Image-Based Simulation for Industry 2024
(IBSim-4i 2024)

21–25 October 2024
Institute of Physics, London, UK

iop.org

IOP Institute of Physics

Welcome

On behalf of the organising committee of the seventh Image-Based Simulation for Industry event (IBSim-4i 2024), we are delighted to welcome you to this initiative to develop the community of image-based simulation users and developers for industrial applications.

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

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

Information for Speakers

Keynote speakers will have 45 minutes (including Q&A) and other presenters are given 25 minutes (including Q&A).

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

Supporting Organisations

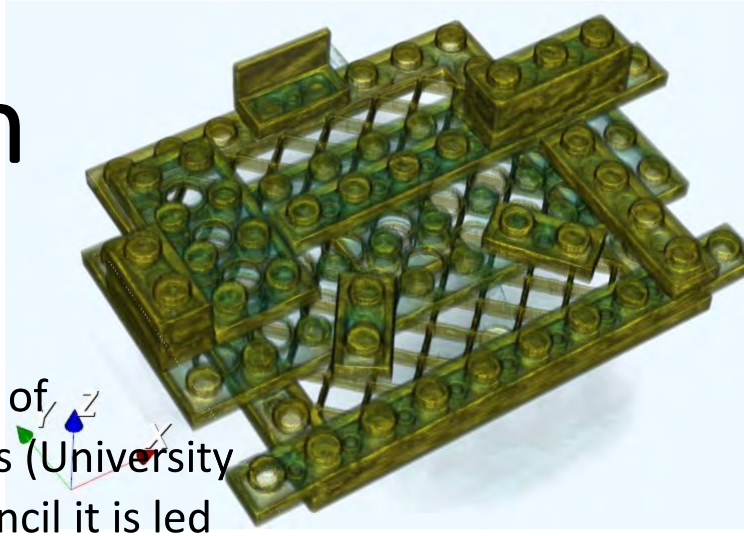
We would like to thank the following organisations for their generosity in supporting this event:

IOP Institute of Physics
Materials and Characterisation Group

IOP Institute of Physics
Applied Mechanics Group

CCPi
TOMOGRAPHIC IMAGING

Collaborative Computational Project in Tomographic Imaging www.ccpi.ac.uk



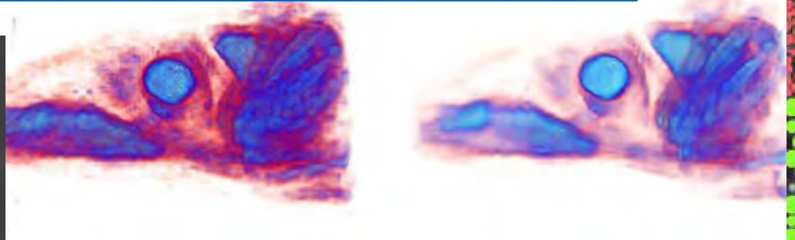
CCPi provides the community with a toolbox of algorithms increasing the quality and level of information that can be extracted by computer tomography. Chaired by Prof Philip Withers (University of Manchester) and co-ordinated by staff within the Science and Technology Facilities Council it is led by a working group of experimental and theoretical academics with links to the Diamond Light Source, EPAC, ISIS Neutron Spallation Source and Industry.

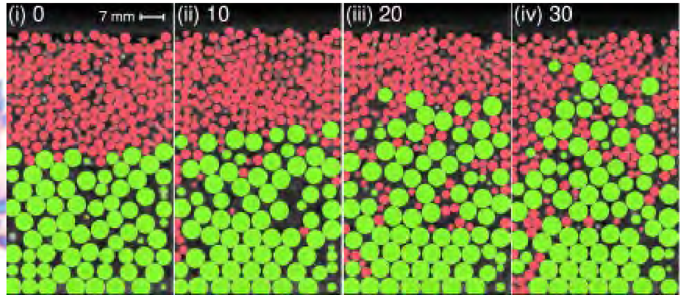
- **Creating and supporting best practice from the national facilities to lab based systems**
- **Python based framework development: the Core Imaging Library** https://www.ccpi.ac.uk/CIL

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**

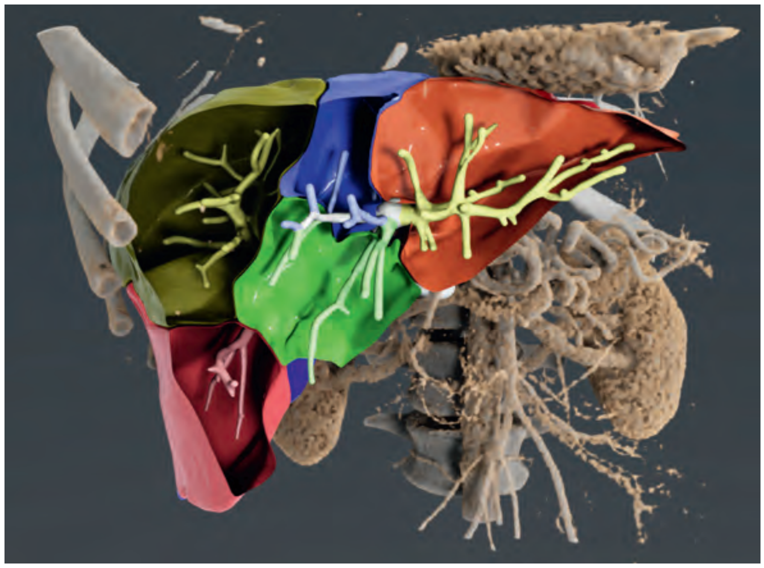
Join over 400 Tomographic Imaging practitioners: discord.com/invite/9NTWu9MEGq

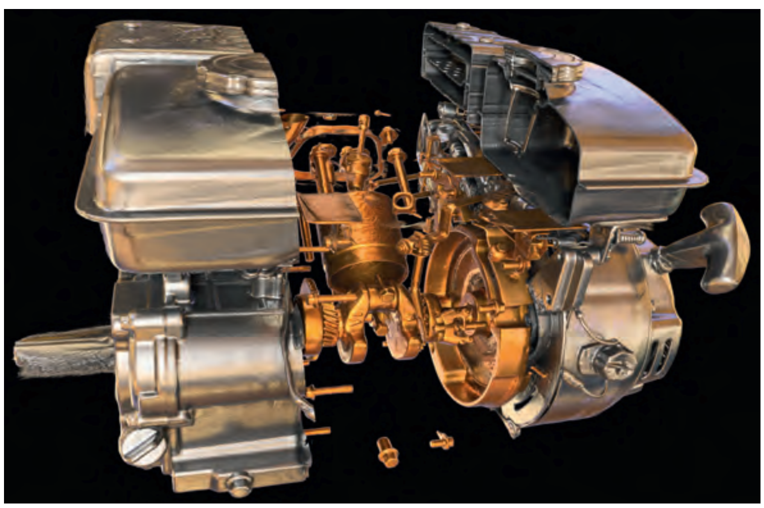




MeVisLab
Development Environment

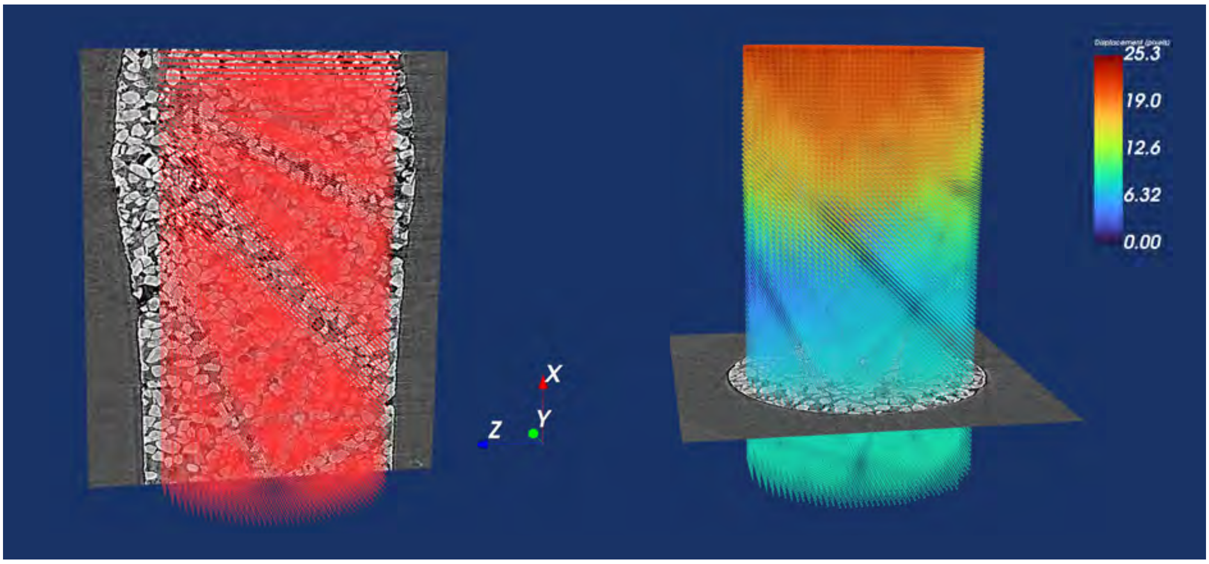
Rapid prototyping and product development of medical and industrial imaging applications





MeVis

iDVC: interactive software for Digital Volume Correlation



DVC enables the quantification of internal displacements and calculation of strain fields from in situ tomography experiments

For beginners and experts

Free training sessions

UKRI Science and Technology Facilities Council Scientific Computing
CCPi Tomographic Imaging
CoSeC
diamond
alc ada lovelace centre
Oregon State University

Keynote Speakers

Dr Sam Cooper
Dyson School of Design Engineering, Imperial College London

Machine learning for the characterisation and design of battery electrodes

Dr Sam Cooper is a Reader in the Dyson School of Design Engineering at Imperial College London. He leads a group focused on the application of machine learning to the characterisation and design of advanced materials such as battery electrodes. His group have released many open-source software tools that can be found at https://tldr-group.github.io/. Most recently, Sam has spun-out a company, Polaron, who are building a generative AI toolkit for materials design https://polaron.ai/.

Professor Christian Gasser
KTH Royal Institute of Technology, Stockholm

The biomechanics-based rupture risk assessment. Patient selection through FEM-based postprocessing of medical images

Christian Gasser is Professor of Biomechanics at KTH Royal Institute of Technology, Stockholm. He holds a Master of Mechanical Engineering (1997) and a PhD in Civil Engineering (2001), both from Graz University of Technology, Austria. The development and application of advanced numerical techniques to solve realistic (bio)engineering and clinical problems, is Gasser's main research objective. Constitutive models for anisotropic finite strain materials have been implemented in all major Finite Element simulation packages, such as ANSYS, ABAQUS, COMSOL, etc, and Gasser's translational biomechanics research led to A4clinicsRE, commercial biomechanical-based simulation software for clinical decision making. In 2022 he has been listed as KTH's most influential researcher in Biomedical Engineering, and his work led so far to more than 16k Google Scholar citations. He received a Humboldt Research Award from Germany, and Gasser is designated 2024 Odqvist lecturer, a distinction awarded by the Swedish national mechanics committee. He is Associate Editor of Int. J. for Num. Meth. in Biomed. Engrg, in the editorial board of Mechanics of Soft Materials and a EMMCC member, principal founder of ARTEC Diagnosis AB and VASCOPS GmbH, and serves a legal expert for skiing accident reconstruction at Oberlandesgericht, Graz, Austria.

Programme

Monday 21 October 2024

Training Course

9:30 AM - 10:00 AM	**Registration and Refreshments**
10:00 AM - 11:00 AM	**Session 1** Introduction into MeVisLab, Types of Modules, Building your own networks, Loading and viewing images and basic Image Processing
11:00 AM - 11:15 PM	**Morning Break**
11:15 AM - 12:45 PM	**Session 2** Rapid Prototyping and Macro Modules, Python scripting
12:45 PM - 1:45 PM	**Lunch**
1:45 PM - 3:15 PM	**Session 3** Data Objects: Masks, Markers, CSOs (Contours), WEMs (3D Meshes)
3:15 PM - 3:30 PM	**Afternoon Break**
3:30 PM - 5:00 PM	**Session 4** Segmentations: Basic (Region Growing, Thresholds), Advanced (using AI in MeVisLab)
5:00 PM - 7:00 PM	**Drinks Reception**

Tuesday 22 October 2024

Training Course

8:30 AM - 9:00 AM	**Arrival and Refreshments**
9:00 AM - 10:15 AM	**Session 1** Introduction to iDVC - algorithms behind the code
10:15 AM - 10:30 AM	**Morning Break**
10:30 AM - 12:00 PM	**Session 2** Getting started with iDVC
12:00 PM - 1:00 PM	**Lunch**
1:00 PM - 2:30 PM	**Session 3** Hands on: prepare for the DVC analysis
2:30 PM - 2:45 PM	**Afternoon Break**
2:45 PM - 4:15 PM	**Session 4** Hands on: run DVC and show the results

Wednesday 23 October 2024

User and Developer Forum

9:30 AM - 10:00 AM	**Registration and Refreshments**
10:00 AM - 10:15 AM	**Welcome** Franck Vidal
10:15 AM - 11:00 AM	**Keynote 1: Christian Gasser, KTH** The biomechanics-based rupture risk assessment. Patient selection through FEM-based postprocessing of medical images
11:00 AM - 12:10 PM	**Session 1: Presentations** **Sascha Heckmann** - Imaging in MeVisLab – Focus on your innovation… **Samir Mohamed** - X-ray CT Reconstruction of 3D-printed Sample Using a Simulated Prior Generated from G-code File **Sunday Nwokolo** - Advanced Computational Techniques for the Recovering of Partially Damaged CT Dataset
12:30 PM - 1:30 PM	**Lunch**
1:30 PM - 3:10 PM	**Session 2: Presentations** **Iwan Mitchell** – Comparing CAD models with actual samples using experimental CT data, X-ray simulations, and mathematical optimisation **Liang Yang** - Unfitted Finite Element for Image Based Simulation **Brian Bay** - Relating Data from Microstructure-Based Digital Volume Correlation to Analytical Models
3:10 PM - 3:40 PM	**Afternoon Break**
3:40 PM - 5:30 PM	**Session 3: Presentations** **Elena Syerko** - Image-Based Computation of Permeability of Anisotropic Multi-Scale Porous Materials by the Software Suite "PoroS" **Vincent Maes** - BASIC: Benchmark Activity for micro-Structure Image-processing of Composites **Yang Chen** - High-performance FFT based homogenisation method of dual-scale flow for permeability prediction in textile fabrics **James Le Houx** – Introduction to DIAMOND synchrotron and ISIS Neutron and Muon source
5:30 PM -8:00 PM	**Networking Reception and Buffet Dinner**

Thursday 24 October 2024

User and Developer Forum

9:00 AM - 9:30 AM	Arrival and Refreshments
9:30 AM - 10:15 AM	**Keynote 2: Samuel J Cooper, Imperial College London** Machine learning for the characterisation and design of battery electrodes
10:15 AM - 10:40 AM	**Session 4a: Presentations** **MIRASLAU BARABASH** - Micro-CT Image-Based 3D Modelling of Lithium-Sulfur Batteries
10:40 AM - 11:10 AM	Morning Break
11:10 AM - 12:25 PM	**Session 4b: Presentations** **John M. Hanna** – Macroscale image-based permeability prediction based on physics-informed and convolutional neural networks **Victoria Hann** - Exploring the Impact of Structural and Textural Realism in Synthetic Micro-CT Data for Machine Learning Model Training
12:25 PM - 1:30 PM	Lunch
1:30 PM - 2:45 PM	**Session 5: Presentations** **Mikhail Matveev** - Research Object Cataloguing - a case of CT images of composites **Chen Liu** – 3D EBSD/SEM tomography of creep damage and the effect of crystal microstructure **Lewis Griffin** - Deep Learning Based Ply Segmentation For Composite Laminate Analysis
2:45 PM - 3:15 PM	Afternoon Break
3:15 PM - 4:30 PM	**Session 6: Presentations** **Nalin Gupta** - Generation of procedural digital phantoms in gVirtualXray **Rakhul Raj** - MODVORTEx: A software for probing magnetic domain dynamics **Ronan Docherty**– Upsampling DINOv2 features for weakly supervised (bio-) materials segmentation
4:30 PM - 5:00 PM	Closing Remarks

Friday 25 October 2024

Collaborative workshop

9:00 AM - 9:30 AM	Registration and Refreshments
9:30 AM - 10:45 AM	**Session 1**
10:45 AM - 11:15 AM	Morning Break
11:15 AM - 12:30 PM	**Session 2**
12:30 PM - 1:30 PM	Lunch
1:30 PM	**Conference Close**

Keynote Speakers

The biomechanics-based rupture risk assessment. Patient selection through FEM-based postprocessing of medical images

<u>Professor Christian Gasser</u>[1]
[1]KTH Royal Institute of Technology, Stockholm

Keynote 1, October 23, 2024, 10:15 - 11:00

An Abdominal Aortic Aneurysm (AAA), the balloon-like expansion of the aorta, is a common disease in the elderly. If the risk of aortic rupture exceeds the interventional risks, elective clinical treatment (AAA repair) is indicated and generally performed when the largest transverse aortic diameter exceeds 5.5cm in males or 5.2cm in females [1]. However, such a diameter-based risk assessment has a very poor specificity and many AAAs that would not rupture during lifetime, are currently repaired, while at the same time aortas keep rupturing below said thresholds. In contrast, the biomechanics-based rupture risk assessment (BRRA) assumes the aorta to rupture as soon as the aortic wall stress exceeds wall strength. It is a generic concept and allows the integration of multiple risk factors, thereby providing a more individualized AAA risk assessment [2]. From a patient treatment perspective, the BRRA may be seen as (Finite Element Method-based) postprocessing of Computed Tomography-Angiography (CT-A) images that have been acquired by routinely clinical examinations. The present talk reviews the state-of-the-art of the BRRA, where key elements are illustrated by following the workflow of commercial software (A4clinicsRE, Vascops GmbH, Austria). The validity of the underlying model assumptions is scrutinized and the value of clinical validation studies discussed. As supported by a significant body of clinical and bioengineering research, the BRRA is now on the verge of being integrated within the clinical decision-making process.

[1] Wanhainen et al. Eur J Vasc Endovasc Surg 57, 2019
[2] Gasser et al. Int J Num Meth Biomed Engrg 28, 2022

Machine learning for the characterisation and design of battery electrodes

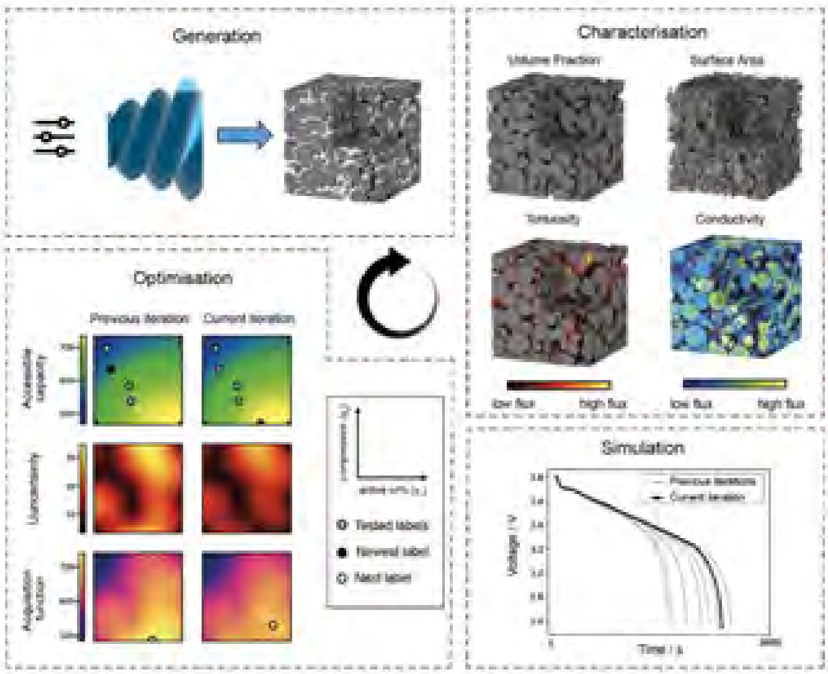
Dr Samule J Cooper[1]
[1]Dyson School of Design Engineering, Imperial College London

Keynote 2, October 24, 2024, 09:30 - 10:15

Battery companies want to know the relationship between their manufacturing parameters and the performance of the resulting cells so that they can optimise their products for particular applications, reduce costs, and improve yield. The literature contains many examples of physics-based models of the various manufacturing processes (including mixing, coating, drying, and calendaring), but these systems are hugely complex, and as a result they are expensive to simulate and hard to validate.

Recent advances in generative machine learning (ML) methods have allowed the relationship from manufacturing parameters to microstructure to be directly learned from data.

In this talk I will present a modular approach to the cell optimisation cycle that makes use of these ML methods, in combination with GPU accelerated metric extraction (TauFactor 2), electrochemical cell simulation (PyBaMM), and Bayesian optimisation. In addition, I will be introducing a new *kintsugi* SEM imaging method for accurately observing the nanostructure of the carbon binder domain; “VoxCel” an open-source, voxel-based, GPU-accelerated, multi-physics cell simulation;



ML methods for generating 3D data from 2D images, as well as, inpainting artefacts in image data; and a data fusion method for combining multi-modal datasets using GANs. Lastly, I’ll present a webapp that normalises the data obtained from testing cells in a lab for easy comparison to commercial cells: cell-normaliser

We are always looking for new collaborations and new data so please get in touch! If you’d like to use any of our suite of open-source tools, then head to our website: https://tldr-group.github.io

We’ve also just spun-out a company from Imperial, called **Polaron**, to bring these tools to market. Check out our website (www.polaron.ai) and get in touch: info@polaron.ai

Oral Presentations
Session 1

X-ray CT Reconstruction of 3D-printed Sample Using a Simulated Prior Generated from G-code File

Samir Mohamed[1], Dr Sam Tammas-Williams[1], Dr Amer Syed[1], Dr Ian Butler[1]
[1]University of Edinburgh

Session 1, October 23, 2024, 11:00 - 12:10

Since its inception in the 1970s, x-ray computed tomography (CT) had revolutionised the field of diagnostic medicine, not to mention the attention garnered in other spheres from material science to cultural heritage and even forensics. Of particular interest to this work is the application of x-ray CT to the field of additive manufacturing (AM), especially fused deposition modelling (FDM), where x-ray CT had been utilised for nondestructive evaluation (NDE) of components as well as for monitoring and controlling the AM process. For high throughput inspection, however, the use of x-ray CT typically poses a bottleneck to the AM process due to large acquisition and processing times, particularly with the number of projections required for traditional reconstruction techniques such as filtered backprojection (FBP) or Feldkamp-Davis-Kress (FDK). While such traditional (analytical) reconstruction techniques are computationally fast, the recent rise in affordable processing power in modern GPUs enables the application of more advanced reconstruction methods, particularly iterative and deep learning algorithms, that allow for complex scanning geometries (e.g. few-view and limited-angle CT) and the incorporation of prior knowledge into the reconstruction process. This paper explores the effect of incorporating a prior image (based on the G-code file) into the reconstruction process (i.e. via regularisation), thereby supplementing the undersampled projection data to maximise reconstruction quality and minimise acquisition time. A Python script was written to parse through the G-code file generated by slicing an STL model, thus yielding prior images that simulate ideal x-ray CT slices. A review of prior-image-based reconstruction (PIBR) techniques has been produced, though it should be noted that PIBR research is mainly concerned with diagnostic medicine, where minimising radiation dose/exposure is a priority. Some PIBR approaches remain relevant, however, as one method of reducing accumulated radiation exposure is to acquire less projections in subsequent scans. To evaluate the performance of various regularisation strategies, x-ray CT data from an FDM sample is reconstructed using the Core Imaging Library (CIL), and the extent to which the number of projections acquired can be reduced is discussed.

Advanced Computational Techniques for the Recovering of Partially Damaged CT Dataset

Mr Sunday Nwokolo[1], Prof Franck Vidal[2,1]
[1]Bangor University, [2]Science and Technology Facilities Council

Session 1, October 23, 2024, 11:00 - 12:10

Porosity defects challenge the structural integrity of additive manufactured materials, especially under fatigue loading. This study evaluates a novel computational method for reconstructing incomplete computed tomography (CT) projection data of a cylindrical rod with porosities subjected to cyclic loading. The initial dataset contained 1583 CT projections in the rod's original state. After cyclic forces were applied, a second dataset had approximately 60% of the data missing due to limited angles. In-situ testing destroyed the sample, preventing a re-scan and necessitating the salvage of the corrupted dataset. Using the Core Imaging Library (CIL), we reconstructed both datasets. Initial attempts with the Feldkamp-Davis-Kress (FDK) algorithm resulted in strong streak artefacts, prompting the use of iterative reconstruction with Total Variation (TV) regularization. We segmented the volume reconstructed with FDK to assess its utility in reconstructing missing angles. We developed an image registration workflow optimised with the Covariance Matrix Adaptation Evolution Strategy (CMA-ES) to accurately register real and simulated datasets. Leveraging on Virtual X-Ray Imaging Library on GPU (GVXR), we successfully simulated and recovered the missing projections. Our method shows promising early results, and we are now benchmarking it against iterative methods, in particular with TV regularisation. Results clearly defined the porosities, demonstrating that our method effectively salvages incomplete projection data and enhances CT data analysis accuracy.

Session 2

Comparing CAD models with actual samples using experimental CT data, X-ray simulations, and mathematical optimisation

Iwan Mitchell[1]
[1]Bangor University

Session 2, October 23, 2024, 13:30 - 15:10

We investigate methods of assessing how a manufactured part differs from a reference CAD model, using a part of an in-situ tensile testing machine designed to be used with a scanning electron microscope. CAD drawings are available, and the 3D surface is exported. After manufacturing, a CT scan was acquired with the DTHE scanner at INSA-Lyon. The challenge was how to compare the manufactured part with its original CAD model. Several options are available:

- Manual measurement from the CT volume Vs Cad drawings.
- CAD model vs a 3D surface derived from a CT volume
- CT scan of the manufactured part Vs Simulated CT scan of the CAD model.

The first option is easy to perform, but is time-consuming and susceptible to human judgement and error. The second option involves subjecting measurements to segmentation and meshing methods, that introducing sources of measurement uncertainty into the process. The final method requires CAD registration and accurate simulation techniques.

A practical method to accurately register CAD models onto experimental CT data is demonstrated. Using X-ray simulation performed with gVirtualXray within the objective function of the registration algorithm allows i) a direct comparison of the two 3D surfaces using Hausdorff distances, and ii) to reconstruct the CT volume of the CAD model. In turn, making a direct comparison of the experimental CT volume with a CT of the registered CAD model is possible, e.g. using traditional image metrics on direct radiographs. Additionally, a digital volume correlation (DVC) analysis with iDVC is performed.

Unfitted Finite Element for Image Based Simulation

Liang Yang[1,2], Jianhui Yang[2]
[1]Cranfield University, [2]Voxshell limited

Session 2, October 23, 2024, 13:30 - 15:10

Flow, solid, and radiation simulations on 3D images reconstructed from CT/MRI scans are valuable in many industrial and biomedical applications. Research shows that Finite Element (FE) and Cartesian meshes must be at least twice as fine as the original image resolution to achieve mesh convergence. To reduce computational costs, we present the unfitted boundary method that integrates an FE numerical model with a conformal mesh, eliminating the need for expensive and complex mesh generation processes.

The unfitted boundary method embeds the domain of interest into a larger computational domain that is easier to mesh. It utilises an additional transformation map in addition to the Finite Element reference map. The well-posedness of the method is ensured by a positive Jacobian. Several numerical examples with high-resolution images illustrate its advantages.

Relating Data from Microstructure-Based Digital Volume Correlation to Analytical Models

Brian Bay[1], Catherine Disney[2]
[1]Oregon State University, [2]Diamond Light Source

Session 2, October 23, 2024, 13:30 - 15:10

Digital Volume Correlation (DVC) is commonly implemented as a volumetric full-field deformation measurement technique, with a homogenized interpretation of material behaviour derived from simple, often grid-based point clouds. The fine-scale image texture used for point tracking is seen as analogous to digital image correlation speckle, an indicator of but not a participant in sample deformation. However, in many materials used for DVC the image texture derives from mechanically significant microstructural features, often with non-random, even semi-periodic organization. In our experience the structure of a point cloud and the microstructure of a material can interfere, generating results that are difficult to interpret and even misleading.

The point cloud underlying DVC measurements offers a solution. At their most basic, image correlation techniques, whether 2D, 3D-stereo, or volumetric, track changes in point locations between image data sets based on small subregions of image data surrounding a point. If the subregion is an appropriate size and contains suitable fine-scale texture, the point will track. Full-field data interpretation evolves from tracking multiple points within a region. Structured point arrangements may facilitate DVC algorithms and data post-processing, but they are not a requirement of the DVC process.

We have seen, particularly in studies of biological tissues, that pre-processing of image data to generate points clouds coordinated with sample microstructure produces more useful DVC results. Biological tissues are not easily homogenized as they often contain microstructural features of a spatial scale significant with respect to sample size. This occurs in bone tissue, where pores are large, and fibrous soft tissues such as intervertebral disc, where tissue layers and collagen fiber bundles are prominent. Dense, contoured point clouds that avoid pores, and curvilinear point clouds that follow individual fibres, are extremely useful in these cases. Examples from recently published and ongoing work will be presented.

In addition to point cloud structure, the method of strain calculation is an important consideration when the goal is comparison with analytical models. Points clouds optimal for DVC are generally of different densities and organization than their analytical counterparts, and displacement variability in measurement results must be managed. A simple process of local polynomial fitting to unstructured point neighborhoods has proven successful in many image correlation settings, yet this is quite different than structured strain calculation from dense element configurations with nodal values presumed free of variability. Methods of accommodating these disparate results will be discussed.

Session 3

Image-Based Computation of Permeability of Anisotropic Multi-Scale Porous Materials by the Software Suite “PoroS”

Elena Syerko[1], Paris Mulye[1], Christophe Binetruy[1], Adrien Leygue[1]
[1]École Centrale Nantes, Nantes Université, CNRS, GeM, UMR 6183, F-44000

Session 3, October 23, 2024, 15:40 - 17:20

In porous media science and engineering permeability is one of the key properties that quantifies the capacity of porous structure to be impregnated by a fluid. Fibrous materials used as reinforcements in structural composites can be considered as the most complex class of porous media due to their anisotropic multi-scale character. Experimental determination of permeability of fibrous materials is time-consuming, requires a specialized equipment, and is hardly possible to perform at the micro-scale. On the contrary, numerical characterization of permeability allows to reduce material waste and to study the impact of the microscale parameters on it.

There is still no widely accepted numerical approach for permeability prediction due to challenges such as the choice of the RVE, boundary conditions, permeability identification, as revealed in the first international virtual permeability benchmark on fibrous media[1],[2]. This motivated the development of a novel scientific software named 'PoroS' [3],[4],[5] consisting of efficient matrix-free iterative solvers specifically designed to predict the saturated permeability of anisotropic porous materials based on 3D images.

The first version of the software PoroS 1.0 computes the permeability of single-scale porosity materials. To overcome the difficulties of image-based computations related to the choice of boundary conditions and consideration of material samples with unknown flow principal directions, a specific approach of flow being induced by a volumetric body force is implemented in PoroS.The full 3D permeability tensor is then calculated from velocity fields by the full-field homogenization.

After the validation,predictions by PoroS 1.0 were compared to the results of the first stage of the virtual permeability benchmark [1]. Computations were performed on a 3D volume representing the yarn microstructure composed of ~400 slightly misaligned fibres. PoroS results fell within the main cluster of benchmark results, being very close to the mean value. Moreover, unlike the majority of benchmark results,PoroS was capable to capture the influence of important microstructural parameters on permeability[4].

The second version of the software PoroS 2.0 [5] addresses the permeability of dual-scale porosity materials and was used in the benchmark second stage[2] dedicated to the mesoscopic scale of a textile. Its results fell within the main cluster of benchmark results.

[1] Syerko E. et al. Composites Part A: Applied Science and Manufacturing, 167,2023,107397.
[2] Syerko E. et al. In: Proceedings of the 21st European Conference on Composite Materials (ECCM-21), Nantes, France, 2024. doi: 10.60691/yj56-np80
[3] PoroS 1.0. IDDN.FR.001.400009.000.S.P.2022.000.20600.
[4] Mulye P. et al. Materials, 17(12),2024,2873.
[5] PoroS 2.0. IDDN.FR.001.390014.000.S.P.2023.000.20600.

BASIC: Benchmark Activity for micro-Structure Image-processing of Composites

Vincent Maes[1], Onur Yüksel[2], Robin Hartley[1], Guillaume Broggi[2], Silvia Gomarasca[2], Théo Baumard[3], Adrien Le Reun[3], Arthur Levy[3], Clemens Dransfeld[2], Bariș Çağlar[2], James Kratz[1]
[1]University Of Bristol, [2]Delft University of Technology, [3]Nantes Université

Session 3, October 23, 2024, 15:40 - 17:20

Composite structures have long been described using homogenized macro (i.e. laminate level) quantities, including fibre volume fraction, ply thickness, and fibre angles. While these quantities are useful in early sizing and design work for determining basic material properties used in calculations, they fail to fully characterize the true micro- and meso-structural features present in all composite parts. To resolve the material at a more refined scale, the composites community is increasingly deploying micro- and meso-scale analyses using various imaging techniques. Several studies have shown improved predictions of material properties when accounting for micro- and miso-structural features.

Obtaining micro- and meso-scale images for analysis is primarily achieved through micrograph (2D) and tomograph (3D) inspection. Irrespective of the imaging technique used, image analysis tools are needed to process the imaging and extract the desired feature data. As the interest in micro- and meso-structural analysis grows, alongside advancements in hardware and software capabilities for acquisition and processing, this field has witnessed significant developments in recent decades. There has, however, been limited effort devoted to benchmarking and comparing the performance of the different algorithms and approaches used to process the images. As such there are also currently no guidelines to enhance consistency between researchers and enable early-stage researchers to accurate and confidently perform microstructural image analysis.

This study begins addressing these gaps by comparing the analysis results from three micrographs, obtained using a confocal scanning microscope from the same polished sample. Each micrograph followed a distinct protocol representative of techniques used by composite laboratories worldwide. Multiple images were acquired to scan a cross-sectional area ranging from 2mm to 3.8mm, using three different objectives (50x, 20x, and 20x extra-long working distance) to obtain varying pixel densities and illumination. These micrographs were then shared between the University of Bristol, the Université de Nantes, and the Technical University of Delft for analysis in a blind format, with each participant using in-house algorithms and methods that had not been used and/or trained on the three micrographs prior to the benchmark activity. The resultant datasets of microstructural metrics were compared using various statistical analyses to comprehend the variability in the captured microstructures. The trends across the different micrographs and participants allow for novel insight into the practical implications of the different approaches which are the first step to standardisation.

High-performance FFT based homogenisation method of dual-scale flow for permeability prediction in textile fabrics

Yang Chen[1]
[1]University Of Bath

Session 3, Oct 23, 2024 15:40PM-17:20PM

Permeability of fibre textiles is an important and long-standing challenge in composites manufacturing using liquid composites moulding technology. The dual-scale porous structure of fibre textiles exhibits strong geometrical variability, hence necessities a comprehensive characterisation. Numerical simulations are used for this purpose relying on a recently proposed FFT based method solving the Stokes-Brinkman equation. The solver is capable of handling large-scale simulations and enable the efficient application of high-performance computing. Geometric models are constructed using textile microstructures either artificially generated or extracted from 3D tomographic images. In this talk, I will first present the numerical algorithm of the FFT solver, which is enhanced with a convergence acceleration technique. Then, some examples, including image-based simulations of dual-scale flow in woven and non-crimp fabrics, will be presented to showcase its capability in large-scale computation using HPC systems. Although it has been developed in the context of composite manufacturing research, this solver can readily be applied to other problems where bi-porous structures need to be considered, such as mass transport in partially fractured and vuggy rocks, which are of interest in petroleum industry or for geological disposal of radioactive waste.

Introduction to DIAMOND synchrotron and ISIS Neutron and Muon source

James Le Houx[1]
[1]STFC UKRI

Session 3, Oct 23, 2024 15:40PM-17:20PM

This presentation will explore the opportunities available for researchers and companies to access advanced imaging techniques at the UK's National Facilities: Diamond Light Source, ISIS Neutron and Muon Source, the Henry Royce Institute and the National X-ray CT Consortium. We will discuss the capabilities of X-ray Computed Tomography (CT) and other imaging methods, such as Neutron CT, and highlighting their applications in various scientific and industrial fields. Attendees will learn about the process for gaining access to these facilities, including proposal submission, peer review, and collaboration opportunities. By showcasing successful case studies, we aim to demonstrate how these facilities can be used to enable image-based modelling in the wider community.

Session 4

Micro-CT Image-Based 3D Modelling of Lithium-Sulfur Batteries

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Session 4a, October 24, 2024, 10:15 - 10:40

Lithium-sulfur (LiS) batteries are expected to supersede the intrinsic limits of Li-ion technology, particularly in the aerospace and heavier electric vehicles industries [1], thereby advancing the UK Battery Strategy 2030 [2]. Describing, optimising and designing the properties of LiS batteries thus represents a cutting-edge challenge with significant industrial and socio-economic impact. 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 [3] based on 3D X-ray CT images with sub-micron resolution (Figure, A) to describe the spatio-temporal dynamics of discharge in LiS cathodes (Figure, B). 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 LiS cathodes, on battery performance at varying C-rates, exceeding the capabilities of the respective volume-averaged 1D electrochemical model (Figure, B). Next, we cross-compare the discharge performance of two samples – a commercial and a lab-fabricated one, with essentially different microstructural properties (porosity, tortuosity, 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. Lastly, we deploy pore network modelling [4] to reduce computational burden and enable a realistic representation of large electrodes in our models.

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

Figure: (A) Example of a segmented X-ray micro-CT image of a pristine LiS cathode. Yellow depicts original sulfur deposition, grey shows the carbon binder domain (CBD), and voids represent the electrolyte-accessible volume. Electrochemical reactions evolve on the particles' surfaces represented by 3D tetrahedral mesh. (B) Discharge performance of a LiS cathode at three different C-rates (solid curves), modelled using the full 3D X-ray micro-CT image-based framework [2] and corresponding 1D model (dashed curves). Image adapted from Ref. [2].

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Macroscale image-based permeability prediction based on physics-informed and convolutional neural networks

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Session 4b, October 24, 2024, 11:10 - 12:25

Permeability is a key property of porous media that quantifies how easy the flow goes through the media. It is an important quantity that is an input to flow simulations in porous media. One key application to the quantification of permeability is liquid transfer molding process for composite manufacturing. Despite its key importance, there is no standard numerical or experimental technique that measures this quantity. Moreover, the available methods offer an estimation of only the average permeability assuming homogeneity over the whole macroscale porous media (fibrous textile), which leads to inaccurate simulations. In this work, we offer a methodology to predict the permeability tensor as a field directly from textile images (before fluid injection). The methodology is based on physics-informed and convolutional neural networks. Data from central injection experiments, including flow front images and inlet pressure sensor, is used for the training process. While during employment of the model, only the textile image is needed for predictions. The proposed model is tested by comparing simulation using the predicted permeability and unseen experiments. It can be concluded that the proposed model has superiority in achieving realistic digital-twin to the experiment when compared to simulations using permeability obtained through classical techniques.

Exploring the Impact of Structural and Textural Realism in Synthetic Micro-CT Data for Machine Learning Model Training

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Session 4b, October 24, 2024, 11:10 - 12:25

The use of machine learning (ML) for image analysis is now standard across many research domains. However, ML models typically require a significant amount of annotated data for training which is rarely available in specialist research areas. In biosciences, for example, image datasets are often small because of complex imaging processes, and fully annotated datasets are less common because of the complexity of manually labelling the images. Synthetically created data can be used to increase the size of a dataset for training with an ML model while maintaining the relevant features and information of the original images. Segmentation masks can be created automatically during the synthetic image generation process, removing the need for tedious manual annotation and ensuring high accuracy of the labels. However, if the features are represented poorly within the synthetic dataset, it can negatively impact the quality of the segmentation. Synthetic dataset creation methods should consider the original dataset's visual features, biological properties and imaging modality.

We present an adaptable pipeline for creating annotated synthetic micro-computed tomography (micro-CT) volumes at scale using the 3D modelling tool, Blender (https://www.blender.org/). The approach can be separated into three main tasks: generating the foreground object of interest, simulating the background medium, and rendering the slices to simulate planes through a micro-CT volume. The first stage is to create the foreground by generating a 3D model of the target sample. We use a plant root system as an example of a complex biological problem. The second stage is to create the surrounding materials – soil in our case – and add realistic textures to simulate the relative density of the materials in which the object is embedded. The final stage is to render the images by slicing the volume at defined regular intervals generating both the synthetic micro-CT image and the corresponding labels at each slice. Using our example dataset, we present the overall process of creating synthetic images and using them to increase the size of the dataset for training a segmentation model. We then explore how varying the complexity of each stage impacts the segmentation quality, focusing on the biological accuracy in the structure of the 3D model and the level of detail and realism in the textures of the generated surrounding material. We present a series of experiments with various texturing methods in both 2D and 3D to evaluate the impact on the segmentation quality.

Session 5

Research Object Cataloguing - a case of CT images of composites

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Session 5, Oct 24, 2024 1:30PM-2:45PM

Composite materials have complex internal structures due to their multi-scale composition (ranging from fibres to tows to reinforcements). Additionally, the internal structure is influenced by processing conditions. Consequently, conducting image-based simulations to characterize composite materials, such as across various fibre volume fractions, would typically require a time-consuming experimental program followed by multiple microcomputed tomography scans. However, most of the images obtained from these scans are not documented in a way that allows for reuse in other projects.

Our project aims to develop a research object catalogue, or database, that facilitates data sharing between different projects and institutions. The first step is to create a rich metadata format that is tailored to the needs of the composites community while aligning with the established practices of the experimental tomography field. Once the format is defined, it will be implemented in a web-based catalogue that allows users to search data using a variety of key identifiers. This catalogue will improve the Findability, Accessibility, Interoperability, and Reuse of composites-related micro-CT data.

3D EBSD/SEM tomography of creep damage and the effect of crystal microstructure

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Session 5, October 24, 2024, 13:30 - 14:45

Understanding the effects of crystal microstructure and loading condition on the creep damage mechanism of engineering materials helps develop effective models in predicting the behaviour and lifecycle of component, which is particularly important in nuclear industry applications. However, the accuracy of modelling using 2D characterisation is normally limited because of spatial variability in grain structure. It is therefore desirable to obtain representative volumetric microstructure information (grain shape, orientation and damage) to assist the crystal-plasticity finite element modelling for damage evolution analysis. In this talk, we will present the approach to characterise and reconstruct the 3D microstructure of 316H steel after creep test from a series of slice scans using FIB, SEM and EBSD. Volumetric crystal microstructure, such as grain morphology and orientation, boundary type and misorientations are segmented. The influence of microstructure and loading conditions will be determined via the correlation to the creep cavities and microcracks identified by back-scattered electron microscopy and machine learning tool. The insights from 3D characterisation will support and validate the digital tool (e.g., 3D CPFE modelling) to achieve a cost-effective approach in monitoring the efficiency and safety of components in industry.

Deep Learning Based Ply Segmentation For Composite Laminate Analysis

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Session 5, October 24, 2024, 13:30 - 14:45

As the aerospace industry increasingly adopts composite materials, refining manufacturing methods becomes imperative. The rise in demand has led to higher rate targets, necessitating the development of more efficient manufacturing methods. One such method for achieving these goals is new out-of-autoclave (OOA) approaches. These approaches eliminate the autoclave – a significant production bottleneck – by integrating deposition, compaction and curing into a single manufacturing step. However, these methods introduce new complexities, such as varying temperature and pressure histories for each ply placed, which can affect the dimensional accuracy of the resulting components.

Dimensional accuracy is already a significant challenge in aerospace manufacturing. Components often require shimming or trimming to fit correctly with other parts, reducing design strength and increasing aircraft mass [1 - 2], which in turn reduces efficiency. With the introduction of variable processes in OOA methods, precise parameter control becomes even more critical. Currently, to measure the effect of process parameters on the composite microstructure, microscopy images are taken, manually segmented, and then measured between the ply boundaries. This is a time-consuming and labour-intensive process.

This project proposes an automated solution using a MATLAB-based deep learning instance segmentation method (See Figure 1). The model, based on a ResNet50-SOLOv2 architecture, was trained using a custom dataset created with an in-house sub-sampling method aimed at reducing labelling efforts. This is paired with a post-processing script which extracts the ply boundaries and returns metrics such as average ply-thickness. This method has shown over 300-times faster segmentation when compared to a manual user approach.

Future developments could extend this method beyond ply thickness metrics to include other metrics such as boundary porosity [3], providing a more comprehensive overview of sample quality and further streamlining process development.

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Session 6

Generation of procedural digital phantoms in gVirtualXray

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Session 6, October 24, 2024, 15:15 - 16:30

Computed tomography is one of the most widely used imaging methods in fields ranging from medical imaging to biomedical and material sciences research, using both laboratory apparatus and synchrotron beamlines for these applications. In the case of synchrotron setups, limited beamtime access makes it difficult for researchers to tune experimental parameters to the samples being studied and necessitates prior judgement on the data that might be obtained. This makes it hard for new users to gain experience and submit successful beamtime applications.

X-ray simulations have gained importance because of this, allowing researchers to gain preliminary insights before carrying out any experiment. One of these simulation software packages is gVirtualXray (gVXR), a C++ library which simulates X-ray images by simulating the attenuation through 3D polygon meshes in real-time using the Beer-Lambert law. A Python wrapper is available. gVXR can be deployed on a wide range of systems, from laptops to supercomputers and cloud infrastructure. It also provides an API to programmatically tweak parameters and a user-friendly graphical user interface (GUI).

Prior versions of gVXR required the user to import the 3D meshes from files or create them from primitives (cubes, cylinders and spheres) without the ability to use Boolean operations. As such, the process of making meshes which resemble experimental samples is quite tedious. Furthermore, in beamline experiments, samples can morphologically be categorised broadly as foam, fibres, powders etc. which are harder to construct using this workflow.

This work showcases functions added to gVXR which can procedurally generate digital phantoms of common experimental sample types. A function for foam was created by utilising implicit modelling techniques and functions for creating general fibres are compared to experimentally obtained images. Along with this, a function for creating radiological step wedges is also shown to illustrate the importance of having these procedural phantoms within gVXR by comparing beam hardening and other artefacts in simulation and experimental data. Other phantoms in development (such as powders and composite materials) are also discussed.

MODVORTEx: A software for probing magnetic domain dynamics

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Session 6, October 24, 2024, 15:15 - 16:30

This work presents a comprehensive software solution for automating domain wall velocity measurements in magnetic materials using Magneto-Optic Kerr Effect (MOKE) microscopy. Building upon our previous work on bubble domain structures, we introduce a versatile graphical user interface (GUI) that accommodates arbitrary domain shapes and employs advanced computer vision techniques. The software provides different methods for domain wall detection and velocity calculation, catering to various domain structures. Our approach significantly reduces the time and effort required for data extraction, transforming a process that previously took weeks of manual work into a task completable within minutes. We provide the details of the algorithmic implementation which is organized into preprocessing, domain wall detection, displacement measurement, and velocity extraction. This tool is applicable to a wide range of scenarios, including bubble domain dynamics, Dzyaloshinskii-Moriya interaction studies in perpendicular magnetic anisotropy systems, and current-driven domain wall motion in patterned strips. By providing GUI, command-line interface and local application programming interface, our software offers flexibility for integration into existing measurement systems and adaptability for specific research needs. This automation promises to accelerate research in spintronics and magnetic materials, enabling more comprehensive and accurate studies of domain wall dynamics.

Upsampling DINOv2 features for weakly supervised (bio-)materials segmentation

Ronan Docherty

Session 6, October 24, 2024, 15:15 - 16:30

Segmentation of micrographs is a prerequisite for most image-based simulations, and these segmentations must be of high-quality for the resulting simulations to be meaningful. Interactive segmentation, where a classifier is trained to map from classical image features (local intensity, edges, etc) to user labels, is a popular paradigm in materials and biological segmentation for its speed and generalisability. Unfortunately, these features have limited expressive power and can struggle with more complex tasks, requiring a sample-specific model to be trained. We upsample the coarse features produced by self-supervised Vision Transformers (ViTs) like DINOv2 and use them as our feature set for interactive segmentation. These 'deep features' greatly improve segmentation performance across a range of tasks, including biological cells, battery electrodes, alloys, and oxides. We expect this workflow to not just improve segmentation performance but other tasks like denoising and (spatialised) property prediction.

Image-Based Simulation for Industry 2024 (IBSim-4i 2024)

21–25 October 2024

Institute of Physics, London, UK