

Image-Based Simulation for Industry 2026

(IBSim-4i 2026)

gVXR User Meeting

12-16 October 2026

Institute of Physics, London, UK



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IBSim-4i

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Welcome to the IBSim-4i + gVXR User Meeting.

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.

IBSim topics:

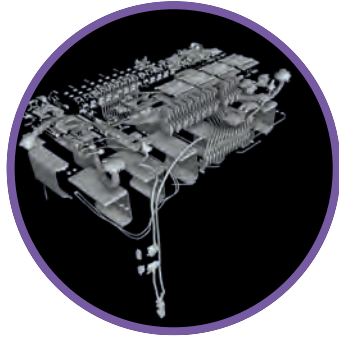
- 3D image acquisition methods (X-ray / neutron tomography, laser scanning etc.)
- 3D image reconstruction, processing, and segmentation
- Computer vision
- Artificial intelligence and machine learning
- Image to simulation mesh techniques
- Finite element analysis (FEM/FEA)
- Computational fluid dynamics (CFD)
- High-performance computing / supercomputing
- Large-scale scientific visualisation
- Advanced / high value manufacturing
- Industry 4.0
- Smart factories

gVXR topics:

- Industrial applications
- Medical and biomedical applications (radiography, CT, interventional imaging, training)
- Simulation-driven system design and optimisation
- Synthetic data generation and AI/ML integration
- Hybrid approaches combining simulation and experimental data
- Digital twinning
- User case studies and software extensions

Event Overview

- **Days 1–2: Training Courses**
 - *Grano*: A free C++/ Python discrete element workbench
 - Digital Volume Correlation (DVC) in Avizo
- **Days 3–4: IBSim-4i Forum**
 - User and developer conference with keynote speakers
 - Focus on **multidisciplinary aspects of image-based modelling**
- **Days 4–5: gVXR User Meeting**
 - Talks, town hall discussions, and interactions with developers and users



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Oral Presentations

A robust registration method for partially overlapping point clouds from different optical modalities

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October 15, 2026, 11:15 - 11:45

In the framework of automated inspections of mechanical parts, tools using optical cameras and laser scanning devices constitute an important mean for ensuring the conformity of the manufactured products. To this aim, measured point clouds have to be compared to a reference model. This requires to register point cloud to a reference within a common reference frame. However, acquired point clouds are often noisy and only partial because of the limited angle of view of the acquisition device. To overcome this challenge, an extensive set of methods have been developed through the years. For instance, the Iterative Closest Point (ICP) and its generalizations, methods based on local geometric features (LGF) or large dominant structures like planes (LDS), and spectral based methods (SBM) [1]. In the context of the registration of partially overlapping point clouds obtained from different modalities, the above methods have to overcome different limitations: good initial guess for ICP methods; matching geometric features from different modalities is a hard problem for LGF methods; LDS methods are limited to cases presenting large plane patches; while SBM are challenged for determining 3D rotations when only partially overlapping data are available.

The present contribution proposes a robust technique for determining 3D rotations for noisy and partially overlapping data. As for SBMs, two given point clouds are first voxelized and the 3D Fourier transforms of both resulting images are computed. Rotation is then decoupled from translation by taking the moduli of the Fourier transforms (the equivalent of a translation in the physical space is a phase shift in the Fourier space). Contrary to SBMs which attempt to determine a global maximum in the 3D correlation image, it is proposed here to only select in both 3D moduli images voxel positions which values are high (typically the highest 1% amongst all voxel values). Selected voxel positions are further condensed using the K-means clustering algorithm. The two sets of centroids extracted from the K-means clustering are then rotated by sampling the 3D rotation space. The rotation minimizing the root mean square distance between the two sets of centroids is kept and translation is determined as in SBMs after the selected rotation has been factored out. The proposed technique has been successfully tested on two different optic modalities (camera and laser scanners) and was successfully able to register noisy, partially overlapping, theoretical and experimental point cloud data.

[1] Bulow, Int. J. Computer Vision, 126(7), 731-750

A web-based scan-planning tool for beam-hardening minimisation in X-ray computed tomography using gVirtualXRay

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October 15, 2026, 14:35 - 15:05

Beam hardening is an intrinsic consequence of polychromatic X-ray imaging: low-energy photons are preferentially attenuated, the mean beam energy rises with path length, and reconstructions develop cupping and streak artefacts that are most severe in multi-material samples. The conventional response is corrective and post-acquisition: linearisation, filtering, iterative and dual-energy schemes applied once the data are already acquired, treating beam hardening as something to repair rather than to avoid.

We have previously introduced and experimentally validated the Beam Hardening Predictive Index (BHPI), a pre-acquisition scalar metric that ranks candidate X-ray spectra by the beam-hardening severity they will produce. BHPI-guided spectra reduced artefacts and improved intensity uniformity without degrading noise performance. Because BHPI requires no full reconstruction for each candidate, a large space of tube-voltage and filtration combinations can be screened before scanning.

Here we present the delivery of this validated metric as a web-based scan-planning tool, offered as a software demonstration to the IBSim-4i and gVXR communities. The tool wraps a gVirtualXRay (gVXR) simulation backend behind a browser interface built using Trame, Kitware's reactive Python framework for VTK-based visualisation and deployment across desktop, client-server and cloud environments. The user uploads a two-dimensional segmented image of the specimen, specifies material zones interactively, and selects the digital twin of the imaging system. The tool then evaluates combinations of tube voltage and filtration and returns candidate spectra ranked on a BHPI-peak signal-to-noise ratio (PSNR) performance landscape, with photon starvation and under- or over-exposure automatically excluded. Results are presented through embedded Pareto-front and parallel-coordinate views, alongside reconstructions produced with the Core Imaging Library (CIL), allowing the user to move from specimen description to assessment of candidate acquisition conditions within a single interface.

By exposing BHPI-based planning through a browser, the tool removes the local simulation, installation and scripting barriers that have kept the metric away from operators who choose scan settings. It shifts beam-hardening mitigation from reactive, post-acquisition correction to a proactive choice made before scanning, making image-quality-aware planning usable at the point of decision.

We will describe the architecture and planning workflow, demonstrate the interface, and report on initial deployment. Ongoing work is expanding support to a wider range of imaging systems and moving the tool towards everyday use in scan planning.

Keywords: beam hardening, BHPI, computed tomography, scan planning, web-based software, gVirtualXRay

An image-based DVC-driven finite element simulation framework for multiscale analysis of fibre-reinforced composites

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¹Ku Leuven, ²3Dmagination

October 14, 2026, 13:30 - 14:00

The accurate prediction of deformation and failure mechanisms in fibre-reinforced composites requires access to both experimentally measured kinematics and mechanically consistent stress and strain fields across multiple length scales. While the combination of X-ray Computed Tomography (XCT) and Digital Volume Correlation (DVC) enables full-field three-dimensional measurements of internal displacements and strains [1, 2], direct quantification of stress distributions and load-transfer mechanisms remains inaccessible from experimental observations alone. Establishing a robust link between measured deformation and the underlying mechanical fields governing damage initiation and propagation therefore remains a key challenge in composite mechanics.

This work presents an image-based DVC-driven finite element (FE) framework that reconstructs mechanically consistent stress and strain fields directly from experimentally measured XCT-DVC displacement data. The methodology integrates in situ XCT testing, global DVC measurements, voxel-conformal image-based FE mesh generation, and direct application of experimentally measured displacement fields as boundary conditions within a unified experimental–computational workflow. By preserving the geometry and material architecture captured in the XCT images, the framework translates volumetric experimental observations into mechanically meaningful simulations.

The methodology is demonstrated on three composite configurations spanning multiple length scales and loading conditions: a uniaxially loaded glass–epoxy cross-ply laminate, a biaxially loaded angle-ply glass–epoxy laminate imaged at the microscale, and a single-glass-fibre epoxy specimen investigated at the nanoscale. For all configurations, the FE simulations reproduced the measured DVC kinematics with high fidelity, yielding low displacement residuals throughout the loading sequence. The reconstructed mechanical fields revealed localisation phenomena associated with ply interactions, interlaminar deformation, gauge-corner failure, and fibre–matrix stress transfer.

Comparison with XCT observations and DVC residual analyses demonstrated a strong spatial correspondence between simulated stress concentrations and experimentally observed damage initiation regions. Importantly, the results show that DVC-derived boundary conditions are essential for reproducing the actual loading state, including experimental imperfections, load asymmetries, and local deformation heterogeneities that are not captured by idealised boundary conditions.

The proposed XCT–DVC–FE framework provides a direct pathway from volumetric imaging data to full-field stress and strain distributions, enabling multiscale damage assessment, model validation, constitutive law calibration, and predictive image-based modelling of composite materials under complex loading conditions.

[1] S. E. Madi et al., *Composites Part B: Engineering*, p. 112815, 2025.

[2] S. E. Madi et al., *Composites Part B: Engineering*, p. 113744, 2026.

Coupling image-based simulation with NDT experiments in RT and UT laboratory courses at INSA Lyon

Jean Letang

October 16, 2026, 10:20 - 10:50

Non-destructive testing (NDT) is a core competency for mechanical and materials engineers, yet laboratory courses are often constrained by safety, cost, and the limited variety of defects and geometries that physical specimens can offer. Image-based simulation offers a complementary pathway: by generating virtual inspection images from well-defined physics, it allows students to explore the domain of validity of each NDT technique systematically. This contribution presents an integrated laboratory course in which image-based simulation (jupyter notebooks) is coupled with hands-on Radiographic Testing (RT) and Ultrasonic Testing (UT) experiments, delivered to students of the Mechanical Engineering and Materials Science & Engineering programmes at INSA Lyon (France). For RT, the Monte Carlo code GATE (based on Geant4) first serves as a high-level physics reference for better understanding the photon transportation and interactions. More specifically, Compton scattering is studied on simple PE step-wedges to understand the air-gap technique in the reduction of the scattering contribution. The course then focuses on gVirtualXRay (gVXR), a deterministic ray-casting tool using tabulated linear attenuation coefficient databases to rapidly predict radiographs and CT reconstructions of 3D specimens. Through gVXR simulations, students can investigate the detection sensitivity to the crack orientation and systematically visualize artefacts such as beam hardening and photon starvation. By toggling monoenergetic vs. polychromatic beams and varying the photons statistics, students gain a mechanistic understanding of why these artefacts occur and how they degrade quantitative CT measurements—insights that are difficult to disentangle in a single physical experiment where multiple factors co-vary.

For UT, SimSonic—a finite-difference time-domain (FDTD) solver of the elastodynamic equations—is employed primarily to visualize wave propagation and mode conversion. Students compare SimSonic-generated pulse-echo traces with measured A-scans to understand how incident longitudinal waves convert to shear/transverse modes (and vice versa) at interfaces, defects, and geometric discontinuities. This mode-conversion analysis explains characteristic features observed in experimental A-scans (arrival times, amplitude variations, echo splitting).

In the course, students first study via simulations the expected output images and scans, then perform the corresponding NDT measurements and compare quantitatively (image and signal characteristics). This loop anchors discussions on the limitations and complementarity of each NDT technique. Teaching experience shows that this simulation–experiment coupling is significantly more engaging than isolated approaches, and crucially provides students with a concrete, mechanistic grasp of the domain of validity and applicability of NDT techniques, particularly regarding 3D CT artefact origins and ultrasonic wave-mode interpretation.

DVC in action: mapping deformation across multiple scales from batteries to violins

Kamel Madi

October 14, 2026, 14:30 - 15:00

Digital Volume Correlation (DVC) is a powerful technique for measuring three-dimensional, full-field displacement and strain maps at the continuum scale from volume images acquired during the deformation of materials. Designing a DVC experiment, however, requires a systematic approach and a careful balance between multiple experimental and computational parameters. With the addition of the fourth dimension (time) data processing and visualization become increasingly important for extracting the mechanical information hidden within large and complex 4D datasets.

This talk will provide an overview of the critical parameters governing DVC measurements and present an optimized workflow for their implementation in a DVC software. A range of challenging academic and industrial applications will be used to illustrate the capabilities of the approach across different length scales and levels of complexity, including core collapse in Li-ion batteries, assessment of the structural integrity of Niccolò Paganini's famous violin, damage of composites and the manufacturing of high-zirconia ceramics for glass furnaces.

Particular emphasis will be placed on visualization and data-reduction strategies that transform large 4D datasets into actionable mechanical insights. Finally, the integration of DVC measurements with numerical simulations will be discussed, highlighting how experimental data can be used to validate simulations, calibrate and improve numerical models.

Experimental method for rubber deformation analysis using in situ X-ray tomography and digital volume correlation with FEM validation

Jérôme ADRIEN¹, Joël LACHAMBRE¹, Aurélien SIBELLAS¹, Justine PAPILLON¹, Rémi BRUANT², Gaetan MAUREL², Eric MAIRE¹

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October 14, 2026, 14:00 - 14:30

The grip and rolling resistance of car wheel tires on a road surface are strongly influenced by the mechanical properties of the rubber and especially by the deformation of this rubber during indentation by the road asperities. The phenomena involved are difficult to observe using conventional techniques such as optical microscopy, due to the opaque nature of the elements concerned. The aim of this work was to develop a new methodology to measure the deformations, in the bulk, of a rubber exposed to indentation-type stresses.

To this purpose, advanced techniques such as X-ray computed tomography (XRCT) combined with Digital Volume Correlation (DVC) were used. The ability of XRCT to provide directly and non destructively three dimensional (3D) images of various materials makes it a valuable tool to study quantitatively the deformation mechanisms during in situ loading. However, some constraints must be taken into account before accurate measurements can be made.

The main difficulties are linked to the attenuation of the materials used (i.e. high attenuation for the soil and much lower for the rubber), the large deformations to be achieved, and the complexity of a road surface. In addition, DVC requires the presence of a speckle in the material's microstructure. In order to validate our approach, an in-situ indentation test using a low X-ray absorbent plastic ball was first conducted to evaluate the performance of DVC algorithm. Analytical rubber samples, specifically produced for this study, made of a SBR type rubber (Styrene Butadiene Rubber) and representative of a tread of a commercial passenger vehicle tire were used. Silica large particles were added to serve as markers and reinforcement of the rubber. The experimental results were compared with numerical simulations in Abaqus.

The results of these analyses will be presented first. Next, research carried out in order to better reproduce the real conditions of contact between the rubber of a passenger car tire and the road will also be discussed.

From Atomic Force Microscopy Maps to Macroscopic Mechanical Properties: An Image-Based Prediction of Tomato Fruit Cuticles Stiffness

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October 14, 2026, 16:00 - 16:30

Tomato fruit cuticles represent a thin multifunctional biocomposite that constitutes the fruit primary protective barrier against water loss, mechanical damage and fruit cracking. Ensuring a mechanical resistance is essential for maintaining fruit integrity throughout development, harvest, transport and storage, making the mechanical properties of tomato fruit cuticles an important determinant of fruit quality and post-harvest performance. Recent experimental studies [1] have shown that the cuticles have local mechanical heterogeneity, which can be revealed by Atomic Force Microscopy (AFM) through high-resolution maps of the local Young's modulus. Understanding the relationship between the heterogeneous microstructure of the cuticle and its macroscopic mechanical response is therefore of major interest for breeding programs, quality assessment, and the development of more resilient crop varieties.

In this study an image-based computational methodology is applied for the prediction of the effective elastic stiffness of tomato fruit cuticles directly from AFM modulus maps. Heterogeneous modulus maps are converted into numerical domains in which each pixel is assigned its experimentally measured local elastic modulus. To replace the conventional mechanical testing, the numerical framework consists in solving a set of independent numerical problems on each specimen under appropriate boundary conditions. By applying the full-field homogenisation method to the resulting stress-strain responses the full equivalent elasticity tensor of a cuticle sample is subsequently determined.

The predicted effective stiffness is compared to the experimental measurements obtained from Dynamic Mechanical Analysis (DMA) tests performed in the small-strain elastic regime. This comparison assesses the capability of the proposed numerical methodology to reproduce the macroscopic behaviour from local mechanical measurements alone.

We propose a numerical approach that enables the mechanical properties of tissue to be estimated from AFM maps. This approach can provide macroscopic values for samples that are fragile or small and, therefore, difficult to handle in DMA or tensile tests. Furthermore, the image-based numerical framework provides a better understanding of how local mechanical heterogeneity contributes to the overall response, thereby offering insights that cannot be obtained solely through mechanical testing of the material as a whole.

[1] Reynoud, N., Geneix, N., D'Orlando, A., Petit, J., Mathurin, J., Deniset-Besseau, A., Marion, D., Rothan, C., Lahaye, M. and Bakan, B. (2023), Cuticle architecture and mechanical properties: a functional relationship delineated through correlated multimodal imaging. *New Phytologist*, 238: 2033-2046.

From X-Rays to Digital Twins: Giving Fusion Power Plants a Nervous System

Lee Margetts

October 14, 2026, 10:15 - 11:00

For centuries, engineers have built machines that are powerful, precise and transformative. Yet even the most advanced machines remain fundamentally passive. They do not truly understand their condition, anticipate their future, or learn from their experience. The next revolution in engineering is changing that.

Advances in imaging, sensing, simulation, high-performance computing and artificial intelligence are converging to create something entirely new: digital systems that can continuously observe, understand and predict the behaviour of complex physical assets. Technologies that once revealed hidden structures through X-rays and laser scanning are now part of a broader vision in which data is transformed into insight, and insight into action.

Fusion energy presents one of the greatest opportunities to realise this vision. Future fusion power plants will be among the most complex machines humanity has ever built. Their success will depend not only on breakthroughs in physics and materials science, but also on the creation of a digital nervous system: a living digital counterpart that continuously senses, learns and anticipates. The future of fusion is not simply about building a star on Earth. It is about giving that star the ability to understand itself.

Fusion is more than an energy challenge. It is a proving ground for a new generation of intelligent engineering systems capable of accelerating discovery, reducing uncertainty and transforming how complex technologies are designed, operated and maintained. If the twentieth century was defined by machines that amplified human strength, the twenty-first may be defined by machines that amplify human understanding.

This talk explores how the convergence of imaging, computation, digital twins and AI is reshaping engineering, and why fusion energy provides a unique opportunity to lead that transformation. The challenge now is not merely to build better reactors, but to create the digital intelligence that will enable them to evolve, adapt and improve. In doing so, we have the opportunity not only to accelerate the path to clean, abundant energy, but also to redefine the relationship between humans, machines and the engineered world.

gVXR based optimisation algorithm for 3D defect positioning in in-line inspection

Vincent Libertiaux

Sponsor Talk: X-Ris, October 14, 2026, 16:30 - 16:45

Industrial X-ray radiography is increasingly required not only to detect defects in manufactured components, but also to localize them accurately in three-dimensional (3D) space. This need is particularly relevant to high-throughput production lines, where inspection systems must combine spatial accuracy with stringent constraints on acquisition and processing time. Conventional tomosynthesis, which relies on acquiring multiple projections over a limited angular range to reconstruct volumetric information, can be too slow for such applications.

We present an algorithm developed at X-RIS for 3D localization of volumetric defects using only two or three radiographic views, substantially fewer than those required by classical tomosynthesis. The method consists of two sequential optimization stages. First, the position and orientation of the part's CAD model are optimized in 3D so that its simulated projections match the acquired radiographs, thereby registering the CAD frame to the measured data. Second, a defect identified manually or automatically in each 2D projection is localized in 3D by optimizing its position and radius within the registered CAD frame.

Both optimization stages rely on the same underlying principle: measured radiographic projections are compared with projections simulated using gVXR, incorporating the known source and detector geometry of the acquisition system while accounting for small measurement uncertainties. This simulation-based approach enables geometric registration and defect localization without requiring a full tomographic reconstruction. The approach is particularly attractive when defect geometry can be reasonably parameterized and projection annotations are available from automated image analysis. Applied to test parts containing defects with known geometry, the proposed algorithm localizes defect position and radius with errors on the order of the detector pixel size. These results demonstrate that accurate 3D defect localization can be achieved from only a small number of radiographic views, providing a substantial reduction in acquisition time and computational cost compared with full tomosynthesis, while maintaining spatial accuracy suitable for industrial quality control.

The proposed approach therefore offers a promising route toward fast, in-line 3D defect localization in high-volume manufacturing environments, where conventional tomographic or tomosynthetic reconstruction is impractical. Ongoing work focuses on extending the method to more complex defect geometries and evaluating its robustness across a broader range of industrial components and acquisition conditions.

Learning composite microstructures: AI for XCT imaging, generation, and evolution

Mahoor Mehdikhani

October 14, 2026, 15:30 - 16:00

Fibre-reinforced composites derive their exceptional mechanical performance from complex microscale architectures, where fibre arrangement, orientation, spacing, defects, and their evolution under load strongly influence macroscopic behaviour. X-ray computed tomography (XCT), particularly synchrotron XCT, provides unique 3D access to these features and their evolution during mechanical testing. However, converting large, high-dimensional XCT datasets into quantitative information and predictive models remains a major challenge. This presentation explores how artificial intelligence (AI) can transform XCT data from images into a basis for quantitative characterisation, microstructure generation, and prediction of microstructural evolution.

The first part focuses on AI-based image segmentation, a critical step in image-based modelling workflows. Different machine-learning and deep-learning approaches are compared for detecting and separating individual fibres in images of fibre-reinforced composites. Building on these observations, interactive deep-learning approaches such as RootPainter, alongside automated instance-segmentation methods, are investigated across XCT and microscopy datasets. The results show that different methods can provide remarkably consistent fibre statistics for well-resolved microstructures, while revealing important challenges for fibres with diameters near the imaging resolution.

The second part addresses AI-based enhancement and generation of composite microstructures. Generative models are explored to learn the statistical characteristics of realistic fibre architectures directly from experimental XCT data. In particular, generative adversarial networks (GANs) and diffusion-based approaches are used to generate physically plausible microstructures while preserving key features such as fibre size, spatial arrangement, and periodicity. Latent spaces provide a route to continuously explore and interpolate between realistic microstructures, opening possibilities for data-driven microstructure design and virtual material generation.

Finally, we explore whether generative models can go beyond reproducing static microstructures and learn their evolution under mechanical loading. A 3D conditional GAN with a U-Net-based generator is trained on XCT time-series data to predict higher-load microstructures from lower-load states. The model successfully reproduces experimentally observed deformation patterns, preserving the overall fibre-bundle morphology while capturing subtle fibre movements during tensile loading.

Together, these studies illustrate a pathway from XCT images to AI-based characterisation, to microstructure generation, and to prediction of microstructural evolution, highlighting both the opportunities and current limitations of AI for image-based modelling of composite materials.

Microstructure Resolved 3D Framework for Modelling Lithium-Sulfur Batteries: Role of multispecies transport in solid phase

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¹University College London

October 14, 2026, 11:30 - 12:00

Lithium-sulfur (Li-S) batteries offer high theoretical energy density but exhibit complex interactions between species transport, electrochemical reactions, and phase evolution that are difficult to capture using conventional continuum-scale models. This work extends an image-based microstructure-resolved three-dimensional finite element modelling (3D FEM) framework (Dai et al., 2022) by incorporating distributed porous-electrode reactions, multispecies ionic transport, sulfur dissolution, and polysulfide precipitation within realistic Li-S cathode microstructures. Ionic transport is described using the Nernst-Planck formulation, while Butler-Volmer kinetics are employed to model electrochemical reactions. The framework also captures local changes in porosity and volume fraction arising from phase transformations during discharge. The model provides spatio-temporal distributions of lithium ions, polysulfides, local current density, and reaction activity within inherently non-homogeneous cathode architectures. Simulations were conducted to investigate the influence of discharge rate, sulfur loading, transport tortuosity, and spatially varying diffusion coefficients on sulfur utilisation and cell performance. Results qualitatively reproduce characteristic Li-S discharge behaviour and reveal the importance of transport limitations in governing lithium depletion, sulfur dissolution, and polysulfide redistribution. Reduced ionic transport within the carbon host leads to lower operating voltage and accessible capacity, while spatial variations in sulfur-species distributions give rise to heterogeneous local reaction behaviour that is not evident from volume-averaged electrochemical metrics alone. A comparison between the expanded porous-electrode framework and the original image-based model is presented to quantify improvements in predictive capability and to assess the associated computational cost. The developed framework provides a versatile tool for investigating microstructure-performance relationships and guiding the optimisation of next-generation Li-S cathode architectures.

X. Dai et al., An Image Based 3D Modelling Framework for Li-S Batteries, ChemRxiv
10.26434/chemrxiv-2022-ektc5-v2 (2022)

Microstructure-Resolved 3D Modelling Framework for Lithium-Sulfur Cathodes

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October 14, 2026, 11:00 - 11:30

Lithium-Sulfur (LiS) batteries represent one of the most promising next-generation candidates, particularly in the aerospace and heavier electric vehicles industries [1], due to their high theoretical capacity, small weight, low cost, sustainability, compared to the current Li-ion technology, thereby advancing the battery development worldwide [2, 3]. 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 battery's macroscale performance. To date, conventional modelling of LiS cathodes has typically relied on a simplified volume-averaged treatment, thus overlooking the influence of the underlying cathode microarchitecture and its properties on the performance of the electrode.

Here, we report [4] an electrochemical finite-element model based on 3D X-ray CT images with sub-micron resolution to describe the spatio-temporal dynamics of discharge in liquid-electrolyte LiS cathodes. Crucially, the model illuminates the dynamics of localization of lithium, polysulfides, precipitation during discharge, and current magnitude, 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 homogenised 1D model. We also elucidate the role of solid-phase porosity, and comment on how the model can be adapted to other classes of conversion batteries (e.g. KS, Zn-air).

Next, we compare the discharge performance of three morphology types--- commercial spherical carbon, electrospun (fibrous), and computer-generated interdigitated 3D microstructures --- with inherently different intrinsic properties (porosity, tortuosity, particle shape, solid-phase surface area), and show how these properties yield different discharge performance. We demonstrate how structural bottlenecks result in localised high-current densities, uneven reaction rates, and preferential Li₂S deposition, leading to potential hotspots and uneven heating potentially causing defects and uneven battery aging. Thus, our modelling framework allows to formulate mitigation strategies and design guidelines to increase the longevity, capacity, and energy density of LiS batteries.

The proposed modelling framework should pave the way towards realistic modelling, optimisation and rational design of manufacturable LiS cathodes to meet the ever-growing industrial energy-storage demand.

References:

1. J.B.Robinson et al., 2021 roadmap on lithium-sulfur batteries, DOI:10.1088/2515-7655/abdb9a
2. UK Battery Strategy 2030, Department for Business & Trade, UK
3. BATTERY 2030+ Roadmap (EU) <https://battery2030.eu/research/roadmap/>
4. X.Dai et al., An Image Based 3D Modelling Framework for Li-S Batteries, ChemRxiv, DOI:10.26434/chemrxiv-2022-2ktc5 (2026)

Mono-material beam hardening correction workflow using gVXR and CIL

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¹STFC

October 16, 2026, 13:20 - 13:50

During X-ray Computed Tomography (XCT) with polychromatic sources, the phenomenon of beam hardening manifests itself as cupping and streaking artefacts in reconstructions, which mask important features in samples and impact dimensional accuracy. While industrial X-ray scanners are accompanied by commercial software with built-in correction methods, custom scanners and synchrotrons need to make use of physical filtration or bespoke software solutions to mitigate these artefacts. We demonstrate a workflow in development that combines two open-source libraries - an X-ray simulation package, gVirtualXray (gVXR), and a CT reconstruction package, the Core Imaging Library (CIL) - to perform physically realistic simulations to correct beam-hardening artefacts in experimental data.

We propose using gVXR to simulate the results of scanning a calibration step wedge made of a similar material to the studied mono-material sample. The scan geometries and source spectral information are used to model the experimental set-up as closely as possible. Comparing the simulation results from polychromatic and monochromatic sources with equivalent energies allows for the fitting of a polynomial correction model which can be used to correct for beam hardening in the sinogram for future datasets on the same scanner with the use of a data processor in CIL.

Tests carried out on simulated phantoms and experimental data indicate a significant reduction in beam hardening related artefacts. Qualitative assessments indicate an improvement in the homogeneity of the corrected reconstructions and reduction of streaks that were present in the uncorrected reconstructions. Quantitative analysis performed on mono-material samples also indicates a general reduction in the standard deviation in homogeneous regions, further validating the qualitative results.

The modularity of this method allows for corrections via partial experimental calibration or from fully simulated systems. While the method is currently limited to mono-material correction, this workflow acts as a foundation for introducing more general multi-material beam hardening correction strategies into gVXR and CIL and incorporating it with gVXR's digital twin functionality to create experiment-ready correction methods.

PHYSICS-BASED SYNTHETIC X-RAY IMAGE GENERATION FOR IMPROVING DEEP LEARNING IN MEDICAL IMAGING

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¹Scalian

October 16, 2026, 09:50 - 10:20

The use of deep learning models has become increasingly common in medical image analysis, yet their performance is often constrained by the size, quality, and diversity of available training datasets. To address these challenges, we developed a physics-based simulation framework capable of generating large-scale, fully annotated synthetic X-ray datasets with controllable anatomical and pathological variability.

By combining the X-ray imaging simulator gVXR [1] with virtual anthropomorphic models [2], we produced realistic radiographic projections. This framework was validated in two use cases: coronary stenosis detection using synthetic coronary angiography and pulmonary nodule detection in chest X-ray and CT imaging.

The pipeline enables precise control over anatomical structures, pathological features, and acquisition parameters, while incorporating organ deformation. For coronary angiography, we generated stenosis of adjustable severity and location. For chest radiography, we introduced synthetic nodules with controlled size, density, and location. After simulation, post-processing was applied to simulate realistic imaging conditions. This approach enabled the creation of fully annotated datasets of 5,000–10,000 images, covering a wide range of clinical scenarios. Object detection models, including YOLOv8, NoduleNet, RetinaNet, and Transformer-based DINO-DETR, were trained on real, synthetic, and mixed (real + synthetic) datasets to evaluate performance.

Models trained on mixed datasets achieved better performance across tasks. DINO-DETR trained on synthetic coronary angiograms demonstrated F1 gains up to 15% and mAP improvements up to 19%. For pulmonary imaging, on 2D-Xray, YOLOv8 demonstrated the most significant performance improvement, with sensitivity increasing up to 19% and mAP increasing up to 7%. Additionally, we observed improvement in the generalization capabilities of a Retina-net model fine-tuned on synthetic data, particularly in terms of sensitivity (+14%) and mAP (+19%).

These results demonstrate that physics-based synthetic image generation provides a fast, cost-effective, and realistic solution to overcome real-world data limitations. By providing control over pathology, anatomy, and imaging parameters, this method enhances model performance, and generalization. Future work will focus on applying this framework to additional pathologies and assessing its effectiveness in real clinical settings.

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Simulating X-ray Computed Tomography: Developing a Virtual Representation and Generating Synthetic Training Data for Deep Learning

Kajsa Fahlgren

October 15, 2026, 14:05 - 14:35

What if time-consuming X-ray scans could be replaced with realistic simulations? This thesis shows how virtual imaging can replicate such scans and generate synthetic data to train machine learning models to segment complex materials accurately.

X-ray computed tomography (XCT) is an imaging technique that allows one to see inside objects without cutting them open. It is widely used in medicine, but also plays a large role in industry. It is, for example, used as a tool by Tetra Pak to analyse the internal structure of paper packaging materials. This is however a very time consuming process and analysing the large volumes that are produced can be very challenging. This thesis explores how to overcome these limitations in two separate objectives.

First, a virtual XCT scanner was developed with the goal of being capable of mimicking the behaviour of a real scanner. By adjusting simulation parameters based on real settings and sample information, the virtual scanner was able to produce data which closely matched real experimental data. This showed that simulation can be used to test scanning settings, saving time by reducing the need for repeated physical experiments. The current model is however limited to specific scanning conditions and further work is needed to make it more generally applicable.

The second part focused on applying the virtual scanner to generate artificial XCT images of fibres. The main advantage of this is that the artificial data includes the exact location of the fibres, which is very difficult and time consuming to find manually in real data. Using this data, machine learning models were trained to automatically identify fibres in real XCT images with great success. This showed that even though the models had been trained on artificial data, they could perform well when applied to real data.

Task-Driven Optimization of Dual-Layer Spectral CT Acquisition Using gVXR for Quantitative Material Decomposition

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October 16, 2026, 11:20 - 11:50

Spectral computed tomography (CT) enables quantitative material discrimination by exploiting energy-dependent X-ray attenuation. However, material-decomposition performance depends strongly on the acquisition configuration, including the source spectrum, filtration, detector spectral response, photon statistics, and attenuation introduced by the scanned object. Consequently, acquisition parameters optimized for conventional image quality may not provide the most informative measurements for a specific material-decomposition task. This work investigates the use of gVirtualXRay (gVXR) as an in-the-loop digital twin for task-driven optimization of dual-layer spectral CT acquisition.

The study builds on our previously developed gVXR-based CT simulation and Core Imaging Library (CIL) reconstruction pipeline for the Lungman anthropomorphic phantom, for which simulated and reference CT volumes showed a zero-mean normalized cross-correlation exceeding 98%. gVXR supports polychromatic spectra, scintillator properties, detector response, photon statistics, and spectral imaging, providing a suitable framework for systematic exploration of spectral acquisition configurations.

In the proposed framework, a dual-layer spectral CT acquisition is parameterized by variables including tube potential, beam filtration, detector-layer spectral response, and photon allocation. For each candidate configuration, gVXR generates paired spectral projections from digital phantoms with known material composition. Material coefficients are subsequently estimated using a fixed polychromatic decomposition model. Rather than optimizing conventional image-quality metrics alone, the acquisition parameters are updated according to a material-specific objective combining decomposition error, cross-material leakage, and noise sensitivity under a constrained photon budget. Controlled two-material phantoms are first used to characterize the optimization landscape, followed by evaluation using the anatomically realistic Lungman phantom to study the effect of object-dependent attenuation on the optimal spectral configuration.

This establishes a closed-loop workflow of simulation, decomposition, task evaluation, and acquisition update, extending gVXR from a synthetic-data generator to a tool for quantitative spectral CT protocol design. The framework provides a basis for future anatomy-adaptive acquisition and joint optimization of spectral imaging and learning-based material decomposition.

Topologically correct *C. elegans* model for deep learning-based reconstruction of limited-angle tomography images

Brun Anna-louise

October 16, 2026, 11:50 - 12:20

Micro-tomography techniques using synchrotron X-rays or proton microbeams give access to three-dimensional (3D) imaging of microscopic structures. For biological applications, the distribution of mass density and/or elemental composition can be achieved at cellular and subcellular scales.

Because these techniques are inherently quantitative, accurate reconstruction is essential for reliable biological interpretation. In practice, most biological samples are deposited on 2D supports. This configuration makes tomographic acquisition severely constrained experimentally, because the sample's support limits the tilt angle. However, at least 180° of angular coverage is theoretically required for complete reconstruction. So, this "missing wedge" in the sinogram leads to symmetric information loss and significant reconstruction artifacts.

Classical approaches to retrieve the missing information, such as interpolation and exemplar-based inpainting are insufficient, and compromise quantitative accuracy. At the same time, the scarcity of experimental data limits the applicability of deep learning methods. However, recent progress in artificial intelligence, particularly context-based autoencoders and diffusion models, has shown promise for limited-angle tomography and sinogram completion, notably in the Helsinki Tomography Challenge [1] with U-Net architectures incorporating rotational priors.

These promising attempts lead us to address the lack of experimental training data, by building a complete synthetic data-generation pipeline based on a mesh phantom of the biological specimen of our interest – *Caenorhabditis elegans* – widely used for diverse applications in genetics. First, we developed a topologically consistent, watertight 3D model derived from the VirtualWorm project [2], and assigned realistic physical properties measured at LP2IB. A custom Free Form Deformation (FFD [3]) framework, driven by an anatomically informed lattice along the organism's medial axis, generates diverse and anatomically valid deformed instances. These deformations were parameterized according to the study of realistic poses of *C. elegans* [4]. Imaging acquisitions were then simulated using the gVirtualXray (gVXR) library [5, 6], producing sinograms under the same limited-angle constraints as the experimental setup. Using this pipeline, we generated a dataset of ~ 4.2 million sinograms with paired ground-truth. Building on our dataset, we investigated deep learning-based approaches for missing-wedge sinogram reconstruction. The pipeline was here developed for proton micro-tomography applications, but it can be adapted to other source types and/or samples, to address for example limited angles or sparse-view industrial CT.

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X-ray Image Generation for Robotic Radiography: a Case Study on Motion Blur in Drone-Based Infrastructure Inspections

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Robotic X-ray imaging systems enable autonomous inspection of the internal integrity of critical infrastructure. However, these systems often suffer from vibrations and unwanted movements that cause motion blur in the resulting radiographs. The impact of this motion blur is often unknown until the first prototype is available and even then requires extensive experimental testing to assess. In addition, tests involving radiation are time-consuming, demand specialized equipment, and pose inherent safety risks. In our work, we propose using X-ray simulation as a tool to complement and replace real images during the development of robotic inspection systems. Our method extends an existing X-ray simulation framework (gVirtualXray) to generate motion-blurred images from any type of motion. We validate the method against an experiment in which an X-ray source and detector were mounted on motion platforms, producing motion-blurred images alongside the motion data that caused the blur. The comparison shows that our method effectively captures the motion-blur effects. The approach is applicable to various robotic systems and we demonstrate its use for a decoupled two-drone system applied to the inspection of critical infrastructure such as wind turbine blades and power lines. This is one of the most demanding applications due to the high degree of freedom of the system components and relatively long exposure times. By coupling the X-ray simulator directly to a robotic simulator, we gain direct feedback on how our system design and control algorithms affect image quality. This coupling offers several benefits. First, it reveals the motion blur sensitivity of the design, helping to pinpoint the degrees of freedom that most affect image quality. Second, it has been key to developing pose-informed deblurring methods, in which robot motion data guides the reconstruction of a sharp image from a blurry one. In this, the simulator serves both as a validation tool for our models and as a source of training and test data. Finally, by mimicking our real X-ray devices, we are working on a tool to predict in advance which settings an inspection will require, or whether inspecting a specific object is even feasible at all.

Posters

Mechanical characterization of hazelnut shell through Finite Element Model Updating

Gardien Guillaume

Each year, around 1 million tons of hazelnuts are produced worldwide. Most of them are industrially shelled. In doing so, a significant number of kernels are broken and lose value. The kernel is indeed affected by the compression of the shell induced by the shelling process. Thus, the mechanical response of the hazelnut shell to uniaxial compression has been studied by several authors [2] [3]. The mechanical response to uniaxial compression of different varieties of hazelnut has been investigated with various environmental and loading parameters such as shell orientation, loading speed, and moisture content. However, although micrographic observations have established the heterogeneous, anisotropic, and cellular nature of hazelnut shell [1], its mechanical properties at the mesoscopic scale remain poorly characterized; the mesoscopic scale being the intermediate scale between the scale of the cells and the scale of the shell thickness. A better understanding of hazelnut mesoscopic mechanical properties will allow the prediction of mechanical response of hazelnut shell under complex solicitations, and lead to an improvement of shelling technologies.

Consequently, the objective of the study is to characterize the mechanical properties of the constitutive material of hazelnut shell in three directions, with various moisture contents and deformation speeds. Lamellas extracted from hazelnut shell in three different directions will be subjected to three-point bending. Force and displacement field will be measured using a load cell and digital image correlation. The data will be processed using the Finite Element Model Updating (FEMU) method. The effect of moisture content and deformation speed will be observed by performing a two-factors campaign of experiments. Two distinct experimental setups are considered: a 2D setup using a camera where only surface displacement field can be computed, and a 3D setup using a micro-CT scanner where internal displacement field can be computed. Those setups are complementary and both needed: on the one hand, the samples exhibit a complex internal geometry, notably including vascular channels, which may significantly influence the internal displacement field; a 3D setup is therefore required to capture these effects. On the other hand, micro-CT imaging does not allow dynamic testing, making the 2D setup necessary to investigate the influence of deformation rate. Regardless of the setup, the geometries used in the numerical models will come from micro tomography and will feature the internal channels.

Multiphysics Modelling of Solid-State Batteries: Effect of Cathode Particle Geometry

Ran An

The solid-state battery (SSB) is a popular research topic. However, after repeated cycling, the performance of the battery tends to degrade due to the loss of close contact between the active material (AM) particles and solid electrolyte (SE) within the cathode [1], changes in the material properties inside the battery in response to temperature fluctuations, and some other issues.

This research focuses on the cathode, examining how the temperature variations and crack will influence the battery performance, as well as which factors influence heat generation during the cycling. After multiple cycles, the reduction in the contact interface between the AM particles and the SE in the cathode leads to an increase the internal resistance and a decrease in capacity of the battery [2]. Furthermore, the reduced contact area results in the formation of more hotspots [2, 3]. At the same time, geometry differences and spatial distribution of the AM particles also give rise to varying hotspots [4, 5]. These hotspots further intensify the heat generation associated with electrochemical reactions, finally these heats affect the battery materials, causing changes in their properties [4, 5].

The objective of this study is to comprehend how the influence of different microstructures within the cathode of lithium-ion SSBs on battery performance following multiple cycles, with a particular emphasis on microstructural changes and the formation of hotspots during this process. In this study, multi-physics modelling of lithium-ion SSBs will be carried out. The model under consideration encompasses three distinct physics: solid mechanics, electrochemistry, and thermal dynamic. Through the integration of these three physical fields, it is possible to observe intuitively the effects caused by the different shapes and spatial distributions of particles, thereby providing guidance for the optimisation of SSB design.

Synthetic 3D Fibre Generation Using a Direction Classifier and Local Orientation Priors

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Realistic 3D fibre reinforced polymer (FRP) digital phantoms are essential for developing, testing, and validating X-ray imaging and reconstruction algorithms, particularly when experimentally measured ground truth is unavailable. However, generating FRP digital volumes that reproduce the structural complexity of real materials remains challenging. Existing approaches often rely on analytically defined growth rules, resulting in predictable trajectories that do not capture realistic local variation. This limitation raises a central question: can locally learned fibre movement, combined with spatially varying orientation information from real data, yield more realistic synthetic volumes than rule-based methods, without a fully generative model?

This work proposes a hybrid data-driven framework for synthesizing more realistic fibre structures by combining a neural-network direction classifier with a spatially varying orientation prior derived from a reference dataset. Within this framework, fibres are modelled as growing upward from the bottom of the volume, with each trajectory seeded from a real starting position near the bottom surface and propagated slice-by-slice toward the top. This bottom-up growth assumption reflects the layer-wise structure of the reference data and provides a natural, physically motivated ordering for sequential direction prediction along the Z-axis.

The proposed method draws on two complementary sources of directional information. First, a directional classifier is trained on real fibre track data extracted from a CT-scanned composite sample. At each point along a trajectory, the model receives the relative X and Y positions of preceding fibre points together with a local Z-position feature, and produces a probability distribution over eight possible in-plane movement directions. Second, the reference fibre volume is partitioned into three-dimensional slabs, within which the dominant local fibre orientation is estimated directly from the track data. This slab-based prior is injected into the classifier's output logits during inference, biasing predicted motion toward the dominant orientation of the corresponding spatial region, without requiring retraining of the classifier itself. Preliminary results suggest the combined classifier-plus-prior approach captures qualitative features of real fibre distributions, including local orientation coherence and controlled curvature, that purely rule-based methods struggle to reproduce.

This approach is intended as an intermediate strategy between purely rule-based fibre generation and fully learned generative modelling. Future work will focus on refining the proposed framework and evaluating the realism and reliability of the generated fibre structures through comparisons with experimental data. The resulting phantoms could support a wide range of studies in X-ray imaging, reconstruction, simulation, and algorithm development when experimentally measured ground truth is unavailable.

Towards GPU-Accelerated Virtual Neutron Imaging in gVXR Using NCrystal

Damian Martín Rodríguez

Virtual imaging is an increasingly useful tool for experiment planning, digital twins, algorithm development and education. The gVirtualXRay (gVXR) framework provides a GPU-accelerated environment for X-ray transmission imaging based on complex 3D geometries, enabling rapid simulation of X-ray radiographic and tomographic acquisitions. While Monte Carlo tools such as McStas and Geant4 are currently used to provide comprehensive neutron transport simulations, a faster complementary approach could be valuable for transmission-dominated virtual neutron imaging and preliminary feasibility studies.

This contribution proposes and discusses a possible future extension of gVXR towards neutron transmission imaging by combining its existing GPU-based ray-tracing capabilities with neutron interaction physics provided by NCrystal [1]. Conceptually, such an extension could retain gVXR's geometry handling, detector modelling and tomography workflows while introducing wavelength-dependent macroscopic neutron cross sections calculated using NCrystal. This could provide a route towards rapid simulation of neutron transmission through crystalline and amorphous materials, including wavelength-resolved radiography and Bragg-edge imaging.

The proposed approach is not intended to replace detailed Monte Carlo neutron transport. Instead, it could provide a computationally efficient complementary tool for generating synthetic datasets and exploring sample geometries, materials, neutron spectra and imaging configurations before undertaking more computationally demanding simulations or experiments. Potential applications include experiment planning, feasibility studies, detector and geometry optimisation, education and digital-twin applications. Such an efficient simulation tool could also provide guidance and support during experiments at large-scale research infrastructures.

A further opportunity would be the simulation of complementary X-ray and neutron imaging using common virtual samples and geometries. This could be particularly relevant to instruments such as ODIN at the European Spallation Source and NeXT at the Institut Laue-Langevin, where complementary neutron and X-ray imaging capabilities can be exploited experimentally and sequentially.

This contribution is intended to stimulate discussion about the feasibility and potential value of such a development within the gVXR ecosystem. A possible implementation strategy, its principal technical challenges and limitations, and the complementarity between GPU-accelerated ray tracing, NCrystal material physics and detailed Monte Carlo simulations will be discussed.

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Using gVXR and McStas to Compare X-ray and Neutron Imaging Techniques

Felix Sjöholm

Due to the different physical nature of photons (X-ray) and neutrons, the interactions with atoms are very different. Imaging techniques based on these two experimental particle methods provide different information and hence contrast mechanisms projected on the detector from the material sample put into the “beam”. While the photon attenuation coefficient has a linear relation/increase with atomic number (Z), the neutron attenuation coefficient is more scattered and unpredictable in comparison (Mass attenuation coefficients of elements on a logarithmic scale for different radiations, <https://doi.org/10.3390/machines11040485>). Moreover, Hydrogen and the “isotope” deuterium are great attenuators of neutrons which allows for many biological materials to be studied. Therefore, the combination of these two imaging techniques can be of great benefit for material science and material development.

This work presented here, conducted during the summer at Tetra Pak, includes a comparison of X-ray and Neutron interactions and imaging techniques. The material sample focused and studied in this work has the application and manufacturing process injection moulding process in mind. In this manufacturing process, the object of importance, often a polymer, is surrounded by a thick metal tool e.g. injection mould. This “non-transparent” metal mould, surrounding the polymer part and creating the cavity where the polymer is injected at high pressure and temperature, makes it impossible for the human eye or a camera system to look into this process with visible light when it is happening, i.e. in situ. However, since the polymer is Hydrogen-rich, neutrons may be able to penetrate the metal mould that stops the majority of the X-ray beam due to the thick thickness of the metal walls.

A Jupyter-Notebook was created in Python during the course of the work that should make the process of loading in an *.stl file and producing an X-ray image in gVXR as smooth as possible. The virtual experiments involved and elaborated with alternating mould thicknesses, mould material, exposure time, tube current and tube voltage to see the effect on the acquired X-ray image.

By using a virtual representation of a Laboratory X-ray equipment, developed in an earlier master thesis project (<https://lup.lub.lu.se/student-papers/search/publication/9243853>) using gVXR, a realistic virtual setup of a XCT scanner was accessible as a benchmark. This work will be continued to create new digital twins of other XCT-equipment's available at Tetra Pak to compare the results obtained. In the future this methodology and developed framework would hopefully be used to create and integrate a virtual beamline of one or some of the Imaging-instruments available at the synchrotron facility based in Lund, MAX IV. For instance, ForMAX, DanMAX, NanoMAX or the upcoming beamline TomoWISE.