Image-Based Simulation for Industry 2023 (IBSim-4i 2023)

9–13 October 2023 Institute of Physics, London, UK



IOP Institute of Physics

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Welcome

On behalf of the organising committee of the sixth Image-Based Simulation for Industry event (IBSim-4i 2023), we are delighted to welcome you to this initiative to develop the community of image-based simulation users and developers for industrial applications.

Image-based meshing is the process by which 3D images (e.g., X-ray CT or laser scanning) are converted into ultrahigh resolution simulations. 3D imaging is increasingly being used in the industrial sector for inspection, nondestructive testing / evaluation (NDT/NDE) and metrology but image-based simulation is still an underutilised technique. Our aim is that the activities of IBSim-4i will facilitate a wider adoption of image-based simulation and provide a platform to discuss the cutting-edge developments in the field.

IBSim-4i will be the ideal forum for the fostering of ideas and the establishing of new collaborative links, helping to build strong networks within UK and at an international level.

Information for Speakers

Keynote speakers will have 45 minutes (35 mins + 10 mins Q&A), other presenters are given 20 minutes (15 mins + 5 mins Q&A).

We would kindly ask that all presenters arrive in the break before their session and introduce themselves to the session chair and to test their presentation.

Supporting Organisations

We would like to thank the following organisations for their generosity in supporting this event:





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- Gain access to expert knowledge in various areas of imaging and simulation research.
- Use AIM, our £10M scientific imaging and characterisation facility, capable of providing imaging and analysis from multiple modalities across length scales ranging from centimetres to Angstroms.
- We have a wide range of material and measurement capabilities to deliver multi-sample, high-throughput testing of advanced materials.

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Keynote Speakers

Professor Fabrice Pierron

Matchid NV, Belgium



Integrating 2D/3D images with numerical simulations for mechanical deformation analysis

Dr Fabrice Pierron has been Professor of Solid Mechanics at the University of Southampton since 2012. He is a specialist of the integration of image-based deformation mapping (like digital image correlation) with inverse identification (like the Virtual Fields Method) to design the next generation of mechanical tests. He has published more than 150 journal articles. He was Editor-in-Chief of the journal Strain (Wiley) for ten years and is a co-

founder of the company MatchID NV (Ghent, Belgium), for which he now also works as R&D Director since 2021. Prof. Pierron is Fellow of the Society for Experimental Mechanics (SEM).

Professor Jean-Charles Passieux INSA Toulouse, France



Generation of analysis suitable B-Spline beam models from digital images

JC Passieux is a full professor of Computational Mechanics at INSA Toulouse, France. He develops high performance computational methods (domain decomposition, reduced order models, local/global coupling, Isogeometric Analysis). He has contributed to the development of finite element based and global digital image correlation (DIC) methods,

identification from digital images, image-based models and data assimilation. He was co-chairman of the international conference Photomechanics 2018 in Toulouse. He is member of the steering committee of the Computational Solid Mechanics Association (CSMA, France). He is one of the founding members of the French PhotoMechanics Association.



Collaborative Computational Project in Tomographic Imaging: <u>www.ccpi.ac.uk</u>

Core CCPi provides the community with a toolbox of algorithms increasing the quality and level of information that can be extracted by computer tomography. Chaired by Prof Philip Withers (University of Manchester) and coordinated by staff within the Science and Technology Facilities Council it is led by a working group of experimental and theoretical academics with links to the Diamond Light Source, EPAC, ISIS Neutron Spallation Source and Industry. **Creating and supporting best practice from the national facilities to lab based systems Python based framework development; The Core Imaging Library:** <u>https://www.ccpi.ac.uk/CIL</u>

The remit is to bring together the imaging community, maximise return on investment in software development and ensure longevity, sustainability and re-use of code:

Software Developer Training/Workshops Tomography software show-and-tells

orkshopsData/Code archive on CCPi zenodo.org collection-tellsIterative reconstruction algorithmsJoin over 400 Tomographic Imaging practitioners

CCPi Flagship and Rich: Reconstruction Toolkit for Multichannel CT Conventional

Computed Tomographic imaging is stuck in a black and white (single channel) era whereas technological breakthroughs in energy-sensitive detectors, missing and noisy data analysis, and time-of-flight methods enable a new era of iterative tomographic imaging in 'colours' (multiple channels) – leading for example to chemical tomography extracting materials linked to their unique k-edge signatures. **The Future is Rich Tomography...**



Credit for images: E. Pasca, M. Turner, B. Searle, R. Atwood, T. Lowe, D. Kazantsev, J. Jørgensen P. Gajjar, E. Papoutsellis, E. Ametova, C. Delplancke, G. Fardell, R. Warr, W. Lionheart, P. Withers





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Programme

Monday 9 October 2023

Training Course

9:30 AM - 10:00 AM	Registration and Refreshments
10:00 AM - 11:00 AM	Session 1 ChopMESH: Introduction to ChopMESH, voxel and voxel-dominated mesh generator
11:00 AM - 12:30 PM	Session 2 Voxel based solver: taichi-LBM3D, PyEFEM and Wyvern
12:30 PM - 1:30 PM	Lunch
1:30 PM - 2:45 PM	Session 3 Voxel based solver: more advanced simulations
2:45 PM - 3:15 PM	Afternoon Break
3:15 PM - 5:00 PM	Session 4 Voxel-dominated mesh on OpenFOAM
5:00 PM - 7:00 PM	Drinks Reception

Tuesday 10 October 2023

Training Course

9:00 AM - 10:30 AM	Session 5 Introduction to AMITEX (overview and installation consideration) for the mechanical simulation of heterogeneous materials
10:30 AM - 11:00 AM	Morning Break
11:00 AM - 12:30 PM	Session 6 a) Geometry for AMITEX : definition and generation b) First simple simulations
12:30 PM - 1:30 PM	Lunch
1:30 PM - 2:45 PM	Session 7 Data inputs (description and examples): a) Material definition b) Loading and output c) Algorithm parameters
2:45 PM - 3:15 PM	Afternoon Break
3:15 PM - 5:00 PM	Session 8 User-defined behaviours: umat and MFRONT

Wednesday 11 October 2023

User and Developer Forum

9:30 AM - 10:00 AM	Registration and Refreshments
10:00 AM - 10:15 AM	Welcome
10:15 AM - 11:00 AM	Speaker: Keynote 1 Fabrice Pierron: Integrating 2D/3D images with numerical simulations for mechanical deformation analysis
11:00 AM - 12:30 PM	Session 1: Presentations 11:00 AM - 11:20 AM Tessa Nogatz: Validation and Verification of Motion Estimation in In Situ Tests 11:30 AM - 11:50 AM Chris Packer: Linking Manufacturing to Porosity and Fatigue Performance in Ti-6AI-4V LPBF Produced Parts Using X-Ray CT
	Techniques 11:50 AM - 12:10 PM Alex Cornell-thorne : Investigating the impact of workflow parameters for a semi-automated image-based simulation methodology using benchmark data based on an international tensile testing standard for metallic materials
	12:10 PM - 12:30 PM Harry Lipscomb and Marti Puig : Characterisation of Surface Roughness for Additive Manufacturing using Deep Learning and X-ray CT
12:30 PM - 1:30 PM	Lunch
1:30 PM - 3:10 PM	Session 2: Presentations 1:30 PM - 1:50 PM Elena Syerko: Results of the Meso-Scale Second Stage of the Benchmark Exercise on the Image-Based Permeability Prediction of Composite Reinforcements
	1:50 PM - 2:10 PM Koussay Daadouch : Computational modeling of fiber- reinforced concrete on the mesoscale: from voxel-based image to finite element mesh
	2:10 PM - 2:30 PM Moritz Weiss: Data-driven Z-rho decomposition in industrial CT
	2:30 PM - 2:50 PM Franck Vidal: New developments in gVirtualXray since IBSim 2021
	2:50 PM - 3:10 PM Walter Villanueva: Melt infiltration into a Particle Bed
3:10 PM - 3:40 PM	Afternoon Break

3:40 PM - 5:00 PM	Session 3: Presentations 3:40 PM - 4:00 PM Rhydian Lewis: VirtualLab: A fully automated, open-source platform for virtual experiments
	4:00 PM - 4:20 PM Benjamin Thorpe : Automating an image-based simulation workflow for component batches with VirtualLab
	4:20 PM - 4:40 PM Umeir Khan: Preform Defect Identification of in-Factory Photographs
	4:40 PM - 5:00 PM Dirk Schut : Joint 2D parallel slice to 3D volume image registration applied to slice photographs and CT scans of apple fruit
5:00 PM - 9:00 PM	Networking Reception and Buffet Dinner

Thursday 12 October 2023

User and Developer Forum

9:00 AM - 9:30 AM	Refreshments
9:30 AM - 10:15 AM	Speaker: Keynote 2 Jean-charles Passieux: Generation of analysis suitable B-Spline beam models from digital images
10:15 AM - 10:55 AM	Session 4: Presentations 10:15 AM - 10:35 AM Sylwin Pawlowski: CFD modelling of flow patterns, tortuosity and residence time distribution in monolithic porous columns reconstructed from X-ray tomography data
	10:35 AM - 10:55 AM Liang Yang : Hex dominated mesh generator for Image Based Simulation
10:55 AM - 11:25 AM	Morning Break
11:25 AM - 12:25 PM	Session 5: Presentations 11:25 AM - 11:45 AM Christian Breite: Enhancing ultrafast in-situ synchrotron radiation computed tomography of composite failure by super-resolution
	11:45 AM - 12:05 PM Ander Biguri : Iterative reconstruction for large scale tomographic problems using TIGRE: discussion on image quality, scanning time and algorithms
	12:05 PM - 12:25 PM Léonard Turpin : Identification of a mechanically based interface from an in-situ experiment
12:25 PM - 1:25 PM	Lunch

1:25 PM - 2:45 PM	Session 6: Presentations 1:25 PM - 1:45 PM Connie Qian: 3D Fibre Architecture Characterisation for Advanced Carbon Fibre Composites through Robust CT Scanning Technology 1:45 PM - 2:05 PM Dongze He: Analysis of the performance of braided composite tubes through X-ray computed tomography image-based modelling enabled finite element analysis 2:05 PM - 2:25 PM Iwan Mitchell: Creating Functional Digital Shadows of X-ray systems 2:25 PM - 2:45 PM Miroslav Yosifov: Generating Physics-Informed and Accurate Training Data through XCT Simulations for Deep Learning Applications
2:45 PM - 3:15 PM	Afternoon Break
3:15 PM - 4:15 PM	Session 7: Presentations 3:15 PM - 3:35 PM Fatih Uzun: Voxel-based full-field eigenstrain reconstruction of residual stresses 3:35 PM - 3:55 PM Grammatiki Lioliou: Two-directional phase sensitivity and isotropic spatial resolution in phase contrast CT: prospects for industrial
	applications 3:55 PM - 4:15 PM Fatima Zahra Oujebbour : 3D U-Net for automatic segmentation of volumes from Multi-energy X-ray Computed Tomography
4:15 PM - 4:30 PM	Wrap-up and Close

Friday 13 October 2023

Collaborative workshop

9:00 AM - 9:30 AM	Registration and Refreshments
9:30 AM - 10:45 AM	Session 1 Personal Introductions
10:45 AM - 11:15 AM	Morning Break
11:15 AM - 12:30 PM	Session 2 Theme Introductions and Identifying Research Challenges
12:30 PM - 1:30 PM	Lunch
1:30 PM - 2:45 PM	Session 3 Research Prioritisation
2:45 PM - 3:15 PM	Afternoon Break
3:15 PM - 4:30 PM	Session 4 Cementing Actions
4:30 PM - 4:35 PM	Close



Keynote Speakers

Integrating 2D/3D images with numerical simulations for mechanical deformation analysis

Dr Fabrice Pierron¹

¹Matchid NV, Ghent, Belgium

Speaker: Keynote 1, October 11, 2023, 10:15 - 11:00

Nowadays, the design of structural components relies mostly on numerical simulations through the finite element method. However, in many cases, the final certification of a structure can only be achieved through experimental tests that aim at validating the simulation. While in the past, this often relied on point sensors like electrical strain gauges or accelerometers, with the advent of digital cameras, deformation imaging has become a technique of choice in this endeavour. Indeed, coupled to image processing algorithms such as Digital Image Correlation, cameras produce near continuous images of the deformation, often named 'full-field' measurements. Such dense measurements have become an ideal counterpart to simulations in terms of richness of information and naturally, engineers and researchers are keen to bring the two together for more efficient validation. However, specific difficulties arise in this process.

First, the complexity of such image-based measurements somewhat matches that of numerical simulations and significant time needs to be invested in training to ensure quantitative measurements can be obtained robustly. Then, while simulations can be spatially converged and subject to minimal computational errors, camera images suffer from electronic noise and have a fixed number of pixels unable to always ensure spatial convergence. As a consequence, quantitively comparing numerical with experimental maps of deformation is a difficult exercise as measurement noise and, more importantly, biases need to be robustly taken into account in the comparison procedure.

This presentation proposes an overview of solutions to rigorously integrate 2D/3D images with numerical simulations to validate structural models and/or identify material behaviour. 2D images typically come from standard white light cameras while 3D images are often obtained through X-ray Computed Tomography. It will particularly focus on the following points:

- How to account for the spatial bias arising from limited camera resolution in 2D/stereo deformation imaging.
- How to deal with 3D (volume images) while avoiding Digital Volume Correlation (DVC curse).

Both items rely on deforming images (2D or 3D) using simulation results to either apply the DIC filter to simulation data to level them up, or to use deformed images in the grey level space to perform the comparison.

Generation of analysis suitable B-Spline beam models from digital images

<u>Jean-charles Passieux</u>¹, Robin Bouclier, Oliver Weeger

¹INSA Toulouse, Toulouse, France, ²Clement Ader Institute, Toulouse, France Speaker: Keynote 2, October 12, 2023, 09:30 - 10:15

Cellular material, namely foams or lattices, are characterized by complex architecture where the material is concentrated in small spans or thin webs, at an intermediate scale between the constituents and the structure. This particularity provides these materials with remarkable specific properties. The recent development of new manufacturing processes (especially additive manufacturing), pushes these materials to a new stage. Many open questions are stirring up the scientific community, in particular, multiscale modelling, characterization of the associated parameters, fast and accurate simulation, and geometric hazard.

In essence, foams have a random architecture, thus their geometry is locally variable and unknown. For lattices, defects inherent to additive manufacturing processes are known to introduce nonnegligible geometric biases. In view of identifying the mechanical properties, the geometric characterization of the sample is therefore of paramount importance to build a digital mechanical twin associated to each individual tested sample.

In this talk, we present different types of image-based modelling techniques and how do they help to bridge mechanical experiments and numerical simulations. We will then focus on techniques that build an explicit geometry based on splines and the corresponding control point fitting procedure. In order to achieve the lightest possible model, and given the morphology of the materials considered, the method aims at building explicit isogeometric beams and isogeometric volumetric models. These models are called analysis-suitable in the sense that they are ready for mechanical simulations. To do so, we propose to extend the Virtual Image Correlation algorithm to the case of branching beams and branching surfaces. We also aim at characterizing the potentially evolving cross-section thickness of each beam. Note finally that we also propose automatic initialization strategies in situation where the topology is unknown a priori, such as foams.

Technically, the sample is described as a set of interconnected quadratic B-Spline beams or surfaces. Two (2D) or three (3D) degrees of freedom (dof) are associated with each control point position. Additional degrees of freedom may be introduced to describe the thickness of the beams. All these dofs are adjusted to minimize a distance between the real image and a synthetic virtual image computed as a function of the dofs.

Oral Presentations

Validation and Verification of Motion Estimation in In Situ Tests

Tessa Nogatz¹, Claudia Redenbach¹, Katja Schladitz²

¹RPTU Kaiserslautern-Landau, Kaiserslautern, Germany, ²Fraunhofer ITWM, Kaiserslautern, Germany Session 1: Presentations, October 11, 2023, 11:00 - 12:30

Combining materials tests and Computed Tomography in so called in situ tests experiences increasing popularity. The motion that a sample underwent during such a test can be computed by methods that operate on the acquired image data. In materials science, such methods are found under the name Digital Volume Correlation (DVC). However, proper validation of the method often falls short, especially compared to 2D algorithms. In so called Optical Flow estimations, plenty of datasets like Middlebury, MPI Sintel or KITTI Vision Benchmark exist. They consist of images with public available displacement field ground truth for debugging and visualization and hidden data for benchmarking. On top, several works reported advantages and disadvantages of different norms for performance estimation.

In DVC unfortunately evaluation based on ground truth displacement is hardly ever found. Though sometimes residuals or error norms are displayed, a proper evaluation is often only done on uncertainty quantification rather than on error evaluation. But without proper validation and, to say so, a plain number to measure the performance, assessment of novel algorithms is nearly impossible. It also complicates the choice of algorithms: Many algorithms in the area of DVC have different approaches on solving the problem. Whereas local DVC is better in resolving jumps and discontinuities, global DVC will provide displacement which can be easily compared to simulations. Hybrid approaches like ALDVC or exotic ones like the equilibrium gap can be used overcome these problems, but can also be very parameter heavy. As DVC calculations are already quite costly regarding computational time, testing of different approaches is usually not an option. Assessment of all algorithms with the same measures to identify the power is therefore inevitable.

In this talk we adapt good practices from 2D and re-evaluate state-of-the-art motion estimation algorithms. We introduce the classical error measures to 3D and shortly discuss advantages and disadvantages. However, our main focus lies on introduction of simulated displacement to estimate the performance of the 3D motion estimation algorithms based on ground truth. We show how such a testbed can not only be used for understanding strengths of algorithms but also to identify weaknesses of existing approaches.

Linking Manufacturing to Porosity and Fatigue Performance in Ti-6AI-4V LPBF Produced Parts Using X-Ray CT Techniques

<u>Chris Packer</u>¹, Dr Sam Tammas-Williams¹, Dr Juan Ahuir Torres², Dr Martin Sharp² ¹ The University of Edinburgh, United Kingdom, ³The University of Liverpool, United Kingdom Session 1: Presentations, October 11, 2023, 11:00 - 12:30

Laser powder bed fusion (LPBF) AM is being increasingly used to manufacture complex parts from a range of metal alloys. The large number of variables that impact the pore population of LPBF Ti-6Al-4V (> 50 by some estimates [1]) means that even optimised samples typically contain some unintended residual porosity. Even at low porosity levels (~0.01%), pores can act as stress concentrators and thus initiate fatigue cracks. Several studies note a correlation between stress (S), pore size (area) and number of cycles to failure (Nf). Typically, larger pores lead to shorter lives[2].

During post-mortem analysis, the initiating pores are typically treated as individual defects, and there has been some success in reducing fatigue life scatter using an equation proposed by Murakami[3] to assign each pore a stress intensity factor, which is higher if a pore is close to a surface.

We will present X-ray CT data to analyse pores morphologies in 3D prior to fatigue testing and relate this to the fatigue performance. This work will help define limitations on how close pores can be before we must consider them as a pair/group rather than individual, as well as predict the performance of such features. We examine whether simple empirical relationships can be effectively used to avoid the need for large FEA models of numerous samples. We also consider how segmentation may influence judgement of material quality. This will help engineers when designing NDT strategies for AM components.

We test specimens manufactured with a range of strategies to test the relationship between process parameters and fatigue performance. A range of overall volume fraction, size and morphology of pores will be tested to quantify the links to fatigue life, including pores in close proximity to each other to examine whether a similar equation to that proposed by Murakami can be used for pores in close proximity.

^{1.} Spears, T. G. & Gold, S. A. In-process sensing in selective laser melting (SLM) additive manufacturing. Integr. Mater. Manuf. Innov. 5, 16–40 (2016).

^{2.} Pessard, E., Lavialle, M., Laheurte, P., Didier, P. & Brochu, M. High-cycle fatigue behavior of a laser powder bed fusion additive manufactured Ti-6AI-4V titanium: Effect of pores and tested volume size. Int. J. Fatigue 149, 106206 (2021).

Investigating the impact of workflow parameters for a semi-automated image-based simulation methodology using benchmark data based on an international tensile testing standard for metallic materials

<u>Alex Cornell-thorne</u>^{1,2}, Wiera Bielajewa^{1,3}, Llion Marc Evans^{1,3}, Rhydian Lewis^{1,3} ¹Swansea University, Swansea, United Kingdom, ²MTC (Manufacturing Technology Centre), Coventry, United Kingdom, ³UKAEA (United Kingdom Atomic Energy Authority), United Kingdom Session 1: Presentations, October 11, 2023, 11:00 - 12:30

The current state-of-the-art in using micro-X-ray CT (μ XCT) for NDT/NDE is to perform analyses such as quantifying flaws, characterising porosity and measuring tolerance deviations. Typically, these analyses pass or fail parts by comparing results against threshold criteria, e.g., maximum allowable defect/deviation size. This does not quantify the impact on performance, e.g., small defects in a critical location may have a greater impact than a large one located elsewhere.

'Image-based simulation' (IBSim) is used to convert µXCT images directly into engineering models able to quantify the 'effect of the defect' under virtual 'in-service' conditions. The IBSim technique's origins are in biomechanics, and it is increasingly being used for characterisation of advanced materials and manufacturing, e.g., composite materials and additive manufacturing, within high-value manufacturing (HVM) sectors. Despite this, it is still underutilised and not yet considered a mature technology. A recent review identified that for IBSim to become more widely accepted, particularly in heavily regulated sectors like nuclear and aerospace, there needs to be verification processes focused on internationally recognised and industrially relevant benchmarks.

Recent work proposed a 'digital twinned' mechanical benchmark based on an international tensile testing standard for metallic materials (BS EN ISO 6892-1:2016). Three 'identical' batches of ten Ti-6AI-4V, Grade 5, samples were fabricated according to the standard with the inclusion of controlled defects of varying sizes. The samples were physically tested with measurements taken using a conventional strain gauge and with digital image correlation (DIC). Before physical testing occurred, the exact same samples were digitised via µXCT and converted into finite element meshes. Thus, direct comparison of physical experimental and virtual simulation results is possible for verification, validation, and uncertainty quantification (VVUQ) of IBSim workflows.

The data for the benchmark were generated using CT Pro (Nikon Metrology NV) for image reconstruction, image segmentation and meshing used Simpleware (Synopsys Inc.), finite element analysis used Code_Aster (EDF S.A.) and data analysis with ParaView (Kitware Inc.).

This study investigated which workflow parameters impact the accuracy of a semi-automated IBSim approach. The IBSim results using various parameters (e.g., those used during segmentation) are compared against the physical experimental values and those from idealised CAD-based simulations.

Characterisation of Surface Roughness for Additive Manufacturing using Deep Learning and X-ray CT

Mr Harry Lipscomb¹, Mr Marti Puig¹

¹University of Manchester, Manchester, United Kingdom

Session 1: Presentations, October 11, 2023, 11:00 - 12:30

Surface roughness is a critical parameter to consider when evaluating friction, durability, or fatigue lifetime of an object. The application of a convolutional neural network called U-Net to CT scanners is proposed to enhance the scanner's capability to characterise surface roughness. The study demonstrates successful training of U-Net using synthetic data generated through ImageJ and training data constructed using a digital twin of a CT scanner at the Henry Moseley X-Ray Imaging Facility. The digital twin was constructed using ray-tracing software called gVXR. Initially, the accuracy by which the digital twin reflects features of a real XCT scanner scan was investigated. This comparison showed the digital twin successfully reproduced common artifacts found in XCT such as streaking and beam hardening. Throughout the study, the primary difference between real and virtual scans was the lack of simulated background noise within the virtual scans, omitted for computational efficiency. The results show that U-Net significantly improves the segmentation of scanned images and reduces beam-hardening artifacts. After U-Net is applied to gVXR scans, the neural network's output has a mean absolute error of 1.92% relative to the ground truth. This is 17 times lower than for the virtual scans alone. However, the model's performance in correcting streaking artifacts and Poisson noise is limited due to the inadequate representation of these factors in the training data. It is concluded that deep learning neural networks are a promising pathway to improve rough surface visualisation through XCT imaging.

Results of the Meso-Scale Second Stage of the Benchmark Exercise on the Image-Based Permeability Prediction of Composite Reinforcements

<u>Dr Elena Syerko</u>¹, Christophe Binetruy¹, Tim Schmidt², David May² ¹Nantes Université, École Centrale De Nantes, CNRS, GeM, UMR 6183, Nantes, France, ²Leibniz-Institut für Verbundwerkstoffe (IVW), Kaiserslautern, Germany

Session 2: Presentations, October 11, 2023, 13:30 - 15:10

In manufacturing processes of composite materials, where a reinforcing preform is impregnated with a liquid resin, a key parameter for the impregnation of reinforcements is their permeability. Experimental measurements of permeability are not standardized yet [1]. Moreover, they are time-consuming and require specialized equipment. A benchmark exercise devoted to the numerical characterization of permeability was organized as a promising alternative for the determination of this parameter.

Multiple studies have been carried out in the field of numerical permeability prediction in recent years. However, there is no currently well-established methodology. This was confirmed by a large variety of approaches used in the first stage of the Virtual Permeability Benchmark [2]. The main concept of this benchmark study is to perform the computations based on real 3D images of textile composite reinforcements, rather than idealized digital twins, which allows to address an important feature of this class of materials – their high variability. While this approach was applied to other classes of porous media, this benchmark exercise is the first contribution to the real fibrous materials.

The first stage of the benchmark consisted in the prediction of permeability at the scale of fibres. The focus of the second stage is the permeability computation at the scale of textiles, which are composed of tows themselves composed of fibres. The permeability of tows computed in the first stage serves as an input for meso-scale calculations of flow through the textile to predict its mesoscopic permeability.

As both stages of the benchmark use the same material from the experimental permeability benchmark[1],the numerical prediction results can be compared to experimental measurements at the corresponding fibre volume fraction. A global fibre volume fraction of $^{5}54\%$ was chosen. For this fibre content the presence of a non-negligible flow at both scales – inter-tow and intra-tow – is expected. It allowed thus to investigate the potential of multi-scale approaches. The image-based computations of the second stage of the benchmark were based on a 3D scan with a nominal resolution of 8 μ m/voxel that represented a stack of 14 layers of a glass woven textile to approach the real processing conditions. From the point of view of representativeness of the material pattern on one side, and the computational cost on the other side, a volume of 700x680x345 voxels was provided to the participants.

Outcomes from this second stage of the Virtual Permeability Benchmark will be presented in details in this talk.

Computational modeling of fiber-reinforced concrete on the mesoscale: from voxel-based image to finite element mesh

<u>Koussay Daadouch</u>¹, Vladislav Gudžulić¹, Günther Meschke¹ ¹Structural Mechanics - Ruhr University Bochum, Bochum, Germany Session 2: Presentations, October 11, 2023, 13:30 - 15:10

This contribution focuses on generating computational concrete models at the mesoscale level, with a particular emphasis on the methodology utilized to arrive at finite element models from the voxelized images. Computational concrete specimens are discretized using a tetrahedral finite element mesh that effectively captures the three distinct phases: aggregates, air pores, and the cement matrix. Creating finite element models from the voxel-based Computational Tomography (CT) images of actual or virtually generated concrete samples [1] requires an initial image segmentation step. This process relies on a meticulously calibrated set of image analysis tools, including adaptive thresholding, active contouring, and watershed algorithms. The conversion process starts by identifying each inclusion and triangulating its surface, which is subsequently smoothed to ensure accuracy and improve the overall quality of the mesh. The obtained triangulated geometries must be carefully examined to identify and resolve any intersections of neighboring inclusions. The boundaries of the concrete specimen are constructed employing a constrained Delaunay triangulation approach to optimize computational efficiency and avoid expensive boolean operations. A method to efficiently segment fibers and resolve fiber-to-fiber intersections in images of fiber-reinforced concrete based on image morphological operations are proposed. The fibers are approximated as straight-line segments embedded within the cement matrix. These line elements are discretized using Timoshenko beam finite elements, enabling the incorporation of a bond-slip law that governs the mechanical interaction between the fibers and the cement matrix. Zero-thickness interface elements equipped with a traction-separation law are employed to simulate fracture behavior. These elements allow for a discrete representation of fracture in the numerical model. Several experimental scenarios are reanalyzed, and the results are compared against available data [2] to validate the capabilities of the proposed model. This demonstration showcases the framework's effectiveness in capturing and reproducing the mechanical behavior of high-performance fiber-reinforced concrete. This framework paves the way for developing improved models and design techniques in the future by providing a comprehensive understanding of the material's behavior at small scales. It enables researchers and engineers to leverage the advancements of high-performance and ultra-high-performance concrete to enhance durability and optimize material usage in construction applications.

References:

[1] Holla V., Vu G., Timothy J. J., Diewald C., Gehlen C., Meschke G., Computational generation of virtual concrete mesostructures, Materials, Vol. 14, 2021.

[2] Schäfer N., Gudžulić V., Breitenbücher R., Meschke G., Experimental and numerical investigations on high-performance SFRC: Cyclic tensile loading and fatigue, Materials, Vol. 14, 2021.

Data-driven Z-rho decomposition in industrial CT

Moritz Weiss^{1,2}, Nick Brierley², Mirko von Schmid², Tobias Meisen¹ ¹Bergische Universität Wuppertal, Wuppertal, Germany, ²diondo, Hattingen, Germany Session 2: Presentations, October 11, 2023, 13:30 - 15:10

Dual-energy computed tomography (DECT) is widely used in clinical settings including material decomposition using the X-ray absorption properties of different materials as a characteristic fingerprint (K-edge absorption).

As shown by Heismann et al. and So et al. these methods cannot be applied to material systems with more than two components without additional assumptions due to the unavailability of characteristic K-edges [1,2]. Last year at the IBSim-4i, we were able to show the transfer of a datadriven method operating on clinical data proposed by Abascal et al. to simulated datasets in an industrial scan setup. This approach is limited to fixed material combinations, which is a major constraint for a general-purpose use case.

In this work, we propose a Z-rho (atomic number - density) decomposition algorithm, which is driven by a newly developed deep-learning model with superior performance in comparison to any convolutional neural network published before. The model follows an encoder-decoder structure while the encoder is a vision transformer derived from the Swin-T model proposed by Microsoft. The decoder uses skip connections from the encoder and up-sampling convolutions comparable to a U-Net. This newly created model is called U-Transformer.

Using this approach, a wide range of materials can be distinguished by a single model. In the first instance, we lose the ability to decompose mixtures into their components. Nevertheless, the newly developed model can be fine-tuned for a certain use-case, which is a subject of current research. The model is trained exclusively on simulated data but computes correct predictions from experimental test scans. Additionally, the model implements uncertainty-awareness to give the user feedback on the prediction's reliability.

The utility of the model is demonstrated using scans of a phantom consisting of aluminum, steel, copper and Inconel. Since the approach is vulnerable to beam-hardening artifacts, a 6-MeV X-ray source was used, which can also be tuned to 3.9 MeV to provide a second energy channel.

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New developments in gVirtualXray since IBSim 2021

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Session 2: Presentations, October 11, 2023, 13:30 - 15:10

gVirtualXray (gVXR) is an open-source framework that relies on the Beer–Lambert law to simulate Xray images in realtime on a graphics processor unit (GPU) using triangular meshes. Recent developments in the simulation code are of interest for the IBSim community.

gVRX is cross-platform. It runs on Windows, GNU/Linux, and MacOS computers, whether they are laptops, desktop PCs or supercomputers. It even run cloud infrastructures, including STFC Cloud, Google Colaboratory and Code Ocean. gVXR has been successfully used in Docker containers. A wide range of programming languages (C/C++, Python, R, Ruby, Tcl, C#, Java, and GNU Octave). Its Python package "gVXR" is listed on the Python Package Index (https://pypi.org/project/gVXR/). An intuitive JSON format has been designed to describe simulation parameters.

Infinitively small point sources and actual focal spots are both supported to define cone-beam geometries. They replicate LabCT scanning geometries. For synchrotron sources, parallel beams can be used. Incident beams can either be monochromatic or polychromatic. In the latter case, xpecgen (https://github.com/Dih5/xpecgen) and Spekpy

(https://bitbucket.org/spekpy/spekpy_release/wiki/Home) have been integrated to define the tube spectrum depending on the anode material, voltage and eventual filtration. Poisson noise is now supported. It can be used to mimic exposure times.

A convolution kernel can be specify to model the impulse response of the detector. A look-up table can be defined to mimic the energy response of the detector due to the use of a scintillator. More recently, photon counting detectors were implemented to simulate spectral imaging.

Scanned objects can be modelled using surface meshes (triangles) in most popular file formats (eg. STL) or volume meshes (tetrahedrons) in the Abacus format (experimental). Multi-material objects can be simulated. The material properties supported are: chemical elements (e.g. the symbol W or the atomic number 74 for tungsten); compounds, e.g. H₂O for water; mixture, e.g. Titanium–aluminium–vanadium alloy, Ti9OAI6V4; and Hounsfield units (for medical applications). Xraylib (https://github.com/tschoonj/xraylib) has been integrated to compute the photon cross sections associated with the materials.

For ease of use, CT acquisition can be specified in an easy manner. Flat field images, with or without Poisson noise, can be generated to improve realism. A plugin for CIL (https://ccpi.ac.uk/cil/) is provided to reconstruct the corresponding CT data.

In a quantitative image comparison study, we compared images created using gVXR to both Monte Carlo simulations and experimental images of realistic phantoms. We demonstrated that accurate images can be generated in milliseconds with gVXR when scattering can be ignored.

Melt infiltration into a Particle Bed

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Session 2: Presentations, October 11, 2023, 13:30 - 15:10

Flow through porous media is a common occurrence in nature such as rainwater penetrating a soil and in other applications such as composite manufacturing, printing technology, powder technology, nanoscience, and nuclear reactor safety. Complex processes exist and of particular interest here is the infiltration of melt into a heated particle bed followed by solidification, and then possibly re-melting which can initiate further infiltration. The effects of thermal gradients in this process competes with the hydrodynamic effects. Fluid infiltration, solidification, and remelting in a particulate debris is particularly relevant as it can occur in the lower head of a reactor pressure vessel during a severe accident in a nuclear reactor. In this talk, I will present an experimental data on the infiltration of a molten Sn-Bi into a pre-heated particle bed of cylindrical geometry with 112 mm in diameter and 280 mm in length. The particle bed consists of 1.5 mm metal spheres. A non-linear kinetics of melt infiltration is revealed by measurements from thermocouples, fiber Bragg grating sensors, and observations from video cameras. Extracted ingots from the experiments are also shown. Finally, methods of extracting information on the porous structure of the ingots from simple sliced 2D image to 3D scanning to get information that can be used for porous media flow modelling and simulation are discussed.

VirtualLab: A fully automated, open-source platform for virtual experiments

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Session 3: Presentations, October 11, 2023, 15:40 - 17:00

Most, if not all, branches of science and engineering use virtual data generated by means of computational models to guide decision-making. Often referred to as simulations, this virtual data is extremely useful in circumstances where the real data is insufficient. Generating large quantities of virtual data is often prohibitive, meaning that sensitivity analysis in high dimensional space or creation of surrogate models is infeasible. VirtualLab is a platform which streamlines the production of virtual data of physical systems, enabling improved insight and understanding to support better decision-making.

Central to the vision of VirtualLab are the three P's; parameterisation, parallelisation and portability. Parameterisation of the workflow enables key variables to be easily changed, making it easier to collect data from across the parameter space. Parallelisation allows simulations to be performed concurrently, which when deployed on supercomputers enables data to be generated in a fraction of the time. The easy portability of VirtualLab ensures that its deployment and use is the same regardless of the computer system, whether it's a Windows personal computer or a Linux supercomputer.

The use of VirtualLab has enabled much better insight into the performance and suitability of heat exchanger components. The Heat by Induction to Verify Extremes (HIVE) experimental facility uses induction heating to replicate the in-service thermal loads experienced during routine operation of a fusion device. To assess a component's suitability for a fusion device, knowledge of its mechanical performance while subjected to large thermal loads is desirable. Due to operational constraints, only a limited quantity of experimental data relating to the thermal response of the component is recorded in HIVE.

Through VirtualLab, large quantities of data were rapidly collected and used to generate surrogate models of the thermal and mechanical response of the component. Using these surrogate models in tandem with optimisation algorithms has enabled the handful of point temperature measurements to be enhanced to the full temperature and stress field of the component, providing much greater insight regarding the component and it's intended application.

Automating an image-based simulation workflow for component batches with VirtualLab

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Session 3: Presentations, October 11, 2023, 15:40 - 17:00

One of the biggest challenges facing precision manufacturing is component qualification. In other words, how do you ensure that the manufactured components behave within spec and are fit for purpose? The traditional approach has always been to test randomly sampled components of the production line. This approach, however, is costly, time-consuming and can only give you so much information. This technique is also component specific. Therefore, it cannot be applied if the tests are destructive or if the performance can vary between parts due to manufacturing tolerances, micro-cracks, pores etc.

Image-based simulation (IBSim) enables us to perform virtual destructive experiments, which are digital equivalents of real-world laboratory engineering tests, on 'as built' components. However, IBSim is conventionally manually intensive and, thus, not suitable for production line non-destructive evaluation.

This talk will discuss the latest additions to VirtualLab, an open-source platform, that facilitates an automated IBSim workflow. That is, the conversion of X-ray computed tomography (XCT) data into a finite element mesh and subsequent analysis. The main challenge for automation in this workflow is considered to be segmentation (or labelling) of the greyscale XCT image. This presentation will focus on a novel automated segmentation workflow which uses a priori knowledge of the component being analysed (i.e., it's CAD drawing) to generate synthetic XCT data via gVXR (a XCT simulation library) which in turn is used to train a machine learning model via Volume Segmantics (a UNet library).

Preform Defect Identification of in-Factory Photographs

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The aerospace industry faces a growing demand for faster delivery of future aircraft. Achieving these production targets requires innovative approaches to composite manufacturing. A promising rateenabler is preforming and infusion of biaxial Non-Crimp Fabrics (NCF's) for primary aerostructures [1]. NCF's have been considered for both their superior mechanical performance over woven fabrics (due to stitching between layers) and ability to deposit multiple orientations at once [2]. An additional trend is the move towards highly integrated structures. These offer the benefit of shorter assembly times at the cost of more complex geometries.

Preforming of dry fabrics is a key step pre-infusion; involving the arrangement of 2D reinforcements into 3D shapes. The key challenge with preforming over complex geometries is the tendency for defects, such as ply wrinkling and fibre waviness, to occur leading to mechanical knockdown. Current inspection is applied on the shopfloor by photographing defects for evaluation. However, the assessment remains qualitative rather than quantitative. This research aims to address this gap by developing an automated workflow to quantify defects captured in shopfloor photographs.

Defect characterisation is first approached through segmentation of the NCF tow boundaries. The segmentation is achieved using a trained deep learning network (U-Net [4]) to trace the wrinkle profile per photograph. This technique offers advantages over conventional thresholding, namely, being insensitive to the stitching pattern visible on the NCF surface. Finally, each wrinkle profile is characterised in terms of amplitude, wavelength and aspect ratio (Fig. 1).

The next steps will be to verify the out-of-plane wrinkle measurements using 3D scans of the preform, for eventual integration of the preform measurements into a digital twin of the aerostructure.

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Joint 2D parallel slice to 3D volume image registration applied to slice photographs and CT scans of apple fruit

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Session 3: Presentations, October 11, 2023, 15:40 - 17:00

Apples are a natural product and therefore vary in quality. Sorting machines sort the apples so that each apple is used for the application that best matches its quality level. However, internal disorders of the apple (browning, watercore, and bitterpit) can not be detected accurately with the current sorting machines. CT imaging can be used to image the inside of apples and may be used to develop X-ray-based quality control systems. However, the relationship between the internal state of the fruit and image features that can be observed in the CT scans is not fully understood yet. To improve this understanding, we have developed an image registration workflow that can be used to create large datasets of photographs of apple slices and their corresponding CT slices. First, the apple is CT scanned and then it is sliced into parallel slices and each slice is photographed. After that, the photographs and the CT scan are segmented to account for the different appearances of these modalities. Lastly, image registration is used on the segmentation masks to find the corresponding CT slice for each photograph. Our image registration method uses a novel transformation model that incorporates the fact that slices are parallel. Because of this it has parameters shared between slices (rotation, scale, and slice thickness), and parameters unique per slice (x and y offset). Using this transformation model and PyTorch-based automatic differentiation. the image registration of all slices within one apple is optimized within a single optimization problem. This approach outperformed an approach where the image registration was performed separately for each slice. The image registration workflow was applied to a dataset of 1347 slice photographs acquired from 107 'Kanzi' apples with several internal defects. On this dataset, the inplane registration error of the endpoints of the apple core was 1.47 mm (+- 0.40).

CFD modelling of flow patterns, tortuosity and residence time distribution in monolithic porous columns reconstructed from X-ray tomography data

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In this work [1], the morphological structure of a monolith was reconstructed using 3D X-ray tomography data. Subsequently, the OpenFOAM CFD package was used to simulate the essential parameters for monoliths' performance characterization such as velocity and pressure fields, streamlines, shear stress and residence time distribution (RTD). Moreover, the tortuosity was directly assessed by measuring lengths of the streamlines which, in laminar regime and steady state, represent the fluid pathways.

It was observed (for the case of the monolith studied) that fluid transport was dominated by flow heterogeneities and advection, while the shear stress at pore mouths was significantly higher than in other regions, which is especially important in protein separations. The computed tortuosity of the monolith (~1.1) was found to be in the same range of the results obtained by known experimental, analytical and numerical equations. The proposed modelling approach was successfully validated by an experimentally obtained RTD.

It is expected that in a very close future, chromatographic materials will be produced by additive manufacturing (3D-printing). The .stl (stereolithography) files used to give information about geometry of 3D printed objects are the same type of files used in this work to create computational mesh and perform CFD studies. Consequently, the herein presented CFD modelling approach can be used to optimise and virtually test the performance of chromatographic materials before being even printed/manufactured, thus leading to production of target materials.

Note:

Currently, we are also focusing on applying similar approach to evaluate fluid dynamics through microfiltration membranes, as well as we started to use Portuguese advanced computing resources to perform CFD simulations of flow of non-Newtonian fluids, such as flow electrodes and blood, at flow capacitive deionization stacks and medical devices, respectively.

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Acknowledgements

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Hex dominated mesh generator for Image Based Simulation

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In this study, we introduce a novel hex-dominated mesh generator specifically designed for 3D images. While most existing mesh generators for images rely on unstructured tetrahedral meshes, there is a demand for hex meshes or hex-dominated meshes due to their superior numerical accuracy and efficiency. However, creating hexahedral meshes for arbitrary geometries poses a significant challenge.

Our proposed hex-dominated mesh generator addresses this challenge. It automatically generates high-quality hexahedral-dominant meshes from 3D images, allowing for more accurate simulations. The resulting meshes can be seamlessly integrated with the widely-used open-source CFD software, OpenFOAM, enhancing the efficiency and reliability of computational fluid dynamics simulations.

To showcase the capabilities of our mesh generator, we provide several numerical examples to demonstrate the accuracy and efficiency of the new hex-dominated meshes.

Enhancing ultrafast in-situ synchrotron radiation computed tomography of composite failure by super-resolution

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Session 5: Presentations, October 12, 2023, 11:25 - 12:25

Monitoring the microstructure and damage development in fibre-reinforced composites during loading is crucial for understanding their failure behaviour. In this work, we present an innovative approach that combines ultrafast in-situ synchrotron radiation computed tomography (SRCT) [1] and deep learning techniques to enhance the spatial and temporal resolution for microstructural analysis.

In the first step, we address the limitations imposed by photon flux and fibre-matrix contrast on the achievable resolution of ultrafast SRCT. We propose a pipeline [2] based on CycleGAN for unsupervised super-resolution and denoising, and U-Net-id for individual fibre segmentation. By leveraging the power of a 3D CycleGAN over a 2D counterpart, we demonstrate significant improvements in resolution. Our results reveal that the data processed through this pipeline yields comparable segmentation quality to a slow-acquisition, high-quality scan, while reducing the acquisition time by up to 200 times. This breakthrough overcomes a key obstacle in robust data extraction from timelapse ultrafast in-situ SRCT.

In the second step, we focus on the progressive development of fibre breaks in unidirectional composite materials under tension. Although ultrafast in-situ SRCT allows real-time monitoring of fibre breaks, the resolution of the resulting images is insufficient for automated analysis. To address this, we explore the application of the developed super-resolution techniques [3]. We train on datasets of high- and low-resolution images that were statically acquired. The trained networks are then applied to low-resolution, noisy in-situ scans of continuously loaded specimens. Our evaluation of the technique is based on statistical parameters related to fibre breaks, including the number of individual breaks and the number of 2-plets and 3-plets per specimen volume. The fully automated process achieves an average accuracy of 82% in identifying fibre breaks compared to manual identification, while the semi-automated approach reaches 92% accuracy. This demonstrates the effectiveness of our developed approach in enhancing the quality of lowresolution scans without compromising the identification of crucial physical parameters. The proposed pipeline, integrating timelapse ultrafast in-situ SRCT with deep learning techniques, revolutionises the microstructural analysis of fibre-reinforced composites. It enables enhanced spatial and temporal resolution, robust data extraction, and automated identification of fibre breaks. This research paves the way for an improved understanding of mechanical behaviour and potential performance optimisation of these advanced materials.

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Iterative reconstruction for large scale tomographic problems using TIGRE: discussion on image quality, scanning time and algorithms

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Session 5: Presentations, October 12, 2023, 11:25 - 12:25

Computed Tomography is one of the most widely used techniques for imaging for modelling. While with sufficient sampling and scanning time, the standard imaging procedures and reconstruction algorithms produce a very high quality image, these constraints are not always possible or desired. It is well known that undersampling or bad data quality (either from high SNR due to short exposure or other sources, such as beam hardening or scatter) can significantly impact the reconstruction quality, up to uselessness.

In the past decade, the computationally costly iterative reconstruction algorithms had made the jump to industrial scale tomographic images, providing significant image quality improvement in many cases. Slowly buy steadily many of these methods are jumping from the mathematical field that the reside at and being applied to big scale imaging. The TIGRE toolbox is one of the tools that provides these methods, both to mathematicians and applied scientist.

In this work, we showcase TIGRE, and explain how the iterative reconstruction methods and their flexibility to add user constraints (prior information) to accelerate and improve image quality, particularly for image based modelling. We contribute a conversation on when are these algorithms useful and how, including the most recent advances in the field, and what is next.

Identification of a mechanically based interface from an in-situ experiment

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To be able to describe the behaviour of some material it is necessary to take into account their heterogeneity. It is then necessary to define a length scale above which the heterogeneity of the material is considered. This length scale is limited by, either the experimental capacity to access to the actual structure of the material, or computation facilities. The phases defined in the model do not necessarily match which the phases (components) of the material.

We propose a method to identify the interface between the two phases of a model but have no physical existence. The sample is a woven composite parallelepiped, composed on one of carbon tows only and on the other size of a mix of carbon and glass tows. Subjected to thermal loading, the sample shows a bi-metal behavior. This last can be modelled using two phases. This simple model is very powerful because it can reproduce faithfully the behaviour with a very limited number of degrees of freedom. That is why, this kind of model are intensively used by industrial to predict the behaviour of composite with non-homogeneous reinforcements.

The difficulty is then to define the position of the interface between those phases, especially when the fibres of the different phases are intricated. This definition is usually based on the geometry of the part (median plan, etc.). A more relevant way to define it is based on mechanics. Here we consider that the best position of the interface is the one for which the model describes the best the behaviour of the material.

To do so, we carried out μ CT in-situ heating-cooling experiment on the sample. The position of the interface between the two phases of the model is then determined using a dedicated Digital Volume Correlation algorithm. The model with the identified interface provides a very precise description of the sample behaviour. This methodology can be extended to more complicated industrial case, for example aircraft engine turbine blades, offering a sensible improvement of the faithfulness of model for a limited cost, not requiring mesoscale modelling which can be both time-consuming to build and computationally demanding.

3D Fibre Architecture Characterisation for Advanced Carbon Fibre Composites through Robust CT Scanning Technology

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Session 6: Presentations, October 12, 2023, 13:25 - 14:45

Compression moulding of high fibre content, long discontinuous carbon fibre based Sheet Moulding Compound (SMC) is an attractive solution for high-rate manufacturing of high-performance composite structures. SMC flows under compression force to fill the mould cavity, allowing complicated geometry to be manufactured. The process can also incorporate continuous fibre prepreg to manufacture hybrid architecture composites, combining the superior mechanical properties of continuous fibre reinforcements and the superior foamability of SMC.

Understanding the fibre behaviour during the manufacturing process is the key to improve part quality, and to better predict the structural performance of the part. The level of heterogeneity and complicated fibre architecture in SMC and hybrid architecture composites requires 3D analysis of the material's internal structure, therefore radiology-based experimental techniques such as ultrasonic scanning and CT scanning are considered very desirable. However, application of radiological techniques for carbon fibre composites is particularly challenging due to the low contrast between the densities of carbon fibre and polymer matrix.

Several commercial flow simulation software offer the capability of SMC-only compression moulding simulation, where commonly used fibre prediction models include phenomenological models and meso-scale models. The former uses fibre orientation tensors to represent the fibre orientation, while the latter predicts the orientation of individual fibres by modelling the physical movement of each fibre. Because of the lack of experimental methods for quantifying fibre orientation in carbon fibre composites, very limited validation data are available for either type of models.

This paper presents a joint experimental and numerical study for characterising fibre orientation distributions in compression moulded carbon fibre SMC and hybrid architecture composites. A novel and robust experimental method utilising CT scanning and image analysis techniques will be adopted for physically determining the fibre orientation distributions. The new experimental method will be demonstrated using a series of SMC only samples as well as a hybrid architecture sample. The numerical study for fibre orientation prediction focused on SMC-only samples where a meso-scale model available through a commercial compression moulding simulation software was investigated. The fibre architecture predicted by the numerical study was compared against the results from the experimental study to assess the predictive validity of the fibre prediction model.

Analysis of the performance of braided composite tubes through X-ray computed tomography image-based modelling enabled finite element analysis

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Session 6: Presentations, October 12, 2023, 13:25 - 14:45

Pore defects and the deformation of fibre bundles produced during manufacturing have significant influence on the mechanical performances of 2D braided tubular composites relative to idealised structures. A multi-scale X-ray computed tomography (CT) image-based finite element modelling method is developed to investigate the damage behaviour of 1 layer carbon fibre reinforced polymer 2D braided tubular composites. The pores and bundles geometries are measured by micro X-ray CT. Then a novel fibre tracing segmentation method is presented to differentiate differently oriented bundles. The progressive damage microscale models are built based on the fibre volume fraction obtained from the CT scans. The properties of each bundle are predicted by microscale model analysis and applied to mesoscale models. Furthermore, mesoscale models, a) X-ray CT image-based model with pores and b) geometry-based idealised model, are built, and the stress-strain responses, a) experimental test results and b) finite element analysis results, under torsion loads are analysed and compared. This work will delineate the influence of pores and bundle shape on the mechanical performance of the 2D braided tubes, providing clear guidance for designing braided architectures, and also narrow the gap in our understanding of the relationship between mesoscale geometries and macroscale mechanical performance.

Creating Functional Digital Shadows of X-ray systems

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Session 6: Presentations, October 12, 2023, 13:25 - 14:45

With the use of X-ray simulations becoming popular to inform and plan for experiments, the need for accurate scanning environments is increasing. Access to beamtime is limited, but a large amount of time during scanning is wasted tweaking parameters for optimal results. A functional Digital Shadow of an X-ray scanner allows for virtual simulation of the scanner, with representative results from a real machine, allowing for accurate scan planning, saving beamtime. The Digital Shadowing process requires quantifying detector and source characteristics, such as flux, energy purity, detector line spread functions, and optical configuration. This process has been performed on three different scanning environments; Diamond Light Source's I-12 beamline, a Nikon XTEK XTH-225, and the Dual Tube High Energy (DTHE) by RX Solutions at INSA Lyon. The results are three Digital Shadows, with the ability to perform simulations on virtual models with comparable behaviour and defects to the real world. These models give the ability to answer questions regarding the X-ray scanners, such as the feasibility of scanning a sample, or specific feature. The Digital Shadows also enable concurrent virtual users, allowing for interactive user training without the need of an actual device, or answering questions regarding health and degradation.

Generating Physics-Informed and Accurate Training Data through XCT Simulations for Deep Learning Applications

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Session 6: Presentations, October 12, 2023, 13:25 - 14:45

Computed Tomography (XCT) stands as one of the most powerful imaging techniques for analysing porosity and detecting defects in industrial materials. Despite a lot of advancements and progress in the field, one of the most challenging problems in XCT data analysis remains segmentation and feature extraction. While artificial intelligence (AI) techniques are increasingly used for this purpose, the generation of reliable ground truth data for training remains an issue. Training AI, and in particular, deep learning algorithms, with accurate ground truth plays an important role in creating precise models for segmentation and testing.

This research focusses on the generation of accurate ground truth for artificially labelled data from STL model data. The proposed method consists of the following steps: First, well defined sample geometries are generated though size variation of a given STL model. By voxelization the computed STLs are directly converted to binary volumetric masks. In the next step simulated XCT data are generated from these STL geometries with varying quality, specifically involving different projection numbers and noise levels. The generated XCT simulations were subsequently used for the training of deep learning algorithms. Three Convolutional Neural Networks (CNNs) U++, V-net, and a Modified 3D-Unet were trained using 80 volumes for training, 20 for validation, and 100 for testing. Known geometries (spheres and cylinders) and irregular geometries with varying defect sizes were simulated in the training data. Furthermore, we investigate the impact of such artificially generated training data on the final label estimation. We therefore compare the three CNNs against conventional segmentation techniques in terms of their performance and usability of accurate and non-accurate training masks. Voxel discrimination error was calculated for each converted label to assess reliability. This process enables the measurement of segmentation uncertainty and algorithm accuracy across different scenarios, ultimately improving detectability.

Preliminary results indicate that our approach increases both the detection accuracy for segmenting small pores and the correct determination of segmented voxel numbers. To measure the detection efficiency, a probability detection method, structural similarity index and dice coefficient functions were applied. Our study demonstrates that for known and easy geometries, the ground truth generation was highly accurate, exhibiting low relative errors of the labelled volume. However, as the number of triangulations and complexity of shapes increase, the error also rises. Nevertheless, an accurately trained model allows for proper segmentation of complex shapes.

Voxel-based full-field eigenstrain reconstruction of residual stresses

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Session 7: Presentations, October 12, 2023, 15:15 - 16:15

Inverse eigenstrain analysis methods have been shown to be effective for the reconstruction of residual stresses in plane eigenstrain problems (sometimes termed "continuously processed bodies"). The reconstruction of residual stresses in discontinuously processed bodies, or the bodies of complex shape and/or full-field eigenstrain distributions is extremely challenging and necessitates the use of simplifying or regularising assumptions. The voxel-based eigenstrain reconstruction method uses the superposition of eigenstrain radial basis functions together with a set of limited experimental data for model-free (unconstrained) determination of unknown eigenstrain fields. The novel point of this approach is the ability to account for all 6 components of strain in an isotropic body without using simplifying or regularising assumptions. Defining the eigenstrain distribution as a weighted sum of radial basis functions eliminates the limitations introduced by global basis functions such as polynomials. By lifting simplifying assumptions and complex formulation, the fidelity of the radial basis function 3D eigenstrain reconstruction method becomes directly related to the quality and the amount of experimental data used for the reconstruction and proper definition of boundary conditions. This presentation aims to show the fundamental principles of this method using numerical experimentation results along with recent applications of the method in laser powder bed fusion additively manufactured specimens and large-scale welded components using limited experimental data from optical and contact profilometry, and strain tomography sources. Results also include validations by independent measurements using diffraction techniques. This presentation also aims to show the link between the voxel-based eigenstrain reconstruction method and the newly developed eigenstrain tomography method.

Two-directional phase sensitivity and isotropic spatial resolution in phase contrast CT: prospects for industrial applications

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Three-modal x-ray CT scanners enable images with the following contrasts to be obtained: attenuation, phase (refraction), and ultra small-angle scattering. While refraction signals provide higher contrast than attenuation signals at the same statistics, scattering signals arise from sub-pixel structural variations (inhomogeneities) in the imaged sample. A key ambition of the Nikon-UCL Prosperity Partnership on Next Generation X-Ray Imaging is the exploitation of three-modal x-ray CT in an industrial context. This includes e.g. early detection of impact damage, gaining an understanding of crack propagation in composite materials, investigating the early stage of corrosion, cracks, voids and porosity in metals, and performing quality control in additive manufacturing.

Our method to achieving three-modal CT is based on beam-modulation; an amplitude modulator (absorbing mask with an array of apertures) is placed upstream to the sample creating an array of separated beamlets. Either an Edge Illumination (EI) or Beam Tracking (BT) mechanism is then employed for phase and scattering signals detection. Both these approaches impose a trade-off between spatial resolution and scan duration: a spatial resolution defined only by the beamlet size can be achieved when employing "dithering", i.e., step-scanning the sample along one or two directions depending on the modulator design, at each rotation angle, at a cost of increased scan times caused mostly by overheads. A 2D-structured modulator provides refraction sensitivity in two orthogonal directions, which reduces inherent image artefacts associated with phase integration; however, it also requires the sample to be step-scanned in 2D, at each rotation angle, further extending the time for data acquisition.

To overcome the impracticality of 2D dithering, especially in applications where high sample throughput is required, we have designed an amplitude modulator with a 2D array of apertures which, however, under-samples only in 1D, thus requiring only 1D dithering. In this talk, we will discuss the simulation studies performed to assist the design of the modulator and present both simulated and experimental images. We will also discuss the compatibility of this method with cycloidal CT, which is a scanning scheme implemented in a flyscan manner, and its potential benefits for three-modal CT in industrial contexts (e.g., in-line scanning for quality control).

3D U-Net for automatic segmentation of volumes from Multi-energy X-ray Computed Tomography

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3D imaging using X-ray Computed Tomography (XCT) can play a crucial role in various industrial sectors, including quality control, defect analysis, and failure investigation. Unfortunately, handling XCT volumetric images can be quite challenging and time-consuming, and automating the related analysis tasks is difficult to achieve. The test case discussed in this article focuses on an inspiratory flow-driven, multidose powder inhaler. The objective of the study is to develop an automatic classification-aided decision tool based on deep learning, which would determine acceptance or rejection criteria and provide assistance in redesigning through reverse engineering if necessary.

An XCT scan of our test case was performed to assess the integrity of the object. It is a multimaterial object with complex internal shape components and a wide range of material properties, which presents challenges in image appearance and segmentation tasks, particularly due to some components having similar attenuation coefficients. Even with multi-energy XCT scans (using three energy bands: 80Kv, 110Kv, and 150Kv), handling and preprocessing the images remain difficult. Moreover, the large size of XCT images makes storage and processing of each inspection for every single product extremely complicated.

To overcome these drawbacks of XCT and achieve our goals, we implemented a convolutional neural network based on the 3D U-Net architecture, which was trained and tested on our XCT volumetric images. Prior to training, a manual segmentation using 3D slicer was performed to prepare the input dataset for the architecture. We identified and classified 18 classes. The actual accuracies of the training and testing phases are encouraging, and we are looking forward to automating the initial step of segmenting the input data.

As for future perspectives, our aims include generating an STL file to simulate the inhalation process. This will allow us to improve the usability and functionality of the product by optimizing the shape of its internal components. Additionally, we intend to adapt the entire workflow for other industrial applications that employ XCT as an inspection tool.

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