector manufacturers. Uncertainty information is mainly available on derived data (e.g. metrology); aleatoric part of uncertainty can be estimated by repeated measurements, but epistemic error remains unknown ==> Finding: info on uncertainty missing.
- Parameter space analysis: Used in a very focused way for optimizing specific algorithms or specific parts of a quantification pipeline for a new experiment. Parameter space analysis should also be important for materials design. Question: is Parameter space analysis here the correct term or does materials science rather need an analysis of the solution space? Question: What is the solution space ==> highly dependent on the application
- Where can Vis actually help? ==> only where the human is in the loop Data processing for Materials Science ==> characterization of materials Comparative Visualization is a big issue for setting up experiments and analyses
- Can Vis help for DoE (Design of Experiments)? For example more coarse simulation methods (e.g., using surrogate models) can help to reduce the need for extensive and complex simulations but still find the sweet spot. Question: Can automatic DoE algorithms be combined with human (not yet formalized or quantified) knowledge?

- Come up with a pipeline – what is the current pipeline? Measurements ==> raw data ==> scripts/tools to get the info they are after.
- Questions:
  - Can we add to/streamline that workflow?
  - In need of more expertise.
  - What tools are available?
  - What are the bottlenecks?
- Uncertainties:
  - What sources of uncertainty are there?
  - Are we even the right group to address this?
  - Doesn't seem to be much data, so vis is hard
- Parameter Space:
  - All are so different: reconstruction, each material is different, really tricky
  - Try to optimize typically mechanical properties of the final result
  - How can we support this? Can visualization actually support this or are there better mathematical tools?
  - Visualization is out of the game whenever the human is out of the game.
  - But if things are really high-dimensional you will not be doing things completely automatically.
  - Can we help with the design of experiments?
  - Maybe help with questions like how to get the voids smaller or other structural questions.
  - Human is looking for correlations with the hope of finding relations
  - But again – how could we support that?
  - Is visualization used in the design of experiments? Selectively. Some people in materials find it unscientific. More like data science than materials science. But this is going to go railway
  - Cheap preview. Simple simulation to narrow down possibilities. In-silico modeling to reduce cost
  - In an engineering application using simulation/visualization – find places where bad effects occur and what the conditions will be to produce those results.
  - In a science application – situational awareness.
  - Can we look to how wet-labs use simulation?
  - Seems to be some reluctance to use vis.

## 4.2 Working Group Discussion Summary: Image Processing

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The group was lead by a presenter, Wolfgang Heidrich, who summarized topics related to volume correlation, denoising and segmentation. The state of the art for these three areas are summarized as follows:

1. Volume correlation: Local DVC (neighbourhood based), and optical flow in computer vision can be better than local DVC.
2. Denoising: 99% time materials scientists use Median and Gaussian, and Sparsity-based (like TV denoising) from the data processing specialist or non-local means give better results, but are rarely applied in practice
3. Segmentation: Deep learning produces very good results, and transfer learning is frequently used to a pretrained network and update the training.

The needs and barriers in these three areas can be summarized as follows:

1. Volume Correlation
   a. Need: Fibre breaking in a synchrotron CT measurement: loading along the feature direction is difficult to see.
   b. Need: Evaluation of DVC algorithms in realistic conditions.
   c. Barrier: Window problem of optical flow.
   d. Barrier: Missing texture. Introduction of artificial tracer particles is not always easy.
2. Denoising
   a. Need: Faster acquisition gives noisy data.
   b. Need: Killing artifacts and detect hidden features. Get simple examples where denoising helps to find features.
   c. Need: Concrete solution: e.g. publish the algorithm at TomoBank.
   d. Need: Web page / Resource / network with implementations of different algorithms – like TomoBank.
   e. Barrier: Implementations not readily available NLM is available, but other denoising are not.
   f. Barrier: Distinguishing features from noise is hard, real features might be deleted.
3. Segmentation
   a. Need: Multilevel heterogeneity. Fibre material, organised in bundles of fibres. The individual fibres are to small to be detected or segmented.
   b. Need: Superresolution can be used to improve the segmentation..
   c. Need: Theoretical analysis could be useful, but is not available.
   d. Need: Segmentation thresholds have a strong influence on the results. E.g. porosity values are dependent on segmentation thresholds.
   e. Need: Segmentation can be implemented by discrete optimization.
   f. Need: Segmentation of medical data?
   g. Barrier: Superresolution: available processing power.

To summarize, the main barriers expressed during this session were related to accessibility for the material science community and related to real data for verification for those people doing optimization.

## 4.3 Working Group Discussion Summary: Machine Learning

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



**Tools:**

Tools need to be made available with machine learning/deep learning to material scientists. Trying to understand results and limitations.

- Which network architectures are more successful for certain problems?
- Which knobs need to be adapted?

**Discussion Topics:**

We discussed a lot on ground truth and measures of quality and generalizability of network architectures and parameters. The group reflected on the following issues:

- Connectivity of microstructural constituents is important in many cases. How to train and test with respect to connectivity?
- Convolutional CNNs may not work if applied to graph structures?
- Can other information be used in addition to voxel intensities? Surface normals, curvature and depth for example -> use it as input to deep learning. What is the consequence for the required training set?

Segmentation as one of the most urgent issues.

**Tomographic data:**

Typically reconstructed as isotropic data whereas microscopy data can be strongly anisotropic, thus looking in a traversal direction is considerably different from any orthogonal direction. Contrast is often different on different devices; histogram matching as a possible solution or re-training with one slice from the new dataset to adjust weights. Noise reduction and image fusion are other issues for deep learning.

**Training data:**

Transfer learning for similar data. Training data with damages and artifacts, e.g. beam hardening and streaking.

**TomoBank:**

Database with annotated training data and challenges, e.g. streak metal artifacts. Role of data augmentation: U-Net people use distortion and noise. What are the right data augmentation techniques for tomography. Examples where data augmentation was negative in certain cases in terms of accuracy where mentioned. Networks should be uploaded? How? What format? Exchange/share networks with data. Archival of networks/data. Perhaps only little re-training is required.

### SciVis Contest:

Create a visualization contest. Which data/problem is most urgent? What are metrics for the quality of the result? For image analysis: It would be Dice-coefficient, Hausdorff distance? But for a visualization contest. Structural similarity as a quality criterion. Sensitivity/specificity. Insights/hypothesis/influence on problem solving related to material science visualization.

### 2D vs 3D:

Training of the network in 2D vs. 3D. 3D as interpolated from 2D slices.

## 4.4 Working Group Discussion Summary: Materials Science Applications for Visualization Beyond Existing Tools (requirements for vis tools from materials sciences perspective)

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), and Rüdiger Westermann (TU München, DE)*



For these breakout groups, we split the group randomly into two subsets containing both material scientists and visualization scientists. Both groups were posed the same question.

### Materials Science Applications for Visualization Beyond Existing Tools (requirements for vis tools from materials sciences perspective) Working Group Discussion: Group A:

Our lead-off question to this group was as follows: Material scientists: Tell us the science problems you want to solve. Visualization scientists: Where can Vis help solve those particular problems?

The challenges we decided on could all fit within a topic of "Steering Acquisition," but each could be useful as a separate goal. These are:
1. Real time dynamic sensing for data acquisition,
2. Accelerated understanding of the materials state for decision making,
3. Identification of interesting events and accelerated discovery of materials property,
4. Real time design of experiments that is robust to changes in strategies during data collection.

To accomplish this, it is envisioned that we design a challenge to the community that will establish a benchmark problem that can be reused for additional efforts.

Accelerate Discovery and Determination of Material Properties
- How to improve visibility of your structure without losing the context.
- Tracking dynamic phenomena.
- Design of experiments. Why is it not used more regularly? Maybe use visualization to aid the design of experiments.

Detect, track and predict behavior from anomalies
- Identify things that are similar and/or symmetries.

Steering Acquisition
- Dynamic Control
- Early detection of characteristics to steer/optimize further data acquisition.
- Maximize information obtained while reducing the acquisition of “useless” data.
- Tracking dynamic phenomena.
- Combine exploratory approaches with optimization of data acquisition.
- Take advantage of visualization to accelerate useful data acquisition.
- Find a common set of samples/phantoms to work on.

Dynamic Sensing Simulation
- The relevance of simulation to help in optimizing acquisition.

Data fusion
- Visualization as a tool to facilitate and optimize fusion

### Materials Science Applications for Visualization Beyond Existing Tools (requirements for vis tools from materials sciences perspective) Working Group Discussion: Group B:

Our lead-off question to this group was as follows: Material scientists: Tell us the science problems you want to solve. Visualization scientists: Where can Vis help solve those particular problems?

#### Problems and Tasks identified by the Material Scientists

- Overview:
  Get a concise and quick overview of the data right after recording it, show interesting points immediately (holes, pores, cracks), find slices that are of interest. Find interesting points in a volume Find slices with something different than the canonical slices (“first 10”)
- In-situ experiments:
  The in-situ experiments require to adapt several forces to the material (temperature, pressure) and record the results. The application of these forces causes the microstructures in the material to change. Experiments can be very different, taking a long time with only a view changes, or events that happen very suddenly (e.g., brittle material under load, cracks happen soon, in contrast to laser powder melting, stabilize melting). For these experiments, at the long run, an automatic decision system should be available to automatically adjust the experiment parameters. In the meantime, visualization can help to visualize the intermediate steps, for an interactive steering of the process. Visualization can help here in the following ways:
  - Timely feedback during the experiment. Possibility of on-line data reduction and preliminary segmentation during the experiment, to better use beamtime. Especially badly needed for fast experiments. Offline-evaluation of data often leads to the problem, that the data cannot be used in the end (extract characterization quickly from the measurement data to get an overview. Very big volumes, many parameters, need to understand that)
  - Parameter visualization to understand the causality between material and experiment parameters (e.g., how does an experiment parameter affect the physical material properties). For example, there can be more roughness in the prepared material, how does this impact the final part
  - Vector field visualization to understand forces

  - Pore tracking over several timesteps (pore segmentation works fine, but the tracking over several timesteps is still a problem – maybe also integrate physical properties of the pore?)
  - Comparative visualization to understand where and when events occurred in the data
  - Change detection to see which parts of the data that has been recorded during the experiment can be thrown away
  - Prediction to better steer the acquisition times of the machines, trigger when something important is going to happen (more a computational effort, not a visualization topic)
- Visualization or large 3D data structures:
  Apart from large volume data, other large 3D structures like skeletons have to be studied. This is currently a problem due to occlusions in 3D. Other options like projections into 2D space would be of help here, where patterns can be analyzed more easily in 2D.
- Visualization or large 3D data structures:
  Apart from large volume data, other large 3D structures like skeletons have to be studied. This is currently a problem due to occlusions in 3D. Other options like projections into 2D space would be of help here, where patterns can be analyzed more easily in 2D.
- Visualization of clustering parameters:
  When clustering pores with multiple criteria, it is often hard to understand the relation between these pores. Visualizations towards the representation of cluster parameters (e.g., in a graph, similar to MegaMol that Tom Ertl showed in his talk) could help the domain experts to better understand the clusterings.
- Segmentation Crowd Challenge:
  Getting better, faster and more accurate segmentation algorithms is still an open issue. A common crowd challenge on segmentation, including machine learning, would be of interest – how could gamification be included?
- Suggestion from the VIS community: Tensor field data
  Tensor field data is used, data sets are available. New CT techniques like SAXS-CT and Nested tensor tomography allow to record more data (e.g., spectrums) for all data points. However, there not so many applications for these types of CTs yet, mainly because it takes a lot of time to acquire a sample.
- Suggestion from the VIS community: Measurement uncertainty
  Currently material scientists trust their measurements (e.g., for segmentation), so there is no need for the visualization of measurement uncertainty

## 4.5 Working Group Discussion Summary: Multilateral Cooperation

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The discussion group on multilateral cooperation was finished with a list of concrete action items to be pursued after this Dagstuhl workshop:

1. **Benchmarking datasets**
   As a free initiative datasets will be provided in order to facilitate a benchmark across participating groups. The benchmark will contain, datasets, currently applied protocols,

data analysis pipeline as well as parametrization. The goal is to have a documentation of a complete workflow in order to either come up with improved results, to compare with existing results, as well as to improve specific steps in a workflow. Benchmarking and testcases may contain permeability analysis, porosity, fiber breakage, generalization of internal structure (connectivity, topology) as well as other aspects. In this context als a SciVis Contest may be targeted.

2. **Plenary talk at Materials conferences**
   Plenary Talks on Visual Computing in Materials Sciences are planned at Composite Conferences. Conferences of interest will be the European conference on composite materials or the TexComp.
3. **Special issue in journal**
   As a direct outcomes of this workshop two special issues in the domain of Visual Computing in Materials Science are planned. More specifically, "Computer Graphics & Applications", as well as "Materials" will be targeted.
4. **Viewpoints article**
   Visualization Viewpoints article offer detailed technical opinions on trends in visualization?
5. **Dagstuhl seminar report**
   Another direct output of the workshop is a cumulative report of all talks and discussion groups which is found in this report.
6. **Tutorials**
   A tutorial in Visual Computing in Materials Sciences will be targeted in an upcoming conference. As primary venues conferences on Materials will be targeted. Euromat will be the primary candidate for this purpose.
7. **Further workshops**
   An joint workshop is planned in Lund at MaxIV for 2019. In addition the submission of proposal regarding a Dagstuhl workshop, an Erice Workshop or a Banff workshop on this or a related topic will be discussed by the end of 2019.

Additional Materials Provided As Part Of Breakout Sessions:
Here is the link to the SciVis contest which was mentioned in the discussions: http://sciviscontest.ieeevis.org/. Some of the data sets are still available.

The new DFG-funded Collaborative Research Center 1313 at the University of Stuttgart on "Interface-Driven Multi-Field Processes in Porous Media – Flow, Transport and Deformation" https://www.sfb1313.uni-stuttgart.de/index.html will have a dedicated project for providing benchmarks for porous media simulation. https://www.sfb1313.uni-stuttgart.de/research-areas/project-area-d/research-project-d3/. A first version can be found here: https://arxiv.org/abs/1809.06926

## 4.6 Working Group Discussion Summary: Shared Data Set and Benchmark Problems

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



### TomoBank:

All datasets will be available at the following link: https://tomobank.readthedocs.io/en/latest/source/dagstuhl.html The following datasets were added by various members of the workshop as part of a dataset and benchmark problem working group:

- **Dataset 1:** Description: Multiphase engineering alloys: Al-Si alloys, Ti alloys. The data covers 3D networks in the same sample before and after heat treatment [1]. When comparing small regions of the networks [1] before heat treatment and after heat treatment, disconnections have occured in these specific reions.
  Questions: What has changed after the heat treatment? Connectivity? Morphology? How can we visualize the changes in 3D for the whole network? Can we identify/quantify this regions and, more importantly, visualize them clearly in large structures Tasks:
  1. Segmentation of raw data: TBD
  2. Topological descriptors of segmented data
  3. 3D visualization of geometrical features

  Download Link: will be uploaded to tomobank, data also available through direct Contact: Guillermo Requena (guillermo.requena@dlr.de);
- **Dataset 2:** Description: Water migration in one-sided heated concrete. A paper is available here: https://link.springer.com/article/10.1007/s10921-018-0552-7 Concrete bars were heated in one end, which causes the water inside the concrete to evaporate, condense deeper in the concrete in pores and lead to a water wave. This can lead to explosive spallation of the concrete and causes problems (tunnel fire accidents). The data set consists of several consecutive rounds of cone-beam CT while the concrete is heated.
  Tasks:
  - Better reconstruction (SpaceTimeTomography?) that takes into account the sample expansions during the experiment
  - Determination of the water content (by subtracting expansion corrected volume data)
  - 3D / 4D visualisation of the migration of the water. In the paper, there is no "convincing" visualization of the water migration and condensation.

  Download Link: The paper is not open access, but a preprint can be made available upon request.
  Contact: Bartosz Powierza (Bartosz.Powierza@bam.de);

### References

1 K Bugelnig, F Sket, H Germann, T Steffens, R Koos, F Wilde, E Boller, G Requena, Influence of 3D connectivity of rigid phases on damage evolution during tensile deformation of an AlSi12Cu4Ni2 piston alloy, Materials Science and Engineering: A 709, 193-202

## 4.7 Working Group Discussion Summary: Suggestions for further discussions

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



- **Datasets & Tasks**
  From the visualization side, it would be great to get access to datasets and specific tasks. There was the suggestion to upload data to the Tomobank and also attach specific tasks to it, so that visualization people could work on them.
- **SciVis Challenge**
  Starting a SciVis challenge on the topic would also include more visualization people, and hopefully result in many suggestions how to visualize the data (and also many citations, since this data is publicly available and people will use it as a benchmark).
- **Review Paper**
  The material scientists are lacking a better overview on the available software tools and how they could use them. There was the suggestion to write a review paper, with materials scientists as co-authors, published in the material science community, where important tasks are outlined, with suggestions which visualization techniques and software tools to use.
- **Software tools**
  As mentioned above, an overview of available techniques and software tools would be of great help for the material scientists.
- **Pipeline**
  A possible pipeline could be Experiment -> data Processing -> Visualization. Therefore, data processing is the missing link here in this group (machine learning would be a way to avoid image processing).

## 4.8 Working Group Discussion Summary: Time-Varying Data

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The group was formed by two materials scientists and two computer vision people. During the session, the problems in materials science where the evolution can provide much more information were highlighted. Then, selected experiments were shown where the use of 3D + time experiments provide a lot of information that needs extraction and evaluation.

The discussion was oriented to a couple of examples where visual computing could help:

1. Tracking features in consecutive volumes during time: Here, it was mentioned that there are a couple of tracking algorithms that could be used for particle tracking but there is no reliable open source tool for that purpose. Even commercial tools are not so efficient

in that sense. Even more, the possibility to track particles with the ability to filter some of characteristics while tracking was proposed.

2. Link the 2D to the 3D space: With the intention to avoid recording and storing not useful data, it is important to be able to, either detect some changes in the acquisition in 2D or with analysis in in-line reconstruction in 3D. A visual analysis of some parameters should be able to trigger the data collection systems when some important change is detected. This is especially important for fast occurring processes where the data acquisition is a constrain because of memory, storage, or other limitations.

## 4.9 Working Group Discussion Summary: Tools

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- **Tomviz**
  Further information: The Tomviz project is a cross platform, open source application for the processing, visualization, and analysis of 3D tomographic data. It is developed in C++, using Qt, building on VTK, ParaView, ITK, Python, SciPy and NumPy. The complete pipeline of data processing steps from alignment and reconstruction to visualization and analysis of 3D data can be presented, saved, and restored. A suite of Python tools for 3D analysis is packaged to accommodate custom algorithms. The initial focus was on high resolution scanning transmission electron microscopy, but that has been broadened to include improved support for other types of tomographic data. Tomviz can load custom Python scripts in the user's home directory to add new extensions to its menus for processing. Tomviz is tested and packaged on Windows, macOS, and Linux with full source code available on GitHub.
  Link: https://tomviz.org/
  Licencing: 3-clause BSD
  Contact person: Marcus D. Hanwell (marcus.hanwell@kitware.com)
  Datasets: A sample tilt series and reconstruction are included with the package, also links to a Nature Data paper with CC-BY licensed data sets hosted on Figshare.
- **open_iA**
  Further information: open_iA is an open source tool for the visual analysis and processing of volumetric datasets, with a focus on industrial CT datasets. As graphical user interface the cross-platform framework Qt is used, which facilitates an easy to use and attractive interface. In-house visualisation and image processing algorithms are supported by algorithms of the ITK and VTK toolkit, which make open_iA a powerful tool for both 3D visualisation and CT data analysis. open_iA is capable of loading various volume dataset formats as well as different surface model formats. It provides slice by slice navigation in its 2D views, common 3D navigation with arbitrary cutting planes in the 3D view, together with custom views for individual visualization. open_iA is easily extensible and serves as central development platform of the research group computed tomography @ University of Applied Sciences Upper Austria, Wels Campus and therefore integrates all algorithms and methods developed within the group.

Link: https://github.com/3dct/open_iA Licencing: GPLv3
Contact person: Christoph Heinzl (c.heinzl@fh-wels.at)
Datasets: Sample datasets are provided with the respective tools

- **aRTist**
  Further information: Simulation tool for X-ray radiography and CT. A few CT examples are shown on the gallery page: http://artist.bam.de/en/gallery/index.htm
  Link: http://aRtist.bam.de
  Link: https://github.com/ElettraSciComp/Pore3Dcencing
  Licencing: commercial, evaluation licenses available, within projects licenses are usually granted for free for project partners
  Contact person: Carsten Bellon (Carsten.Bellon@bam.de)
- **Super-resolution CT reconstruction**
  Further Information: tomographic reconstruction tool for datasets with very thin features (fibers or sheets). This is research code with datasets, as well as the scientific publications.
  Project page: https://vccimaging.org/Publications/Zang2018SuperResolutionCT/
  Code:https://drive.google.com/open?id=1Ws454D65kopVprnuVP_OMajbtRN0Um24
  License: Creative Commons, attribution noncommercial
  Contact: Wolfgang Heidrich (Wolfgang.Heidrich@kaust.edu.sa)
- **Space-Time Tomography**
  Further Information: tomographic reconstruction of 4D time varying data. Research code + datasets + scientific publication.
  Project page: https://vccimaging.org/Publications/Zang2018Space-timfore/
  Code: https://github.com/gmzang/SpaceTimeTomography
  License: Creative Commons, attribution noncommercial
  Data: https://repository.kaust.edu.sa/handle/10754/627676
  Contact: Wolfgang Heidrich (Wolfgang.Heidrich@kaust.edu.sa)
- **Pore3D**
  Further Information: Pore3D is a software toolbox for processing and analysis of three-dimensional images. The core of Pore3D consists in a set of state-of-the-art functions and procedures for performing filtering, segmentation, skeletonization of 3D data and extraction of quantitative parameters. A full control of algorithms parameters and intermediate results is possible at each step of the analysis.. Easy integration with other sw tools is possible (fro GUI, 3D visualization, ...). Although three-dimensional data can be produced by several techniques (for instance: magnetic resonance, X-ray scattering or confocal microscopy), the library was developed and optimized for Computed Tomography data. Pore3D features are available through the high-level scripting environment IDL and it has been tested with IDL 64-bit from versions 6.4 to 8.5.
  The original project page can be found at: http://www.elettra.eu/pore3d/ but now the sw is available on Github.
  Main bibliographic reference at: https://www.sciencedirect.com/science/article/pii/S0168900210002615 Code: https://github.com/ElettraSciComp/Pore3D License: The project is licensed under the GPL-v3 license
  Contact: Lucia Mancini (lucia.mancini@elettra.eu); (pore3d@elettra.eu)
- **SYRMEP Tomo Project (STP)**
  Further Information: SYRMEP Tomo Project (STP) has been developed for the users of the SYRMEP beamline of the Elettra synchrotron facility (http://www.elettra.eu) to perform the digital image processing required by parallel beam absorption and propagation-based phase contrast CT experiments. This sw is routinely used at by all SYRMEPl users

during CT experiments but the underlying idea is also to let users perform post-beamtime optimization, fine tuning and/or additional tests with common hardware at their home institution. The software has been also developed for teaching and educational purposes. SYRMEP Tomo Project is available only for Windows 64-bit machines.
Main bibliographic references are: http://dx.doi.org/10.3233/FI-2015-1273 and http://dx.doi.org/10.1186/s40679-016-0036-8.
Code: https://github.com/ElettraSciComp/STP-Gui
License: The project is licensed under the GPL-v3 license.
Data: Many datasets from the SYRMEP beamline are available on TomoBank at the link https://tomobank.readthedocs.io/en/latest/

- **PITRE and H-PITRE**
  Further Information: PITRE (Phase-sensitive x-ray Image processing and Tomography REconstruction) is a software developed by INFN Trieste n order to facilitate and standardize the simulation and elaboration of X-ray phase contrast images. The acronym PITRE in Italian is pronounced /'pi.tre/; the pronunciation is the same of "P3", which is then chosen as a logo for the PITRE program. A batch processing manager for PITRE, called PITRE_BM, can execute a series of tasks ("jobs"), which is created via PITRE, without manual intervention.
  H-PITRE (High-performance software for Phase-sensitive x-ray Image processing and Tomography REconstruction) is a fast tomography reconstruction program which uses the parallel computing abilities of NVIDIA GPU (Graphics Processing Unit).
  Code: https://sites.google.com/site/rongchangchen/
  License:
  Data:
- **TTK, Topology ToolKit**
  Further Information: Open-source library and software collection for topological data analysis integrated with visual exploration tools. It is built as a general purpose library, not specific to material science. Easy-to-use plugins for the visualization front end ParaView. All data format and interaction support is available thanks to ParaView. Written in C++ but has bindings (VTK/C++, Python) and command line support.
  Link: https://topology-tool-kit.github.io
  Licensing: BSD
  Mailing List: (ttk-users@googlegroups.com)
- **ASTRA Toolbox**
  Further information: The ASTRA Toolbox is a MATLAB and Python toolbox of high-performance GPU primitives for 2D and 3D tomography. We support 2D parallel and fan beam geometries, and 3D parallel and cone beam. All of them have highly flexible source/detector positioning. A large number of 2D and 3D algorithms are available, including FBP, SIRT, SART, CGLS. The basic forward and backward projection operations are GPU-accelerated, and directly callable from MATLAB and Python to enbale building new algorithms. The source code of the ASTRA Toolbox is available on GitHub.
  Link: www.astra-toolbox.com
  License: GPLv3
  Contact person: Jan de Beenhouwer (jan.debeenhouwer@uantwerpen.be)
- **MegaMol**
  Further Information: Megamol is a visualization framework for large particle data. It originated from research in the DFG Collaborative Research Center 716 and provides

advanced visualization techniques for point-based data like molecular dynamics, SPH, laser point clouds etc.
Link: https://megamol.org/ https://www.sfb716.uni-stuttgart.de/index.en.html
Contact person: Guido Reina (guido.reina@visus.uni-stuttgart.de)

- **Gephi**
  Further information: Open-source tool for the visualization of large graphs and networks.
  Link: https://gephi.org/
  Licencing: Open-source
- **Orange**
  Further information (Daniel Weiskopf): "Data Mining Fruitful and Fun: Open source machine learning and data visualization for novice and expert. Interactive data analysis workflows with a large toolbox." (quote from their web page). A general framework for useful, e.g., for multidimensional data. Comes with interactive visualization As discussed in the breakout group 2 on Thu, multidimensional data analysis could play a role in some applications
  Link: https://orange.biolab.si/
  License: GNU General Public License as published by the Free Software Foundation; either version 3.0 of the License, or (at your option) any later version.

# 5 Panel discussions

## 5.1 Overview Talk and Discussion Summary: Application of Machine Learning tools for quantitative 3D-4D materials science!

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The discussion circled on topics regarding the applicability of the tools and methods which were presented by the speakers. Special interest was seen in the different ML techniques as well as how and where to use them.

## 5.2 Overview Talk and Discussion Summary: Machine Learning for Material Sciences: Computer Vision at Scientific Facilities

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



In the discussion, the different ML techniques were addressed, which the speaker is using for segmentation and classification of their dataset. The core tool was pyCBIR, a python tool for content-based image retrieval (CBIR) capable of searching for relevant items in large databases given unseen samples. Furthermore, techniques and neural networks architectures such as those found in LeNet, AlexNets and U-Net were discussed as well as their applicability for different scenarios. Finally Xi-Cam was briefly introduced by the speaker, a versatile interface for visualization and data analysis providing workflow for local and remote computing, data management, and seamless integration of plugins.

## 5.3 Overview Talk and Discussion Summary: Real-time data analysis and experimental steering: Do we need it? Are we ready for it?

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



The author summarized three challenge areas: 1) capturing ultra-fast and ultra-slow processes; 2) detecting spatially rare events in large volumes at meso/nano scale resolutions; and 3) enabling multi-dimensional enquiry to explore spaces of higher dimension and size. The hope is that real-time data collection and steering can bring the following benefits: 1) collect only relevant data; 2) instrument error correction; 3) optimize temporal and spatial resolution; 4) zoom-in at different length scales; and 5) minimize radiation damage to specimens. It is clear that the user (scientist) is needed in the loop, but the role of the user is changing. Previous generations did lots of hand-tuning of parameters, whereas the current generation relies on smart defaults. Moving forward, tools are needed to both help allow exploration of the data (parameters, solution space, etc.) and to allow specialized enquiry.

## 5.4 Overview Talk and Discussion Summary: Through the micro-CT and what we found there? Quantifying images of fibrous materials

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This talk presented recent advances in the imaging of fiber composite materials. The goal of the work was to determine the internal structure of the fibrous material through images. This was done by inferring a structure tensor from the image data, from which a classification and an orientation of the material can be deduced. Studies were done to understand the impact of image quality on the structural tensor that is inferred. Based upon the structural tensor that is inferred, one desires a quantification of the fibrous structures and a seamless transfer of data to mechanical modeling software, allowing the calculation of various quantities. Questions were related to the similarities between this work and what is done in the medical imaging world, what modeling assumptions were used (such as assuming symmetry of the structural tensor), and concerning the use of higher-order tensors for input into damage models (and how that damage information is used). The speaker proposed a benchmark exercise that could be used by the imaging / visualization community to test their algorithms / tools.

## 5.5 Panel Discussion Summary: The Integrated Visual Analysis Challenge 1

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



In the integrated visual analysis challenge we touched on the core intersection between visualization and materials science. From the talks and upcoming panel discussions it became clear that in the daily work of materials scientists, image processing and feature detection techniques are of very high importance. The discussion focussed on concrete hints to advanced techniques in either field, which can help materials scientists to more accurately and efficiently analyse their datasets. In particular, techniques that can employ temporal coherence in the reconstruction step turned out to be of interest. Due to the complexity of the structures in high-resolution measured data, visual data analysis is considered an important ingredient. To the visualization community it became clear how huge and well-resolved scanned materials can be, and that real-time capabilities often play a central role in large-scale research facilities.

## 5.6 Panel Discussion Summary: The Integrated Visual Analysis Challenge 2

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This session was a continuation of the visual analysis challenge. As mentioned earlier, we touched on the core intersection between visualization and materials science. From the talks and upcoming panel discussions it became clear that in the daily work of materials scientists, image processing and feature detection techniques are of very high importance. The discussion focussed on concrete hints to advanced techniques in either field, which can help materials scientists to more accurately and efficiently analyse their datasets. In particular, techniques that can employ temporal coherence in the reconstruction step turned out to be of interest. Due to the complexity of the structures in high-resolution measured data, visual data analysis is considered an important ingredient. To the visualization community it became clear how huge and well-resolved scanned materials can be, and that real-time capabilities often play a central role in large-scale research facilities.

## 5.7 Panel Discussion Summary: The Interactive Steering Challenge

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This session focussed on the presentation of various computational steering techniques and tools designed for material and engineering design. In all cases, researchers were able to leverage some existing technologies. However, it was clear that considerable effort still needed to be expended to adapt current analysis and visualization tools to the needs of the domain scientists. For instance, acceleration of techniques to enable real-time analysis, visualization and refinement were needed, as well as new APIs to enable efficient data transfer, etc. Questions about the balance between quantitative and qualitative visual comparisons were proposed, as well as how important is it that tools represent solutions which are feasible to manufacture or produce. It is clear that there are many things still needed to bridge current tool technologies and the needs of material science domain experts.

## 5.8 Panel Discussion Summary: The Quantitative Data Visualization Challenge 1

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This session focussed on various visualization algorithms, their application to materials science problems, and the lessons learned. Topics such as the current role of interactivity in procedures that in the future will be automated, uncertainty quantification and its visualization, and the use of novel visualization techniques to displaying both similarities and differences as seen in various material science applications. The questions related to understanding the role of automatic learning (deep neural nets) and interpretability, how material scientists use robustness information, and a greater understanding of how symmetries can be exploited when employing segmentation algorithms.

## 5.9 Panel Discussion Summary: The Quantitative Data Visualization Challenge 2

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This session focussed on various topics related to the quantitative use of analysis and visualization in material science. The first two talks focussed on recent efforts on materials containing fibers; how to interpret, model, visualize and reason about fiber orientations and defects were discussed. We then transitioned to talks about the use of machine learning and image processing / computer vision when doing quantitative analysis of material science data. A consistent issue that was brought up was the need for benchmark problems (i.e. ground truth) and for training data.

## 5.10 Panel Discussion Summary: The Visual Debugger Challenge

*Christoph Heinzl (FH Oberösterreich – Wels, AT), Robert Michael Kirby (University of Utah – Salt Lake City, US), Stepan V. Lomov (KU Leuven, BE), Guillermo Requena (DLR – Köln, DE), Rüdiger Westermann (TU München, DE)*



This session focussed on the use of visual computing as a "debugging" tool within the materials science pipeline. The discussion was mainly about the use of visualization for parameter-space navigation and ensemble visualization. It turned out that in many applications in materials science there is a need for exploring the similarities and dissimilarities between multiple data sets, e.g. from measurements with different doses or reconstruction algorithms. Also the possibility to directly visualize datasets from different measurements or simulation technologies was requested. The discussion was also about which kind of interactivity is required in materials science. It seemed that interactive visual exploration of 3D data sets is desired, yet the community has some experience in this field. Concrete use cases where the different kinds of interaction can be demonstrated are highly appreciated.

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