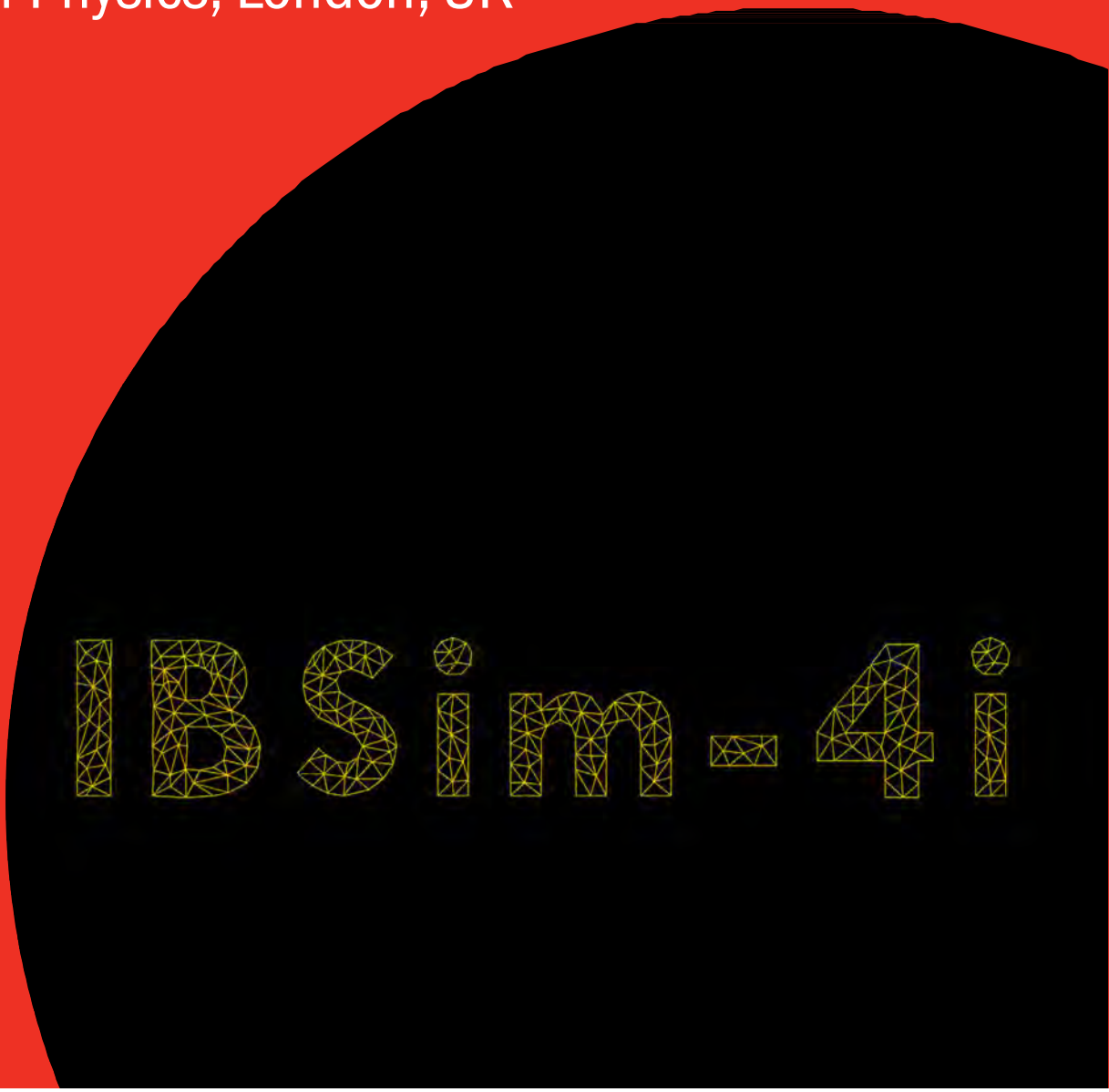
Image-Based Simulation for Industry 2025
(IBSim-4i 2025)

20–23 October 2025
Institute of Physics, London, UK



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Welcome

On behalf of the organising committee of the seventh Image-Based Simulation for Industry event (IBSim-4i 2025), 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

Presentations Timings:
Invited Speakers: 45 minutes (40 min talk + 5 min questions)
Contributed Speakers: 30 minutes (25 min talk + 5 min questions)

Slides for the IBSim-4i Website

If you would be happy for your presentations slides to be available on the official IBSim-4i website, please email them to sarah.evans@iop.org and let us know you would be happy for them to be displayed there.

Supporting Organisations

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

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Materials and Characterisation Group

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CCPi
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3Dmagination
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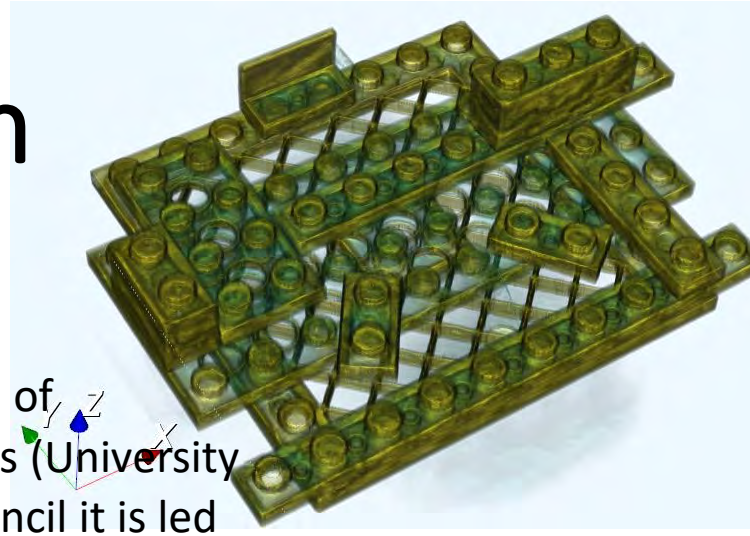
Collaborative Computational Project in Tomographic Imaging www.ccpi.ac.uk



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 co-ordinated 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 https://www.ccpi.ac.uk/CIL**

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**
- **Data/Code archive on CCPi zenodo.org collection**
- **Tomography software show-and-tells**
- **Iterative reconstruction algorithms**

Join over 400 Tomographic Imaging practitioners: discord.com/invite/9NTWu9MEGq

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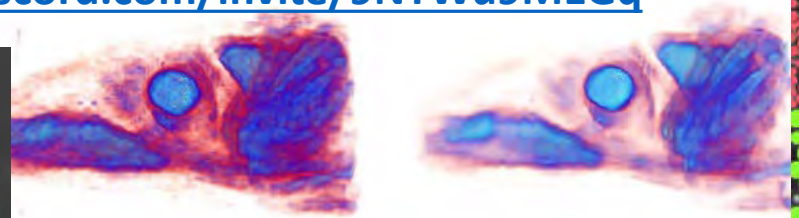

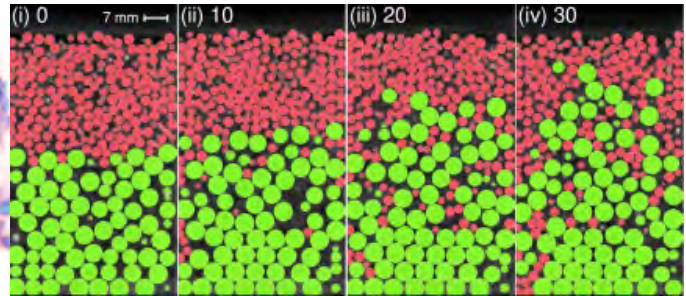

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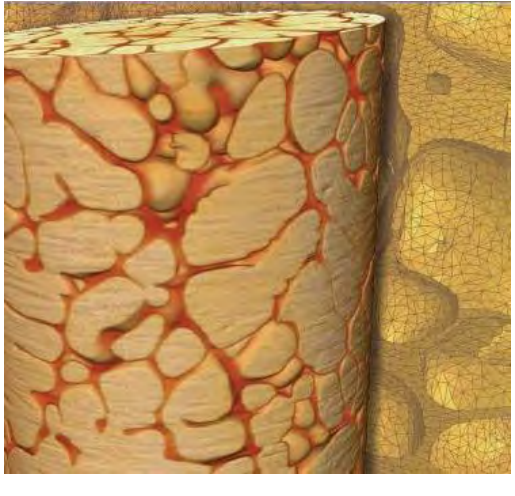
The University of Manchester

CoSeC Computational Science Centre for Research Communities

UKRI Science and Technology Facilities Council

UKRI Engineering and Physical Sciences Research Council



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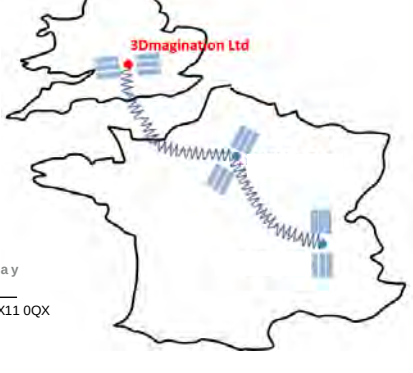

Keynote Speakers

Dr Stepan Lomov
KU Leuven

Stepan V. Lomov (1955) graduated from School N30 in Leningrad (1972), Phys.-Mech of Leningrad Polytechnic Institute (1978). PhD on terminal ballistics (1985), Dr Hab. on textile materials science (1995), St. Petersburg State University of Technology and Design. Since 1999 works in KU Leuven, Belgium, Department of Materials Engineering, coordinator of the Composite Materials Group in 2013 – 2020, Toray Professor in 2015 – 2020. Professor Emeritus since 2020.

Research areas: composites and textiles science and engineering: internal structure, manufacturing, in-service mechanical behaviour, nano-composites, experimental damage mechanics, micro- and meso-level geometrical and mechanical models.

(co-) author of WiseTex and VoxTex software tools for geometrical modelling and XCT analysis of textile composites, (co-) author of 350+ journal papers and book chapters, editor of four books (Elsevier – Woodhead, Wiley), member of Editorial Boards (CSTE …) and Scientific Committees (ECCM …).

Lecture courses in KU Leuven, Scoltech (Moscow), Politecnico di Milano, GIAN (India), International Centre for Mechanical Sciences (Udine), Harbin Institute of Technology.

Promoted 30+ PhD students.

Professor Luisa Silva
Centrale Nantes

Research in advanced numerical techniques used in High Performance Computing: stable/stabilized immersed finite element methods, interface capturing through modified level-set set or phase-field methods, anisotropic mesh adaptation, developments in a massively parallel context.

Expertise fields and software application developments:

- Finite elements and eulerian approaches to solve thermomechanical multiphase problems
- Parallel multiphase computational fluid dynamics of highly viscous to inviscid fluid flows and their phase changes
- Direct 3D image based numerical simulations(X-Ray tomography, point clouds, ...) in several applications fields
- Development of software applications for urban environments, material forming processes and material structure development simulations

Oral Presentations

Session 1

Understanding the Structural Characteristics of the Placenta in Heath and Disease

Avery Pennington[1], Angelos Evangelinos[2,3], Toby Jackson[4], Dolapo Adebo[1], Sam Kersley[1], Paul Brownbill[2,3], Gowsihan Poologasundarampillai[5], Alys Clark[4], Alexander Heazell[2,3], Dr Michele Darrow[1]
[1]Rosalind Franklin Institute, [2]Maternal & Fetal Health Research Centre, School of Medical Sciences, University of Manchester, [3]MAHSC, St Mary's Hospital, NHS MFT, [4]Auckland Bioengineering Institute, The University of Auckland, [5]School of Dentistry, University of Birmingham

Session 1, October 22, 2025, 11:00 - 12:30

Placental diseases show dysregulated physiology and structure within multiple maternal and fetal organs whose physiology can change rapidly during gestation. This remains a significant clinical problem, in part because of our inability to adequately predict or detect vulnerability toward fetal compromise, meaning opportunities for best clinical management are missed.

The work describes a pipeline for sample preparation, imaging, segmentation and structural quantification of placenta samples across imaging techniques and corresponding scales (MRI, HiP-CT, synchrotron micro-CT). This allows investigation of the fetal-maternal interface and fetal-placental vascular network in placentas from normal and pathological outcomes including pre-eclampsia, fetal growth restriction, stillbirth, and maternal diabetes.

Multiple deep learning approaches to segmentation of the synchrotron micro-CT data of the intervillous space (where the maternal blood flows) the placental villous tissue and the fetal vascular network (where the fetal blood flows) have been assessed. An iterative human-in-the-loop active learning approach has been applied to generate the largest dataset of this type currently available.

Quantitative metrics and segmentations from this pipeline have enabled both comparative physiology to describe healthy and disease states and are also used by collaborators to simulate function of the circulatory systems within the placenta with particular focus on oxygen and nutrient transfer between the maternal and fetal circulations.

This work was funded through the Wellcome Leap In Utero program.

Mesoscale Modelling of Sarcomere Structure and Function using Fluctuating Finite Element Analysis

Renee Taylor[1]
[1]University of Sheffield

Session 1, October 22, 2025, 11:00 - 12:30

Fluctuating Finite Element Analysis (FFEA) is a molecular modelling algorithm that supports mesoscale simulations of biomolecular systems, by representing them as viscoelastic solids, subject to thermal fluctuations (Solernou et al., 2018). Unlike atomistic models, FFEA treats molecules as a mixture of 3D volumes comprised of tetrahedral finite elements and 1D rod elements, which can represent biomechanical behaviour across larger timescales (Solernou et al., 2018). In this particular use case, we model the complex protein structure of a muscle sarcomere, which is the smallest unit of muscle. To reduce complexity while preserving the structure of the sarcomere, the model was simplified such that only myofilaments and structural constraints such as the Z-disc was modelled. Myofilament geometries were assembled from stereolithography (STL) meshes, while the mesh representing the Z-disc was built using the 3D design software, Blender. This initiative enables the design and simulation of biologically representative protein structures, which can advance our ability to better understand the function of muscle contraction and potentially other large biological complexes.

1. Solernou, A. et al. (2018) ‘Fluctuating finite element analysis (FFEA): A Continuum Mechanics Software tool for mesoscale simulation of biomolecules’, PLOS Computational Biology, 14(3). doi:10.1371/journal.pcbi.1005897.

On the use of synthetic plant for plant phenotyping based on computer vision

David Rousseau[1]
[1]Université d'Angers

Session 1, October 22, 2025, 11:00 - 12:30

The rapidly expanding field of plant phenotyping, crucial for accelerating crop breeding and understanding plant responses to environmental changes, relies heavily on computer vision techniques. However, the acquisition of diverse, high-quality, and comprehensively annotated real-world image datasets for training robust computer vision models presents significant challenges. These include the variability of natural light, complex occlusions, the vast diversity of plant architectures, and the laborious nature of manual annotation. In this context, the judicious use of synthetic plants emerges as a powerful paradigm shift. By leveraging advanced computer graphics and procedural modeling, we can generate highly realistic virtual plant models with precise control over their morphology, growth stages, and environmental interactions. These synthetic data offer several compelling advantages. We present a panorama of such approaches and discuss their application in Agtech industries while possibly opening also interesting windows for other industrial domains.

Posters
(Session 2)

Modelling the hardening mechanisms of Oxide Dispersion Strengthened steels with crystal plasticity models

Lizzie Mushangwe[1]
[1]University of Oxford

Session 2 (posters), October 22, 2025, 14:00 - 14:30

Oxide dispersion-strengthened (ODS) ferritic/martensitic steels are promising candidates for structural components in future fusion reactors such as the UKAEA's STEP reactor, where materials will be exposed to extreme conditions of high temperature and intense 14.1 MeV neutron irradiation. Under such conditions, a complex spectrum of radiation-induced defects—including dislocation loops, voids (bubbles), and precipitates—interact with dislocations and grain boundaries, leading to irradiation hardening, embrittlement, and loss of ductility. These degradation mechanisms ultimately limit the structural integrity and operational lifetime of reactor components. ODS steels are engineered with a high density of finely dispersed yttrium-titanium-oxygen (Y-Ti-O) nano-oxides, which are theorized to act as defect sinks. By trapping point defects and facilitating vacancy–interstitial recombination, these particles can suppress the formation of defect clusters and stabilize the microstructure under irradiation. Despite their proposed advantages, there remains limited experimental evidence quantifying the extent to which nano-oxides mitigate irradiation-induced hardening in fusion-relevant environments.

This study investigates the irradiation response of ODS steel 14YWT compared to its non-ODS counterpart 14WT under 2 MeV proton irradiation to doses of approximately 0.02 dpa and 0.2 dpa. Post-irradiation nanoindentation was employed to map hardness profiles as a function of depth, providing insight into localized mechanical property changes within the irradiated layer. The non-ODS steel, 14WT, exhibited a pronounced hardness spike (~6 GPa) at depths of 18–19 µm, coinciding with the Bragg peak region where defect production was highest. Beyond 25 µm, hardness returned to baseline levels, suggesting strong defect clustering and localized dislocation pinning within the peak damage zone. In contrast, the ODS variant, 14YWT, displayed a more uniform hardness distribution (~6–8 GPa) across the irradiated region, with a significantly reduced Bragg peak effect. This behaviour implies that Y-Ti-O nano-oxide dispersions enhanced defect recombination, reduced the formation of large defect clusters, and helped preserve mechanical stability under irradiation.

The results provide promising experimental evidence that nano-oxide dispersions improve irradiation tolerance by modifying defect evolution and whilst also mitigating hardening. These findings reinforce the potential of ODS steels as leading candidates for radiation-resistant materials in fusion energy applications. Ongoing work integrates these empirical observations into crystal plasticity finite element models to establish quantitative relationships between specific defect populations and macroscopic hardening behaviour. Such predictive modelling tools will inform the future design and optimisation of advanced ODS alloys with improved fatigue life, reduced swelling, and enhanced long-term performance in the harsh operating environment of fusion reactors.

Developing a digital twin for the validation of packing optimisers used for nuclear decommissioning.

Jean-Claude Bikaku[1]
[1]CDT SATURN (University of Leeds)

Session 2 (posters), October 22, 2025, 14:00 - 14:30

This review outlines the research scope and key concepts with a specific focus on nuclear decommissioning, the application of robotics in decommissioning operations, Digital Twin technology, the Discrete Element Method, and powder characterization."
The primary objective of this review is to establish a practical environment incorporating robotic systems to bridge the gap between real-world operations and digital simulation within a digital twin framework. The digital twin, based on DigiDEM, provides a unified virtual platform for simulating packing arrangements of irregularly shaped components. Packing more irregulars' shapes objects in the container make it achievable regardless the physics law or gravity apply to an object robotically picked and placed in the container. Machine vision sensors embedded within the physical twin enable real-time detection and correction of discrepancies between the physical and simulated environments. This approach specifically addresses limitations inherent in simulation models. A real-time validation system for the packing simulation is currently under implementation, and numerical results will be presented upon completion of various test cases.

Microstructure-resolved 3D Modelling of Interdigitated Lithium-Sulfur Batteries

Zeyan Wang[1,2], Phil Morris[1], Rhodri Jervis[1], Miraslau L. Barabash[1]
[1]Electrochemical Innovation Lab, Department of Chemical Engineering, University College London, London WC1E 7JE, [2]Department of Materials, Imperial College London, London SW7 2AZ

Session 2 (posters), October 22, 2025, 14:00 - 14:30

Lithium–sulfur (Li–S) batteries, which employ abundant elemental sulfur as the cathode material, are among the most promising next-generation energy storage technologies due to their high theoretical energy density and cost-effectiveness [1] – the priorities for the UK's Battery Strategy 2030 [2]. A key challenge is uncovering how microscale battery morphology influences its macroscale performance. This problem can be addressed by employing the image-based continuum modelling approach to capture the realistic battery microarchitectures with adjustable parameters.[3] Unlike conventional 1D modelling, which tends to overpredict discharge performance and neglect the influence of electrode microstructural properties [4] , 3D modelling offers more physically accurate simulations by capturing localised heterogeneities in the electrode microarchitecture. Supported by X-ray CT imaging [4], this in-silico approach captures realistic electrode structures and improves predictive accuracy of the electrochemical behaviour of Li–S batteries.

Here, we apply the newly developed finite-element model (FEM) [4] to 3D interdigitated Li-S cathodes (Fig. 1(a)). This cathode architecture features a piano-like 3D configuration in which the cathode and anode are arranged in an alternating spatial pattern, potentially mitigating the traditional trade-off between energy and power densities. [5] The model enables one to visualise the dynamics of localisation of lithium, sulfur, and polysulfides over time during discharging, as shown in Fig. 1(a), as well as the role of C-rate on the discharging behaviour of the interdigitated Li-S battery, as given in Fig.1(b). We analyse the role of pillars' parameters – e.g. thickness, length, spatial density – to understand their effects on the Li-S battery discharge, lithium diffusion distance, polysulfides' precipitation, and utilisation of active material. We conclude by proposing tentative strategies for maximizing the capacity, energy or power density of this battery architecture.

This study highlights the benefits of image-based modelling, connecting microstructure and battery performance under various internal and external conditions, when formulating the guidelines for manufacturable design of Li-S batteries. We would like to emphasise that accounting for complex microstructures with variable design parameters might only be accomplished through a microstructure-resolved 3D modelling framework. [4]

References:

1. R. P. Fang et al., 2017 Adv. Mater. 29 1606823 https://doi.org/10.1002/adma.201606823
2. Department for Business and Trade 2023 UK battery strategy https://www.gov.uk/government/publications/uk-battery-strategy/uk-battery-strategy-html-version
3. C. Tan et al., 2019 Phys. Chem. Chem. Phys. 21 4145–4154 https://doi.org/10.1039/C8CP04763D
4. X. Dai et al., 2022 ChemRxiv https://doi.org/10.26434/chemrxiv-2022-2ktc5
5. K. Xu et al., 2022 Chin. J. Mech. Eng.: Addit. Manuf. Front. 1(4) 100053 https://doi.org/10.1016/j.cjmeam.2022.100053.

On-the-Fly Meshing and Simulation: A code_saturne-based HPC Pipeline for Industrial XRCT

Jones Harriet[1], Charles Moulinec[1], James Le Houx[2], Stefano Rolfo[1]
[1]UKRI-STFC Scientific Computing, Daresbury Laboratory, Warrington, WA4 4AD, [2]UKRI-STFC ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot OX11 0QX

Session 2 (posters), October 22, 2025, 14:00 - 14:30

To maximise the effective use of Micro-X-ray computed tomography (XRCT) data, particularly during limited beamtime, fast and accurate data processing pipelines are required. Ideally, users would be able to quickly interrogate their data during beamtime, and calibrate their experiments accordingly. Image-based modelling workflows using High Performance Computing functionality display significant promise in this respect. The workflow presented in this poster is based on a pre-existing workflow developed by Le Houx (2021), which uses savu for reconstruction, SuRVos for volume segmentation and OpenImpala, a finite difference package for solving equilibrium partial differential equations directly on image domains. The new workflow will connect HTTomo (an alternative to savu offering in-memory compute on GPUs) with SuRVos2 and a robust and accurate solver from EDF R&D's open-source multi-purpose massively parallel code_saturne (for mesh generation and simulations). code_saturne offers a number of benefits to the user including on-the-fly mesh generation and refinement directly from the voxel dataset, which should reduce preprocessing time and complexity significantly compared with the use of separate software to perform these tasks. The Compatible Discrete Operator (CDO) solver within code_saturne generates accurate results on any type of grid for many numerical operators, making it well suited to the analysis of a wide range of physical properties on complex geometries.

As a significant portion of the user community at synchrotrons and other imaging facilities utilise the HDF5 file format for data processing and storage, the current focus is on developing an HDF5 reader within code_saturne. This is accomplished in serial, with parallel developments in progress. Initial tests involve the use of a bi-layer electrode geometry, relevant for industrial battery research, generated using PoreSpy. This is read into code_saturne, where the mesh is generated on-the-fly and the potential across the geometry calculated using the CDO solver. Preliminary benchmarks performed on the UK National Facility ARCHER2 (Tier-1) show promising results and good scaling with increasing compute, from 10.65 second solve time for a Poisson equation for the potential using $1{,}072^3$ cells on 16,384 cores up to 124.44 seconds using $6{,}670^3$ cells over 524,288 cores. Good performance is also seen when using large datasets on a Tier-2 system, with a solve time of 382.71 seconds for $2{,}144^3$ cells over 4,096 cores. Ongoing work includes full validation of current results, parallelisation and optimisation of all processes, and exploring applications in high-throughput automated analysis to accelerate material characterisation.

Validating Multiscale Models of Irradiation Damage Using Image-Based Simulations

Mr Ethan Edmunds[1], Christopher Race[1]
[1]Department Of Materials Science And Engineering, The University Of Sheffield

Session 2 (posters), October 22, 2025, 14:00 - 14:30

The materials used in nuclear fusion reactors operate under harsh conditions, including irradiation damage, high mechanical stresses, and elevated temperatures, whilst requiring sustained integrity over extended service life. A critical challenge is material creep, a time-dependent deformation often governed by the intricate evolution of dislocation networks. As creep experiments are inherently time-consuming and costly, computational simulations and modelling present an effective alternative.

Multiscale materials modelling provides a hierarchical approach, leveraging diverse simulation schemes across various length and time scales to achieve a comprehensive understanding of material performance. At the atomistic scale, models like classical molecular dynamics offer high-fidelity insights into fundamental mechanisms, such as dislocation mobility and point-defect diffusion. However, their computational intensity limits these simulations to short time scales and small cell sizes. To analyse the evolution of whole grains over longer timescales, researchers use larger-scale models such as crystal plasticity finite element methods (CPFEM). Yet, CPFEM's accuracy is often constrained because its underlying mathematical equations are empirically parameterised from experiments, rather than being entirely derived from first principles. The ambition of multiscale modelling is to create a fully physically-based system, achieved by tuning higher-scale models with insights and quantitative input from lower-scale ones. However, a significant challenge remains: rigorous validation and accurate uncertainty quantification across these vastly different scales are notoriously difficult.

Image-Based Simulation (IBSim) bridges the gap between computational modelling and real-world material behaviour by directly integrating experimentally derived microstructural data into simulations. At larger length scales relevant to continuum models like CPFEM, techniques such as Electron Backscatter Diffraction (EBSD) reveal grain structures, crystallographic orientations, and dislocation densities. Digital Image Correlation (DIC) complements this by providing full-field, non-contact measurements of deformation and strain during in situ mechanical testing, enabling direct comparison between simulated and experimental strain fields. At finer length scales, Transmission Electron Microscopy (TEM) provides detailed insight into individual dislocations and their mobility. Together, these experimental techniques provide the microstructural data essential for performing IBSim. This approach ensures simulations reflect the "as-manufactured" material state, including process-induced defects and heterogeneities, and allows for the replication of complex geometries, enabling robust comparisons with experimental observations. As a result, IBSim supports the direct validation of the predicted deformation behaviour and provides a critical feedback loop to understand the interplay between the microstructure and mechanical performance.

Session 3

RadioSphere: Measuring the 3D kinematic of a dense cluster of spheres using two-view radiographs

Léonard Turpin[1]
[1]Université De Bordeaux

Session 3, October 22, 2025, 15:30 - 17:30

Particle Image Velocimetry (PIV) is a method that allows measurement of the displacement field within a fluid flow using images of particles carried by the flow. In traditional imaging, it only provides information within the plane of the image.
The RadioSphere project [1] aims to extend this method to 3D displacement fields, using radiographic images instead of optical ones. By using monodisperse spheres and a divergent beam, the perspective effect makes it possible to measure the position of a sphere along the axis perpendicular to the image plane. This method also enables the study of the behavior of granular media.
Precise calibration of the setup geometry, as well as the X-ray absorption model, is important. A procedure has been developed that accounts for beam hardening and scattering, based partly on dedicated calibration images and on initial-state images (auto-calibration).
To study dense media, typically granular materials, a setup has been developed that allows for simultaneous radiographs from two different axes. Each axis is calibrated independently, and the relative position of the axes is also calibrated to be able to couple both views.
Finally, a temporal regularization approach has been developed to track dense flows. Physical constraints on the arrangement of the spheres and limitations on displacement jumps make it possible to measure the kinematics of each individual sphere and track them over time. This intrication of the experimental data and a physical model of the media give access to high temporal resolution measurement of a complex flow behaviour.

[1]: Andò, E. et al. Single-projection reconstruction technique for positioning monodisperse spheres in 3D with a divergent x-ray beam. Meas. Sci. Technol., 32, 9 (2021) doi : 10.1088/1361-6501/abfbfe

Hardware based phase-retrieval for hard x-ray imaging

Grammatiki Lioliou[1], Alberto Astolfo[1], Marco Endrizzi[1], Peter Munro[1], David Bate[1,2], Charlotte Hagen[1], Alessandro Olivo[1]
[1]University College London, [2]Nikon X-Tek Systems Ltd

Session 3, October 22, 2025, 15:30 - 17:30

X-ray phase contrast imaging and CT (XPC-CT) offers superior contrast over conventional absorption-based CT at equal dose, particularly for low-Z materials, e.g., carbon fibres and soft polymers, by capturing phase shifts introduced by variations in the real part of the refractive index. Among single-shot XPC-CT approaches, propagation-based imaging with phase retrieval using the Paganin filter is widely used due to its simplicity (no additional optical elements are required) and robustness. Paganin-based retrieval relies on digital filtering in the frequency domain. It is specifically designed to preserve fine structural details while suppressing noise and fringes. However, it requires spatial coherence and is thus typically implemented with low-flux, polychromatic microfocus sources.
We propose an alternative, hardware-based strategy for phase retrieval. Assuming the source blur being a truncated, double-sided exponential (Laplace) distribution, we tune the total system blur to mimic the frequency response of the Paganin filter. We investigate whether adjusting the source size can approximate the effects of the Paganin filter, eliminating the need for digital post-processing. On top of providing a retrieved phase image directly from the CT reconstruction, it allows using a larger focal spot, thereby increasing the available flux.
To assess feasibility, we performed a wave-optics simulations under the Fresnel approximation. The simulation incorporates source shape/size, energy, detector pixel size and PSF, sample thickness, sample material properties (refractive index), and Poisson noise. The system blur is calculated in both real and Fourier space and compared directly to the ideal Paganin filter for a given material imaged on a chosen system. The blur is then tuned by either changing the source size or the source-to-sample distance (affecting the projected source size on the detector, assuming fixed source-to-detector distance). This is also validated experimentally with two propagation-based scans, at different source-to-sample distances, using a microfocus source. Despite non-ideal conditions (Gaussian source and detector blur), simulations and experimental results suggest that the system blur acts as a partial filter, confirming the feasibility of hardware-driven phase retrieval under practical constraints.
This proof-of-concept study lays the foundation for flux-optimized XPC-CT by careful hardware tuning, offering a pathway toward simplified, more efficient XPC-CT without digital retrieval post-processing.

Data-driven interpretation of strain localisation in fibre-reinforced composites: PCA of in situ XCT–DVC biaxial tests

Salaheddine Madi

Session 3, October 22, 2025, 15:30 - 17:30

Accurately predicting failure in fibre-reinforced composites remains a significant challenge due to the complex interplay between fibre architecture, resin morphology, and multiaxial stress states. Conventional failure criteria often fail to capture this complexity, as they rely on homogenised parameters identified from simple uniaxial tests. To move towards predictive models that are both accurate and microstructure-informed, new experimental strategies are required to quantify three-dimensional strain fields and relate them directly to the underlying microstructure.

In this study, we extend our recently developed in situ biaxial testing methodology [1] that combines laboratory X-ray Computed Tomography (XCT) with Digital Volume Correlation (DVC). Two E-glass/epoxy laminates $(0/90)_S$ and $(+45/-45)_S$ layups, were tested under equi-biaxial loading. XCT imaging with a voxel size of 7.5 µm enabled reconstruction of volumes large enough to encompass the homogeneous gauge region of the biaxial sample, ensuring representativeness. DVC provided full-field strain measurements throughout the loading sequence.

A dedicated Avizo plugin was developed to automate the extraction of effective mechanical properties from DVC strain fields, enabling evaluation of stiffness ratios and shear–normal strain couplings. To complement this property extraction, we implemented a Principal Component Analysis (PCA)-based framework to systematically reduce the dimensionality of the strain datasets and highlight dominant deformation modes. This dual approach allows for both quantitative stiffness estimation and the identification of strain–microstructure correlations.

Results show that the $(0/90)_S$ laminate exhibits strong correlations between transverse normal strains and in-plane shear components, reflecting the constraints imposed by orthogonal fibre plies. In contrast, the $(+45/-45)_S$ laminate demonstrates more balanced stiffness and correlations dominated by shear interactions aligned with the ±45° fibres. PCA revealed that the first principal strain mode correlates with fibre orientation and transverse strain localisation, while the second mode captures shear-driven interactions. Clustering of the PCA space further distinguished groups of strain–microstructure couplings, providing a data-driven means of separating deformation mechanisms.

This integrated framework demonstrates the potential of combining automated property extraction with PCA to bridge microstructural variability and macroscopic failure behaviour. The developed methodology provides the foundation for data-driven micromechanical model calibration. In future work, we plan to extend it to SRCT (4D-data), to further enhance both spatial and temporal resolution, thereby enabling more refined and predictive models of composite failure.

[1] S. E. Madi et al., "In situ biaxial tensile testing of composites: coupling X-ray computed tomography and digital volume correlation with finite element simulations," Composites Part B: Engineering, p. 112815, 2025.

A quantitative single-shot method for phase-contrast CT of multi-material

Dr. Andrea Mazzolani, Alberto Astolfo, Marius Didziokas, Pauws Erwin, Mehran Moazen, Peter Modregger, Peter R. T. Munro, Alessandro Olivo
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Session 3, October 22, 2025, 15:30 - 17:30

X-ray phase-contrast imaging (XPCI) reveals soft-tissue and low-density structures invisible to conventional absorption CT by exploiting the unit decrement of the real part δ alongside the imaginary part β of the refractive index. Edge-illumination XPCI (EI) achieves quantitatively accurate retrieval of multi-material samples, at the cost of multiple mask positions per projection to decouple phase and attenuation, leading to elevated dose and long acquisition times. To overcome these limitations, we present a Linear Joint Reconstruction (LJR) method
that requires a single-exposure, retrieving δ and β maps from one acquisition per angle via a convex, non-iterative inversion.

Starting from the full EI forward model, we apply a first-order Taylor expansion of the normalized log-intensity ratio to linearize the inherently non-linear joint reconstruction problem. This transforms the inversion into a convex least-squares system that yields an analytical closed-form solution, obviating the need for iterative Gaussian fitting of the illumination curve. As a result, LJR reconstructs multi-contrast volumes in under one minute from 2000 projections on a 48 GB GPU, over 30× faster than standard multi-shot EI methods, which take approxi-
mately 30 minutes, while reducing both acquisition time and radiation dose by up to five-fold through the elimination of multiple mask steps.

We validate LJR on both simulated and experimental datasets. In a rod phantom made of two different plastics, reconstructed δ and β profiles agree within approximately ≈ 5% relative error compared to multi-shot EI. In a challenging biological specimen, namely an intact mouse brain within its native skull, LJR robustly recovers minute soft-tissue interfaces and high-contrast bone structure. For this sample, the phase CNR increased by approximately 50%, and the attenuation CNR improved by about 15× relative to conventional multi-shot EI acquisitions of the same sample, while maintaining comparable image quality.
By combining a laboratory-compatible phase-contrast modality with a fast analytical solver, LJR makes quantitative, high-throughput XPCI practical for complex multi-material samples in biomedical and materials-science applications. This single-shot approach lays the ground-work for real-time phase-contrast guided simulations, virtual histology, and industrial non-destructive testing under challenging imaging conditions.

Session 4

A synergistic approach to X-ray CT and simulation at the NXCT

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Session 4, October 23, 2025, 10:15 - 10:45

The National Research Facility in lab-based X-ray CT (NXCT) provides access to cutting-edge X-ray CT equipment and capabilities, enabling high-impact science for researchers in academia and industry across a wide range of sectors. We bring together X-ray labs at the Universities of Manchester, Southampton, Warwick and UCL, through a single point of access, providing technical expertise to guide users in designing, acquiring and processing their X-ray CT data. Simulations play an important role in the work of many researchers accessing our facility. From predicting the elastic response in additively manufactured parts, to simulating permeable flow analysis through bio separators and virtually restoring historic pianos, there are a wide range of applications utilising these methods. X-ray CT enables the creation of detailed 3D computerised images of real components, which can then be integrated into simulations for more accurate predictions.

This presentation will provide an overview of the facility and highlight some of our simulation-driven case studies. We will also introduce an ongoing collaboration between the NXCT and Scientific Computing at STFC that aims to utilise the gVirtualXRAY (gVXR) simulation software to enhance user support in innovative ways. This interactive simulation toolkit will allow users to perform realistic X-ray imaging simulations through a control panel that mimics the operation of a real device. It will support our users in hands-on X-ray CT system training, provide opportunities to optimise scans and generate training data for data augmentation in machine learning.

Session 5

pyvale: An open-source toolbox for simulating imaging diagnostics applied to fusion component validation

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Session 5, October 23, 2025, 11:15 - 12:15

Engineering components in a fusion power core are subjected to significant thermal (10's MW/m), mechanical (MN range) and electromagnetic loads (several Tesla) making experimental validation under these conditions challenging. To reduce the cost of simulation validation experiments we have developed a sensor simulation toolbox called `pyvale` (the python validation engine) which is designed to analyse the deployment of imaging diagnostics accounting for measurement uncertainties.

`pyvale` is an open-source python package available on the python package index with the source code here: https://github.com/Computer-Aided-Validation-Laboratory/pyvale . We take inspiration from computer graphics and synthetic image deformation for assessing uncertainties of digital image correlation (DIC) systems and extend the idea to a multi-physics scenarios including thermal (e.g. thermocouples, pyrometers, infra-red cameras) and mechanical sensors (e.g. strain gauges, digital image correlation).

We currently support synthetic image generation through ray tracing and rasterization renderers in Blender as well as a bespoke 2D image deformation tool. This includes specific tools that apply DIC speckle pattern textures to meshes as well as deforming meshes using input finite element simulations. We are also currently in the process of developing rendering algorithms that mitigate the additional errors introduced when converting higher order quadrilateral finite element meshes to linear triangular meshes commonly used in computer graphics applications.

In addition to the synthetic image generation capabilities of `pyvale` we also include a subset based 2D digital image correlation module. Here we support reliability guided and Fourier windowing-based algorithms which we have optimized for memory usage and performance on large scanning electron microscope images for micro-mechanics applications. Specifically, we can correlate a 1 giga-pixel pair of images in ~5 minutes using ~50 GB RAM and an AMD Ryzen Threadripper 7980X with 64 cores. In the future we will also provide support for stereo calibration and stereo DIC.

In designing `pyvale` we aim to provide users with a simple python interface for imaging simulation tools that can be easily installed using `pip install pyvale` without needing to build any compiled code from source or require a specific operating system. For the computationally intensive modules (custom rendering and digital image correlation modules) we are using compiled languages such as Cython, C/C++ and Zig allowing for high performance while wrapping these in a user-friendly python interface. At the conference we will demonstrate the imaging simulation pipeline of `pyvale` using a high heat flux test of a fusion divertor heatsink.

Image-Based 3D Modelling of Electrospun Lithium-Sulfur Cathodes

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Session 5, October 23, 2025, 11:15 - 12:15

Lithium-Sulfur (LiS) batteries represent one of the most promising next-generation candidates, particularly in the aerospace and heavier electric vehicles industries [https://www.doi.org/10.1088/2515-7655/abdb9a], due to their high theoretical capacity, small weight, low cost, sustainability, compared to the current Li-ion technology, thereby advancing the UK Battery Strategy 2030 [https://www.gov.uk/government/publications/uk-battery-strategy]. Thus, describing, optimising and designing the properties of LiS batteries represents a paramount challenge with significant industrial and socio-economic impact. At the core of that challenge is understanding how the battery morphology at the microscale affects the above macroscale properties. To date, conventional modelling of LiS cathodes has typically relied on a simplified volume-averaged treatment, thus overlooking the influence of the underlying cathode microstructures and their properties on the performance of the electrode.

Here, we apply the recently developed electrochemical finite-element model [https://doi.org/10.26434/chemrxiv-2022-2ktc5-v2] based on 3D X-ray CT images with sub-micron resolution to describe the spatio-temporal dynamics of discharge in LiS cathodes. Crucially, the model illuminates the dynamics of localization of lithium, polysulfides, and precipitation during discharge, which are otherwise inaccessible in conventional experimental in-situ and operando techniques. We demonstrate that the model accurately captures the effects of the localised inhomogeneities, inherent to Li-S cathodes, on the battery performance at varying C-rates, exceeding the capabilities of the respective volume-averaged 1D electrochemical model. Next, we cross-compare the discharge performance of two samples -– a commercial spherical carbon and an electrospun fibrous morphology – with inherently different microstructural properties (porosity, tortuosity, particle shape, sulfur particle size distribution) and, using the above model, show how these properties result in the observed differences in the discharge performance of the two samples. Furthermore, we generate in silico and optimize parametrized 3D microstructures, mimicking electrospun LiS cathodes, and propose tentative ways for maximizing the capacity and energy density of LiS batteries. Lastly, we deploy pore network modelling [https://doi.org/10.21105/joss.01296] to reduce computational burden and enable a realistic representation of large electrodes in our models.

We expect this modelling framework and results will pave the way towards realistic modelling, optimisation and rational design of advanced LiS battery cathodes to meet the growing industrial demand.

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Figure: Computer-generated fibrous-carbon LiS-microstructure (inset): simulated discharge. Left: Spatial Lithium-concentration [mol/m^3] with lithium-flowlines (lines, black). Right: current density’s (C-rate’s) impact.

Session 6

evoxels: A differentiable physics framework for voxel-based microstructure simulations

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[1]Imperial College London, [2]Massachusetts Institute of Technology, [3]Karlsruhe Institute of Technology

Session 6, October 23, 2025, 13:45 - 14:45

Materials science inherently spans disciplines: experimentalists use advanced microscopy to uncover micro- and nanoscale structure, while theorists and computational scientists develop models that link processing, structure, and properties. Bridging these domains is essential for inverse material design where you start from desired performance and work backwards to optimal microstructures and manufacturing routes. Integrating high-resolution imaging with predictive simulations and data-driven optimization accelerates discovery and deepens understanding of process-structure-property relationships. The differentiable physics framework evoxels is based on a fully Pythonic, unified voxel-based approach that integrates segmented 3D microscopy data, physical simulations, inverse modeling, and machine learning.

• At its core is a voxel grid representation compatible with both pytorch and jax to leverage massive parallelization on CPU, GPU and TPU for large microstructures.
• Both backends naturally provide high computational performance based on just-in-time compiled kernels and end-to-end gradient-based parameter learning through automatic differentiation.
• The solver design based on advanced Fourier spectral time-stepping and low-RAM in-place updates enables scaling to hundreds of millions of DOFs on commodity hardware (e.g. forward Cahn-Hilliard simulation with 400^3 voxels on NVIDIA RTX 500 Ada Laptop GPU with 4GB memory) and billions of DOFs on high end data-center GPUs (1024^3 voxels on NVIDIA RTX A6000)
• Its modular design includes comprehensive convergence tests to ensure the right order of convergence and robustness for various combinations of boundary conditions, grid conventions and stencils during rapid prototyping of new PDEs

I will discuss the current code design, testing strategies for rapid prototyping of material models and ongoing activities as well as the envisioned development and intended use of the package in the future.

Investigating geometric misalignments in parallel beam laminography using x-ray simulation

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Session 6, October 23, 2025, 13:45 - 14:45

X-ray tomography performed on flat samples can result in reconstruction artefacts due to the anisotropic absorption. A common method to combat these artefacts is laminography, in which the sample and its rotation axis are tilted, equalising the absorption between projections and reducing artefacts. Accurate alignment of geometric parameters, such as the centre of rotation offset and tilt, is particularly important in this geometry to reduce further artefacts in the reconstruction.

This talk will describe investigations into the geometrical alignment of laminography using simulated x-ray datasets created using the gVirtualXray (gVXR) package (https://gvirtualxray.sourceforge.io/). gVXR was used to develop a digital twin of the Dual Imaging and Diffraction (DIAD) beamline at Diamond Light Source, modelling the beamline geometry, pixel size and scintillator response. The energy dependent characteristics of the detector were characterised experimentally, including the point spread function (PSF) using the edge technique and the photon flux. These measurements enable the generation of realistic simulated images with appropriate noise levels across a range of exposures. This method has enabled us to generate accurate simulations of the DIAD laminography setup and could be extended to other beamlines.

We used various simulated samples to investigate typical artefacts in flat sample tomography and laminography, with the aim of demonstrating to users where a particular geometry will be favourable. We also investigated the impact of geometric misalignment in laminography. The simulated datasets allow systematic variation of the tilt and centre of rotation offset, to study their impact on the laminography artefacts. Existing automatic geometry alignment methods for tomography, typically cannot handle the effect of the tilted rotation axis therefore a method has been developed to refine the geometry parameters by minimising residuals between filtered forward projections and simulated data. The simulations have been important tools for the development of alignment strategies and as a guide to improve laminography reconstructions.

Session 7

Image-Based Meshing and CT Simulation of Corrosion Features from SEM Data

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Session 7, October 23, 2025, 15:15 - 16:45

This work demonstrates an image-based simulation pipeline that integrates corrosion morphology extracted from Scanning Electron Microscopy (SEM) data into a fully reconstructable CT phantom. A 2D SEM image was segmented to isolate regions corresponding to distinct corrosion patch and voids. These regions are converted into 3D binary volumes and meshed using voxel-based extrusion, resulting in watertight STL files representing individual corrosion phases and air pockets.
The extracted corrosion and void mesh are embedded onto the surface of a steel cylindrical phantom and imported into the gVirtualXray (gVXR) simulation platform. A polychromatic CT scan is simulated based on realistic scan geometry and source-detector parameters. Simulated radiographs are reconstructed using the Filtered Back Projection (FDK) algorithm within the Core Imaging Library (CIL) framework.
The reconstructed CT volume is visualised with spatial annotations corresponding to the original corrosion types. Full-slice and zoomed-in visualisations reveal the detectability and contrast of Pb, PbO, PbO_2, and Pb_3O_4 regions, providing insight into how corrosion products may appear under industrial CT conditions. Both gVXR and CIL are open source. This reproducible framework enables controlled digital phantom generation and supports future work on defect detection, reconstruction benchmarking, and digital twin validation for material flaw analysis.

Realistic Synthetic CT Dataset for Automated Defect Inspections

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Session 7, October 23, 2025, 15:15 - 16:45

The identification of defects in metallic parts from additive manufacturing (AM) is crucial. Although X-ray computed tomography (CT) is widely used in non-destructive testing (NDT), the inspection process is still repetitive, time-consuming, and often affected by human error, which increases costs. To overcome these limitations, a fully integrated, image-based simulation workflow has been developed to enable scalable, automated defect detection using deep neural networks (DNNs).

Defect features are first extracted and labeled directly from sinogram data using our developed iSHT (iterative Sinusoidal Hough Transform) methodology. To preserve spatial coherence and volumetric realism, the 2D slice extraction is integrated into a 3D framework. Operating entirely in Radon space, iSHT is based on the sinusoidal properties of sinograms to extract defect features with accuracy. Then, the augmentation module implemented is the sinoDAM (sinogram Dataset Augmentation Methodology). It also operates in the Radon space and automatically synthesizes and labels new training data. Defects from the iSHT methodology are inserted into both simplified and industrially complex target objects.

A dual-variability augmentation strategy is implemented. Geometric transformations like rotation, scaling, and translation are applied to 3D defect meshes, while spatial repositioning is performed using controlled distributions to simulate realistic defect scenarios. The developed framework synthesizes new datasets which are both geometrically diverse and statistically representative of defect positioning observed in industrial AM components.

From small real or simulated dataset, the output augmentations from the sinoDAM are conducted in Radon space. Defect sinograms are injected into those of the target object, preserving the fidelity of CT acquisition characteristics. Each synthesized defect is tracked throughout the workflow, allowing for metrology-like inspection and dimensional analysis. This enables precise quantification of defect size, shape, and spatial coordinates. The augmented dataset with 2D cartesian slices was developed for both object detection and instance segmentation tasks for further training and inference on DNNs. The generation of ground-truth coordinates further supports dimensional analysis. Preliminary results indicate a correct accuracy and robustness across varied geometries and defect distributions, validating the effectiveness of the proposed workflow.

This contribution offers a reproducible and versatile framework for Radon space simulation in industrial NDT. By integrating sinogram-level augmentation, automatic labeling, and spatially consistent synthesis, the workflow supports the development of scalable and reliable defect detection systems designed to meet the needs of AM.

Benchmark Activity for micro-Structure Image-processing for Composites: Voids in 2D

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This study brings together several research groups and their tools for segmenting voids on 2D micrographs, see Figure 1. By comparing the generated masks, see Figure 2, and porosity metrics, see Figure 3, regions of disagreement are identified allowing greater understanding of different methods and establishing a foundation from which future improvements and standardization will be made possible.

Improving confidence and consistency in void segmentation is critical due to the significant effect voids have on the performance of composite components [1]. Even small variations in void volume fraction can have pronounced effects on matrix failure strengths. Broad scatter in the trends points to the importance of not just the global metrics but also the meso- and micro-scale variations in void locations, sizes, and shapes [2].

In order to capture these effects in advanced simulation tools and capture local variations, accurate micro-scale segmentation of void regions is needed. This drives the need for image-based analysis to replace more conventional standardized macro-characterization methods such as acid digestion and burn-off [3]. Within image segmentation methods applied to voids detection two primary categories can be distinguished: thresholding-based and more recent machine-learning-based [4]. Both approaches can be used to take 2D, 2.5D, or 3D datasets and generate masks that identify pixels belonging to voids. While the literature contains many examples of such techniques being used, there is limited cross-validation, resulting in uncertainty when comparing results or translating techniques from one study to another.

To enable the collective efforts of the academic community to build towards standardization and consistent void segmentation, this study shared several high-resolution micrographs with a wide panel of participants. Each participant was asked to generate and provide a mask of the voids. No limitations were put on the techniques the participants could use. The masks were then combined and assessed for level of agreement. This highlighted specific regions of high disagreement, specially around large and highly irregular voids. One dataset was also found to be an outlier, having marked a significant amount of small voids not marked by any other set. Further exploration of the disagreement when accounting for methods used may yield insights into the relative biases of specific algorithms or process steps.

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