

AI COMP 26

Artificial Intelligence for Composite Materials Conference

Vancouver, Canada - August 5-7, 2026



Book of Abstracts

Contents

PLENARY

- FROM PROCESS SIMULATION TO QUALITY-AWARE DIGITAL TWINS IN THE AGE OF AI (Anoush Poursartip)
- AI-ENABLED FORWARD PREDICTION AND INVERSE DESIGN OF COMPOSITE MATERIALS (Pavana Prabhakar)
- AI FOR SCIENTIFIC DISCOVERY AND ENGINEERING DESIGN (Steven L. Brunton)

KEYNOTES

- CREDIBILITY OVER ACCURACY: AI; PHYSICAL FIDELITY; AND THE FUTURE OF COMPOSITES SIMULATION (Sunil Acharya)
- ARTIFICIAL INTELLIGENCE-DRIVEN COMPOSITES VIRTUAL TWINS IN THE 3DEXPERIENCE PLATFORM–INDUSTRY WORLD MODELS (Etienne Ardouin)
- FENNM: A HYBRID VARIATIONAL FRAMEWORK FOR ROBUST STRUCTURAL MODELLING AND INVERSE PROBLEM SOLVING (Frédéric Gosselin)
- FROM IMAGES TO INSIGHTS: AI FOR CHARACTERIZATION AND SIMULATION OF FIBER-REINFORCED COMPOSITES (Mahoor Mehdikhani)
- USING AI IN ENGINEERING, RESEARCH, AND EDUCATION (Julia Rubin)

SESSION ONE – AI-driven Design and Industrial Applications in Composites

- AI-DRIVEN DESIGN AND OPTIMIZATION OF ACTIVATED CARBON CANDIDATES FOR CARBON-BASED COMPOSITE SORBENTS IN CO₂ CAPTURE (Saeid Tajbakhsh)
- GENERATIVE DESIGN OF SEMI-AUXETIC CELLULAR LAMINATES VIA PROBABILISTIC MACHINE LEARNING AND BAYESIAN INFERENCE: AN UNCERTAINTY-AWARE DESIGN PERSPECTIVE (Fereshteh Hassani)
- KPC-RAG: A RETRIEVAL-AUGMENTED GENERATION CHATBOT FOR DEMOCRATIZING COMPOSITES KNOWLEDGE (Shayan Fahimi)
- MACHINE LEARNING-ASSISTED DESIGN OF STOCHASTIC VORONOI LATTICES FOR ENHANCED ENERGY ABSORPTION (H. Yazdani Sarvestani)
- PHYSICS-INFORMED BAYESIAN GAUSSIAN PROCESSES FOR ACCELERATED CHARACTERIZATION IN COMPOSITE MATERIALS: FROM FORMULATION TO PERFORMANCE (Paulina Portales Picazo)
- RAPID INVERSE DESIGN OF MESO-ARCHITECTED COMPOSITES USING SEQUENCE-BASED DEEP LEARNING (B. Gangadhara Prusty)

SESSION TWO– AI for Non-Destructive Testing and Structural Health Monitoring

- AI-ENABLED METROLOGY FRAMEWORK FOR DAMAGE ASSESSMENT OF HYDROTHERMALLY AGED UNIDIRECTIONAL GLASS-FIBER-REINFORCED THERMOPLASTICS (Jorge Palacios Moreno)
- IDENTIFICATION OF IMPACT DAMAGE IN COMPOSITE STRUCTURES FROM SPARSE STRAIN SENSOR DATA USING GRAPH NEURAL NETWORKS (Christopher Gorsky)

MACHINE LEARNING INTERPRETATION OF ACOUSTIC EMISSION SIGNALS FOR MIXED-MODE DAMAGE DETECTION IN COMPOSITES (Johannes Reiner)

THE EFFECT OF PHOTO-QUALITY ON PHOTO-LEARNING WAVINESS SEGMENTATION IN NCFS (Umeir Khan)

UNSUPERVISED CLASSIFICATION OF DEFECTS IN AFP PROFILOMETRY SCANS (Harvey Buhagiar)

SESSION THREE– Mechanical Behavior and Failure Prediction with AI

BAYESIAN INFERENCE ON FINITE ELEMENT INPUT PARAMETERS TO SIMULATE VARIABILITY IN PROGRESSIVE CRUSH TESTS OF COMPOSITES (Johannes Reiner)

DATA-EFFICIENT TRANSFER LEARNING FRAMEWORK FOR DIGITAL ALLOWABLES OF OPEN-HOLE COMPRESSION STRENGTH OF COMPOSITE LAMINATES (Xin Liu)

DEEP LEARNING AND MULTI-SCALE STRATEGIES FOR FAILURE MODELLING OF COMPOSITE STRUCTURES WITH COMPLEX MATERIAL ARCHITECTURES (Aewis Kw Hii)

EXPLAINABLE PHYSICS-INFORMED MACHINE LEARNING FOR MECHANICAL PROPERTY PREDICTION AND FORMULATION DESIGN OF RECYCLED POLYMER COMPOSITES (Oumayma Tajir)

GRAPH TRANSFORMERS FOR EFFECTIVE PREDICTION OF PROGRESSIVE FAILURE EVOLUTION IN COMPOSITE STRUCTURES (Luca Patrignani)

IMPACT DAMAGE PREDICTION OF COMPOSITE LAMINATES USING MACHINE LEARNING (Meysam Rahmat)

MODELING SHORT-FIBER REINFORCED COMPOSITES WITH ROTATION-FREE PARAMETRIC DMN (Huidi Ji)

PHYSICS INFORMED NEURAL NETWORKS FOR THE MICROMECHANICAL ANALYSIS OF COMPOSITE AND STRUCTURAL METAMATERIALS (Yunfa Zhang)

REINFORCEMENT LEARNING-DRIVEN IMPACT ENERGY OPTIMIZATION USING TRANSFORMER-BASED SURROGATE MODELING FOR MULTI-MODAL DAMAGE PREDICTION IN CFRP/GFRP LAMINATES (Bal Krishna Raj Vijeta)

ROBUSTNESS ANALYSIS OF DATA-DRIVEN IMPACT LOCALIZATION MODELS IN THE PRESENCE OF EXPERIMENTAL UNCERTAINTY (Emanuel Von Cramon-Taubadel)

USING EXPLAINABLE MACHINE LEARNING TO SUPPORT THE MODELING STRATEGIES OF COMPOSITE STRUCTURES (Marco Petrolo)

SESSION FOUR– Data-drive Surrogate Models and Accelerated Simulations

AI-ENABLED COMPOSITE TEXTILES WITHIN THE UPWARS SUSTAINABLE INNOVATION FRAMEWORK (Mohammad S. Rouhi)

AI-ENABLED MULTISCALE ICME WORKFLOW FOR INJECTION-MOLDED COMPOSITES IN LS-DYNA (Sunil Acharya)

BAYESIAN CALIBRATION AND UNCERTAINTY QUANTIFICATION TO SUPPORT BONDED COMPOSITE TEXTILE MODELING WITH LIMITED DATA (Matthew Kirby)

DATA-EFFICIENT VIRTUAL MATERIALS TWIN FOR TERNARY SHORT FIBER-MAGNETIC PARTICLE POLYMER COMPOSITES VIA AI-CALIBRATED MICROSTRUCTURE-BASED FEA (Yingnan Wang)

DEVELOPMENT OF PROBABILISTIC SURROGATE MODEL FOR UNCERTAINTY QUANTIFICATION IN LOW VELOCITY IMPACT (LVI) OF CARON/EPOXY WOVEN COMPOSITES (Sanghyun Yoo)

FEASIBILITY-AWARE BAYESIAN OPTIMIZATION OF COMPOSITE STRUCTURES WITH FAILURE CONSTRAINTS (Luca Patrignani)

MACHINE LEARNING-BASED MULTISCALE MODELLING OF COMPOSITE LAMINATES FOR EFFICIENT STRUCTURAL SIMULATIONS (Carlos González)

MACHINE LEARNING-ENABLED BAYESIAN INFERENCE FRAMEWORK FOR CONSTITUENT HYDROGEN PERMEABILITIES IN POLYMER COMPOSITES (Mustafa Okumuş)

PHYSICS-LED GENERATION OF MISSING DATA FOR EFFECTIVE USE OF AI/ML (Harika Tankasala)

UNCERTAINTY CHARACTERIZATION OF THERMAL SHOCK PERFORMANCE OF AEROSPACE COMPOSITES WITH PHYSICS-INFORMED NEURAL NETWORKS (Juhyeong Lee)

SESSION FIVE– AI and Statistical Methods for Process Modelling of Composites

BAYESIAN OPTIMIZATION OF NON-GAUSSIAN PROCESS-INDUCED DEFORMATIONS IN AEROSPACE COMPOSITES (Kendall A. Johnson)

GENERATIVE MATERIAL CARDS FOR PROCESS SIMULATION (Goran Fernlund)

MACHINE LEARNING SURROGATE-ASSISTED OPTIMIZATION OF CURE CYCLES IN MULTI-MATERIAL THERMOSET COMPOSITE SYSTEMS (Alberto Mussali)

ROUGHNESS DESCRIPTORS DISCOVERY DRIVEN BY THE PREPEG TAPES CONSOLIDATION PROCESS (Francisco Chinesta)

THREE-DIMENSIONAL KINEMATICALLY ENRICHED HOMOGENISATION FOR AI-ASSISTED CONSOLIDATION ANALYSIS OF DISCONTINUOUS COMPOSITES (Maria Onoufriou)

SESSION SIX– AI for Intelligent Composites Manufacturing and Control

A REDUCED ORDER MODELING APPROACH TO PHYSICS-BASED SIMULATION OF AUTOMATED FIBRE PLACEMENT (Nima Bakhshi)

A SURROGATE MODEL FOR CONTINUOUS RESISTANCE WELDING OF THERMOPLASTIC COMPOSITES (Marco Didone)

COMBINING PHYSICS-BASED AND DATA-DRIVEN METHODS TO OPTIMIZE SUB-MELT CONSOLIDATING THERMOPLASTIC TAPES (OATMEAL) (Joseph G. Kirchhoff)

REAL-TIME FLOW-FRONT MONITORING AND CLOSED-LOOP INJECTION CONTROL IN TRANSPARENT SLA-PRINTED HOLLOW STRUCTURES (Heinrich Pfander)

AI-Enabled Forward Prediction and Inverse Design of Composite Materials

Pavana Prabhakar¹

¹ Charles G. Salmon Associate Professor, Mechanical Engineering
University of Wisconsin-Madison, USA, pavana.prabhakar@wisc.edu

Composite materials offer exceptional opportunities for tailoring stiffness, strength, and failure resistance through microstructural and architectural design. At the same time, this flexibility creates a major challenge as the response of composites depends strongly on heterogeneity, spatial arrangement, weave architecture, and damage evolution, making design exploration computationally expensive when based solely on high-fidelity simulations. For a composites community increasingly interested in AI, the key question is not simply whether AI can fit simulation data, but how it can be used in a way that remains mechanically meaningful and useful for design.

In this talk, I will address that question across several classes of composite materials. I will start with deep learning frameworks for predicting full-field stress distributions in heterogeneous composites, showing how image-based surrogates can capture the influence of volume fraction and spatial randomness while retaining more mechanistic information than scalar property predictions alone. We will then move to learning richer mechanical responses from composite geometry, including parameterized representations of constitutive behavior. Building on these forward models, we will next address inverse design of woven composite architectures, with emphasis on the challenges of non-unique structure–property mappings and the role of interpretable texture-based features in guiding design. Finally, I will extend these ideas to failure-aware design through convolutional neural network surrogates for phase-field fracture simulations, enabling efficient optimization of composite microstructures for improved tensile strength.

The central message of my talk is that AI has the potential to become a practical tool for composite materials research when it is coupled with mechanics, informed representations, and design objectives. Rather than replacing established modeling approaches, AI frameworks complement simulation by accelerating prediction, enabling inverse exploration of large design spaces, and providing new pathways toward data-driven composite design.

AI for Scientific Discovery and Engineering Design

Steven L. Brunton¹

¹ Professor of Mechanical Engineering, University of Washington, USA, sbrunton@uw.edu

This work will discuss several key challenges and opportunities in the use of machine learning for scientific discovery and engineering design. In particular, I will describe how machine learning may be used to develop accurate and efficient nonlinear dynamical systems models for complex natural and engineered systems. I will emphasize the need for interpretable and generalizable data-driven models, such as the sparse identification of nonlinear dynamics (SINDy) algorithm, which identifies a minimal dynamical system model that balances model complexity with accuracy, avoiding overfitting. I will also introduce several key benchmark problems in dynamical systems and fluid dynamics that provide a diversity of metrics to assess modern machine learning techniques. Because fluid dynamics is central to transportation, health, and defense systems, we will emphasize the importance of machine learning solutions that are interpretable, explainable, generalizable, and that respect known physics.

From Process Simulation to Quality-Aware Digital Twins in the Age of AI

Anoush Poursartip¹

¹ Professor, Department of Materials Engineering, The University of British Columbia &
Director of Research and Development, Convergent Manufacturing Technologies, Inc., Canada,
anoush.poursartip@ubc.ca

The vision of a quality-aware digital twin framework linking materials discovery, product development, certification, production control and optimization, and even in-service management is no longer a dream. This is thanks to AI methods which are promising a supercharging of prior digitalization advances in composites processing and manufacturing. These methods include ML surrogate and inverse models, formal uncertainty quantification and propagation methods, and the underlying data science methods for managing and aggregating large and disparate data sets from both simulation and experiment. A quality-aware digital framework can then be rolled up into much broader digital thrusts such as Model-Based Systems Engineering (MBSE). This will enable a step-change in our use of digital tools for composites processing and manufacturing in the near future, reducing risk, timelines, and cost.

Artificial Intelligence-Driven Composites Virtual Twins in the 3DEXPERIENCE Platform– Industry World Models

Etienne Ardouin¹, Florent Savine²

¹ Etienne Ardouin (Dassault Systemes, Woodland Hills, California), etienne.ardouin@3ds.com

² Florent Savine (Dassault Systemes, Velizy, France), florent.savine@3ds.com

The increasing complexity and wider applications of composite materials and their manufacturing processes demands a new paradigm in engineering design — one that transcends conventional simulation-driven workflows and embraces the transformative potential of Artificial Intelligence. This presentation investigates a series of integrated AI applications spanning the full composites engineering value chain, from materials characterization at the microstructural scale through to intelligent manufacturing process planning, all realized within the industrial context of Dassault Systèmes' 3DEXPERIENCE Platform.

At the materials scale, Machine Learning models developed within the BIOVIA and SIMULIA environments are employed to predict constitutive material behavior directly from microstructural descriptors, substantially reducing the reliance on costly and time-intensive physical testing campaigns. These data-driven surrogate models demonstrate strong predictive fidelity across a range of fiber-reinforced composite architectures, offering a computationally efficient pathway to virtual material qualification. At the structural and thermal analysis scale, AI-augmented simulation methodologies within SIMULIA are explored to enable real-time design feedback loops for macroscopic composite assemblies operating under complex multi-physics loading conditions demanded by aerospace and automotive certification standards.

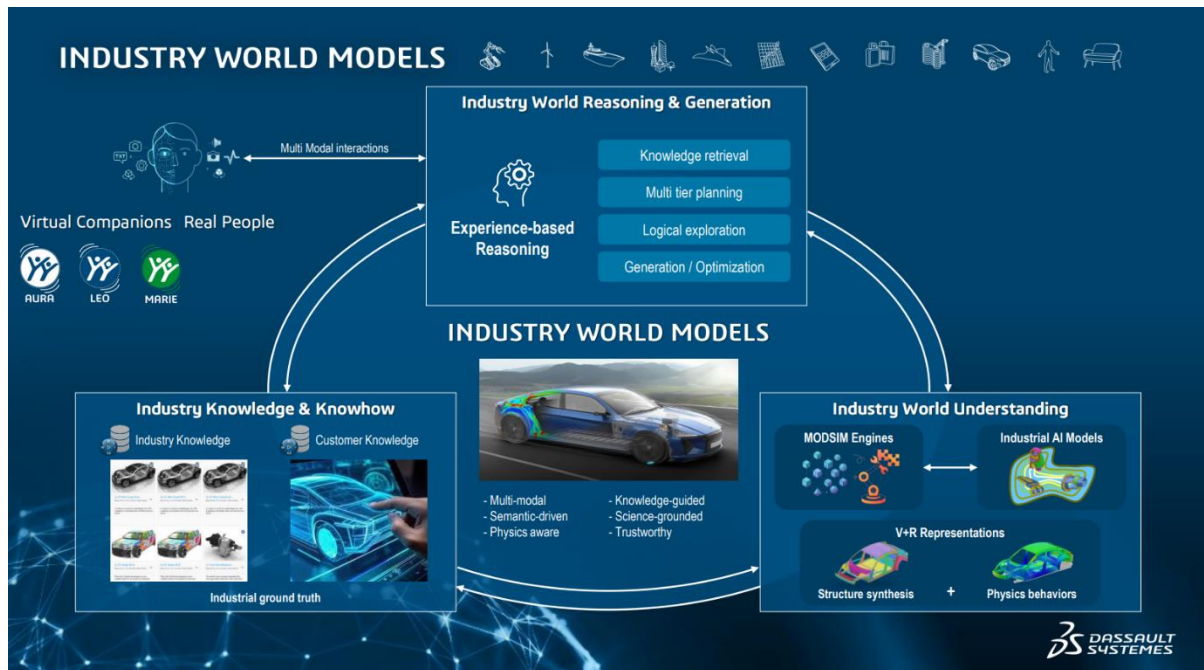
Beyond simulation, this work introduces the concept of Agentic AI in the form of Virtual Companions — autonomous, context-aware AI agents embedded within CATIA for Composites Design Engineering and DELMIA for Manufacturing Process Planning. These companions assist engineers by interpreting design intent, facilitating design change for alternative laminates strategies, flagging manufacturability constraints, and dynamically sequencing production operations, effectively acting as intelligent co-engineers throughout the product development lifecycle.

Collectively, these advances illustrate a cohesive, platform-native AI strategy for composites that is both scientifically rigorous and industrially deployable.

References:

- [1] Dassault Systemes WhitePaper: “[Introducing industry world models](#)”
- [2] V. Oancea, J. Bi, S. Chen “Fine-Scale Feature Preservation-Oriented Geometric Pre-training for AI-Driven Surrogate Modeling” – April 2025 - DOI:10.48550/arXiv.2504.20110
- [3] F. Savine “Explicit composite ply location, orientation and shape optimization via a feature-mapping method” - May 2025 - WCSMO-16
- [4] F. Savine “Simultaneous optimization of unconventional stiffener layouts and composite layups applied to large cylindrical shell structures” - 2022 Phd thesis, Sorbonne Université

- [5] Dassault Systemes WhitePaper: “[AI-Driven Generative Experiences](#)”
- [6] NVIDIA Article: “[How Industrial AI and Digital Twins Accelerate Design, Engineering and Manufacturing Across Industries](#)”



Industry World Models introduction at NVIDIA GTC 2026 Conference

Credibility Over Accuracy: AI, Physical Fidelity, and the Future of Composites Simulation

Sunil Acharya, PhD

¹ Synopsys Inc, Sunil.Acharya@Synopsys.com

The past decade has witnessed an unprecedented, and at times uncritical, expansion of artificial intelligence across the industrial spectrum. From the modernization of legacy manufacturing to the high-stakes development of First-of-a-Kind (FOAK) emerging technologies, AI is fundamentally reshaping the engineering lifecycle. However, beneath the digital transformation narrative lies a fragmented reality where AI adoption is uneven and its physical boundaries are often poorly defined.

This talk provides a practitioner's cross-domain survey of AI applications across the full industrial value chain, including material discovery, product design, manufacturing, and real-time process control. The presentation explores how accelerated computing is redefining the limits of simulation by enabling a shift from static validation to dynamic, real-time insights. The landscape is evaluated through three distinct lenses:

- **Where AI genuinely transforms practice:** This involves utilizing GPU-accelerated surrogate modeling and physics-informed neural networks to achieve orders-of-magnitude speedups in multi-physics coupling.
- **Where AI is applied in hybrid form:** This involves creative use of AI with complementary methodologies to enhance existing workflows.
- **Where AI faces fundamental barriers:** This includes addressing data scarcity in high-capital FOAK projects, the "black box" interpretability crisis, and the challenge of enforcing rigorous physical laws within learned models.

A critical observation of this survey is the existence of "borrowed successes," which are proven AI methodologies from fields such as fluid dynamics and structural health monitoring that offer high applicability to composites but remain largely underutilized. Central to this discussion is the role of digital twins for predictive maintenance and uncertainty quantification (UQ). In safety-critical workflows where experimental data is often prohibitively expensive, model credibility must be the operative standard rather than mere predictive accuracy.

Drawing from these broad industrial lessons, the session argues that the most productive role for AI in composites is as an intelligent interface layer. This framework manages uncertainty across scales, ensures reliable lifecycle monitoring, and enables transferability across evolving material systems. The talk concludes by defining the validation frameworks and data infrastructure necessary to move toward trustworthy, certification-ready AI integration in composite simulation.

FENNM: A Hybrid Variational Framework for Robust Structural Modelling and Inverse Problem Solving

Mohammed Abda¹, Lucas Berthet¹, Mohsen Hamed¹, Elsa Piollet², Christopher Blake²,
Bruno Blais³, Frédéric P. Gosselin^{1*}

¹ Laboratory for Multiscale Mechanics (LM2), Department of Mechanical Engineering, Polytechnique Montréal, Canada

² Maya HTT, Canada

³ CHAOS Laboratory, Department of Chemical Engineering, Polytechnique Montréal, Canada

*Presenting Author frederick.gosselin@polymtl.ca

Many of the important challenges in the modelling of composite materials and their processing can be formulated as inverse problems: identifying the rheological properties of a resin from observations on how it flows into a real part, identifying the multi-scale properties of a composite part from micro- or macro-scale observations, or tuning the fracture mechanics of a model based on experimental observations. While Physics-Informed Neural Networks (PINNs) offer a promising framework for combining experimental data with mathematical models to solve these inverse problems, they often lack robustness in practical engineering settings. Standard PINNs are sensitive to initialization and typically require extensive problem-specific tuning to balance competing loss terms, which can hinder convergence for stiff or highly nonlinear systems [1, 2].

To address these limitations, this research introduces the Finite Element Neural Network Method (FENNM), a hybrid solver that integrates the data-driven flexibility of deep learning with the rigorous formalism of the finite element method (FEM). FENNM is developed within the Petrov-Galerkin framework, where a neural network generates the global nonlinear space of trial solutions while the test functions are selected from the nonvanishing Lagrange shape function space.

Unlike previous variational PINN variants that utilize vanishing test functions—thereby losing critical interface information—FENNM explicitly incorporates flux terms at element boundaries. This architectural choice allows natural boundary conditions and point loads to be embedded directly into a single residual loss function, significantly enhancing training stability. To maintain computational efficiency, we utilize tensor product operations to evaluate Gauss quadrature integration across the domain as detailed.

The method's efficacy is demonstrated through case studies pivotal to composite structural modelling. We showcase FENNM's ability to solve inverse and parametric identification problems, identifying unknown physical properties—such as surface absorptivity in a thermal panel model—using as little as a single data point. Furthermore, FENNM is shown to function effectively on irregular meshes generated by standard industrial tools like Gmsh. By bridging the gap between machine learning and traditional numerical methods, FENNM provides a robust framework for the next generation of structural modelling tools in the aerospace and construction industries.

References:

- [1] Abda, M., Hamed, M., Piollet, E., Blake, C., Gosselin, F.P. “The Finite Element Neural Network Method: One Dimensional Study” Next Research, 2, 4, 100885 (2025)
- [2] Abda, M., Berthet, L., Hamed, M., Hibatullah, D., Piollet, E., Blake, C., Blais, B., Gosselin, F.P. “The Finite Element Neural Network Method: Leveraging Non-Vanishing Shape Functions in Space-Time-Parameter Framework”, Research Square Preprint [<https://doi.org/10.21203/rs.3.rs-7702801/v1>]

Learning Composites Microstructure Evolution from XCT Time-Series Using 3D Conditional Generative Models

Xiangyu Lu¹, Abraham George Smith¹ and Mahoor Mehdikhani²

¹ Department of Computer Science DIKU, University of Copenhagen, Denmark

² Presenting Author Department of Materials Engineering (MTM), KU Leuven, Belgium,
mahoor.mehdikhani@kuleuven.be

Understanding the microstructural evolution of fibre-reinforced composites under mechanical loading is essential for predicting damage and failure in structural applications. Fibre-reinforced polymer composites exhibit complex microscale behaviour in which local deformation and damage mechanisms develop progressively before macroscopic failure occurs. Recent advances in synchrotron X-ray computed tomography (XCT) enable in situ imaging of composite microstructure during mechanical testing, producing high-resolution 3D datasets that reveal fibre-level structural evolution. However, analysing and predicting the evolution of such large 3D datasets remains challenging. In this work, we investigate whether deep generative models can learn to predict microstructural evolution directly from XCT time-series data, enabling the generation of physically plausible future states of a composite microstructure under increasing load.

We formulate the problem as a 3D conditional image-to-image translation task, in which an XCT volume representing the composite microstructure at a given load level is used to predict the corresponding microstructure at a higher load state. The dataset in this study consists of a synchrotron XCT time series of a unidirectional glass/epoxy composite subjected to in situ tensile loading. The dataset contains high-resolution 3D volumes acquired at progressively increasing load levels. At this spatial resolution, individual fibres can be clearly resolved, allowing detailed observation of fibre arrangement and microstructural deformation as loading increases.

To learn this transformation, we implement a 3D conditional generative adversarial network (cGAN). The generator adopts a 3D U-Net-based encoder-decoder architecture, which is well suited for volumetric image translation tasks. The encoder progressively compresses the input volume through stacked 3D convolutional layers, capturing hierarchical structural features of the fibre microstructure. The decoder then reconstructs the predicted higher-load microstructure using transposed convolutions. Skip connections between encoder and decoder stages preserve high-resolution spatial information, which is critical for accurately representing individual fibres and fine microstructural details. The discriminator is implemented as a 3D convolutional classifier that distinguishes between real XCT patches and generated predictions, thereby encouraging the generator to produce outputs that are statistically consistent with the real data distribution (Fig. 1).

Training is performed using a combination of adversarial loss and reconstruction loss, encouraging the generator to produce outputs that are both structurally accurate and statistically realistic. The reconstruction loss is implemented using voxel-wise similarity metrics such as mean absolute error (MAE) and mean squared error (MSE), which help maintain correspondence between generated and ground-truth volumes. Because full XCT volumes are prohibitively large for direct training, the data are decomposed into smaller overlapping 3D patches, which significantly increases the effective number of training samples while keeping memory requirements manageable.

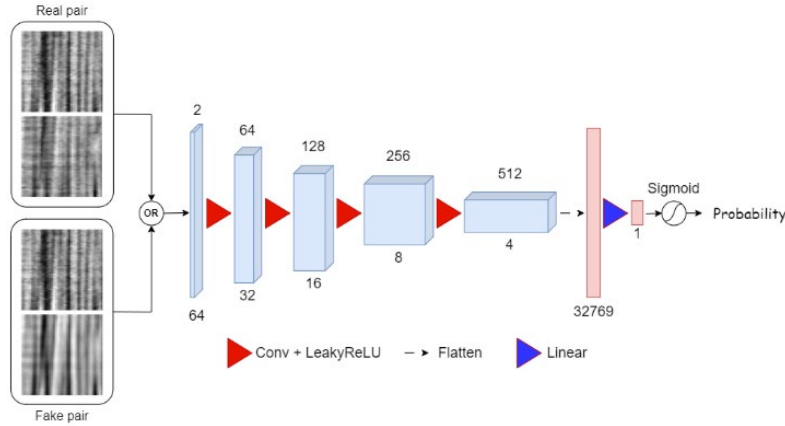


Figure 1. Discriminator architecture. The input is an image pair concatenated along the channel axis.

A key aspect of the proposed methodology is the evaluation of multiple training configurations and dataset pairings. Instead of training only on consecutive load states, the framework is tested using several input-target combinations representing different levels of microstructural change. For example, models are trained to predict moderate microstructural evolution between nearby load steps as well as more significant transformations between early loading states and states closer to failure. This approach allows us to assess the generalization capability and robustness of the generative framework across varying prediction difficulties and structural differences. In addition, several independent training runs and dataset are explored to evaluate the stability and reproducibility of the learned generative mappings.

The results demonstrate that the proposed 3D cGAN framework is capable of learning important aspects of composite microstructure evolution. In particular, the model successfully reproduces deformation patterns observed in the XCT time series (Fig. 2). Generated volumes preserve the overall morphology of the fibre bundle and realistically capture subtle shifts in fibre positions as the material deforms under increasing tensile load. Both quantitative reconstruction metrics and qualitative visual comparisons indicate that the generated microstructures closely resemble the ground-truth XCT data. These findings demonstrate that deep generative models can effectively learn continuous structural transformations of complex 3D fibre architectures from experimental imaging data, at least for small deformation regimes.

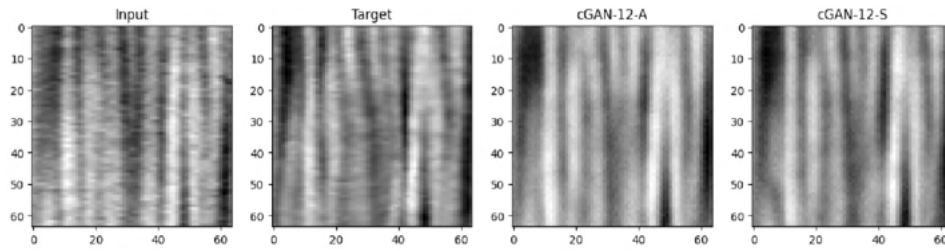


Figure 2. A generation example of cGAN-12-A and cGAN-12-S on 00-to-12 validation set.

Future work will extend this framework toward more advanced predictive capabilities. In particular, further studies will investigate the integration of physics-informed inputs, such as stress or strain fields, and the development of physically motivated loss functions to enable the prediction of localized damage mechanisms and failure processes within fibre-reinforced composites. Such developments could ultimately contribute to data-driven modelling approaches for understanding and predicting microscale deformation and failure in advanced composite materials.

References:

- [1] M. Mirza and S. Osindero, “Conditional generative adversarial nets,” arXiv preprint arXiv:1411.1784, 2014.

Using AI in Engineering, Research, and Education

Julia Rubin¹

¹ Department of Electrical and Computer Engineering, University of British Columbia, Canada,
mjulia@ece.ubc.ca

As Generative AI (GenAI) techniques are rapidly transforming virtually every area of our lives, the responsible, critical, and effective use of these techniques becomes more important than ever. This talk will discuss observations and lessons learned from a number of studies my research group and I have conducted to examine experiences and strategies for effective human-AI collaboration in areas such as software development, legal analysis, and scientific research. We will also discuss pedagogical interventions we devised and our observations of students' experiences with GenAI within the scope of an upper-level undergraduate course on software engineering. Our analysis results lead to a number of suggestions for future researchers, educators, and industry practitioners seeking to deploy human-in-the-loop AI frameworks.

Session One

1 AI-DRIVEN DESIGN AND INDUSTRIAL APPLICATIONS IN COMPOSITES

AI-Driven Design and Optimization of Activated Carbon Candidates for Carbon-Based Composite Sorbents in CO₂ Capture

Faezeh Hajiali¹, Saeid Tajbakhsh², Naoko Ellis³ and Bhushan Gopaluni⁴

¹ Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, BC, Canada, Faezeh.hajiali@gmail.com

² Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, BC, Canada

³ Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, BC, Canada & Bioproducts Institute, University of British Columbia, Vancouver, BC, Canada

⁴ Department of Chemical and Biological Engineering, The University of British Columbia, Vancouver, BC, Canada & Bioproducts Institute, University of British Columbia, Vancouver, BC, Canada, bhushan.gopaluni@ubc.ca

The development of high-performance carbon capture materials requires efficient strategies for identifying promising sorbent candidates within large and complex design spaces. Activated carbons derived from sustainable and low-cost precursors are attractive for CO₂ capture because their adsorption performance depends strongly on pore structure, surface chemistry, and other physicochemical characteristics. In carbon-based composite sorbent development, selection of the activated carbon phase is a critical design step, yet conventional experimental screening remains resource-intensive and slow.

This work presents an AI-driven design and optimization framework for accelerated selection of activated carbon candidates for CO₂ capture applications. The approach combines a multi-headed one-dimensional convolutional neural network (MH1DCNN) with multi-fidelity Bayesian optimization (MFBO) to improve search efficiency while reducing dependence on expensive high-fidelity evaluations. The MH1DCNN learns nonlinear relationships between physicochemical properties and CO₂ uptake and is used as a low-cost predictive model. Literature-reported data from 841 activated carbon samples are treated as high-fidelity evaluations, while MH1DCNN predictions provide low-fidelity guidance. These information sources are integrated through a probabilistic surrogate model that balances exploration of uncertain regions with exploitation of promising candidates.

The proposed framework reduces the number of required high-fidelity evaluations by more than 75% and identifies top-performing candidates using only 13 high-fidelity acquisitions. The study demonstrates how multi-fidelity AI can support data-efficient material selection and optimization, providing a practical computational workflow for the design of carbon-based sorbent systems and related composite formulations for CO₂ capture.

Keywords: Composite Sorbents; Activated Carbon; CO₂ Capture; Machine Learning; Multi-Fidelity Optimization

References:

- [1] Hajiali, F., Ellis, N. & Gopaluni, B. From biomass waste to CO₂ capture: a multi-fidelity machine learning workflow for high-throughput screening of activated carbons. *npj Comput Mater* 11, 363 (2025).
- [2] Wang, J., Pu, Q., Ning, P. and Lu, S. Activated carbon-based composites for capturing CO₂: a review. *Greenhouse Gas Sci Technol*, 11: 377-393 (2021).

Generative Design of Semi-Auxetic Cellular Laminates via Probabilistic Machine Learning and Bayesian Inference: An Uncertainty-Aware Design Perspective

Fereshteh Hassani^{1,2}, Huilong Fu³, Navid Zobeiry³, and Sardar Malek^{1,2}

¹ Department of Civil Engineering, University of Victoria, Canada, fhassani@uvic.ca

² Centre for Advanced Materials and Related Technology (CAMTEC), Canada

³ Department of Materials Science and Engineering, University of Washington, USA

Cellular materials are widely used in lightweight applications because their mechanical properties can be tailored through geometric design [1]. Achieving low structural weight without sacrificing mechanical performance is a longstanding objective in applications such as aerospace, where structural mass directly affects performance and fuel efficiency. To address this trade-off, researchers have proposed various cellular microstructures and topologies, as well as performance optimization strategies to improve performance-to-weight efficiency [2, 3]. Recently, semi-auxetic cellular laminates have been introduced to enhance the performance of lightweight materials by stacking hexagonal and re-entrant honeycomb layers [4]. These laminates harness the opposing deformation behaviour of auxetic and non-auxetic layers to activate a stiffening mechanism without a significant weight penalty. Prior work established the concept of 3D-printed semi-auxetic laminates and demonstrated that a parametrically designed Positive-Negative-Positive (PNP) architecture can achieve remarkably enhanced mechanical efficiency compared with its constituent honeycomb layers alone. Through combining finite element simulations, surrogate modelling, multi-objective optimization, and experimental validation, it was proven that geometric design can be used to tailor stiffness and density in cellular laminates.

This study presents a probabilistic inverse-design framework for targeted geometry discovery in 3D-printed semi-auxetic laminates. The design space is defined by six geometric input parameters, corresponding to the unit-cell features of the semi-auxetic laminate, and one targeted mechanical output associated with stiffness-to-weight performance. A Gaussian process regression (GPR) surrogate model is first trained to learn the nonlinear mapping between geometry and performance, enabling rapid prediction across the design space. The workflow further incorporates Sobol sensitivity analysis to quantify the relative influence of the six geometric parameters on the targeted response, thereby identifying which parameters dominate the inverse-design landscape. The GPR surrogate is then embedded within a multi-stage Markov chain Monte Carlo (MCMC) framework to infer posterior distributions of feasible geometric designs that satisfy a prescribed target response (defined by a mean value and standard distribution) rather than a single deterministic optimum. The resulting posterior predictive distributions reveal not only likely high-performing geometries, but also the uncertainty and identifiability of each design variable under the imposed performance objective.

The proposed framework moves beyond conventional forward optimization by introducing a Bayesian generative-design strategy for semi-auxetics. Instead of returning only a Pareto-optimal boundary, it provides a distribution of candidate geometries consistent with a desired modulus-efficiency target, offering improved robustness for design exploration and manufacturability assessment. Overall, this work establishes a new data-driven route for geometry optimization of architected semi-auxetics by integrating surrogate modelling, probabilistic posterior sampling, and global sensitivity analysis. It opens the door to uncertainty-aware design of next-generation 3D-printed cellular composites.

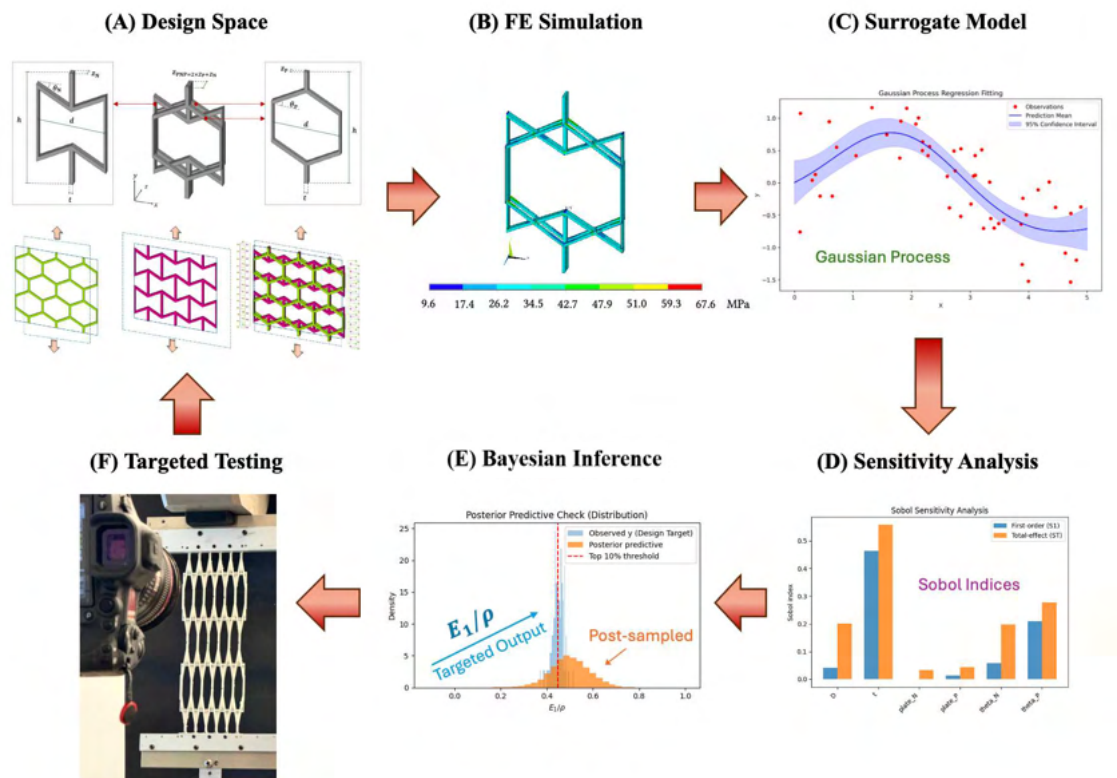


Figure 1 Bayesian Inverse Design of Cellular Semi-Auxetic Laminates

Keywords:

Semi-auxetic cellular laminates, finite element method, probabilistic machine learning, sensitivity analysis, Bayesian inference

References:

- [1] M. F. Ashby, The properties of foams and lattices, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences 364 (1838) (2006) 15–30. doi:10.1098/rsta.2005.1678.
- [2] P. Wang, F. Yang, B. Zheng, P. Li, R. Wang, Y. Li, H. Fan, X. Li, Breaking the tradeoffs between different mechanical properties in bioinspired hierarchical lattice metamaterials, Advanced Functional Materials 33 (45) (2023) 2305978. doi:10.1002/adfm.202305978.
- [3] P. Zhang, F. Bai, Y. Liu, Y. Ma, W. Zeng, Y.-J. Yang, L. Liu, W. Wang, Design and optimization of high stiffness tetrahedral lattice structure, Additive Manufacturing 102 (2025) 104719. doi:10.1016/j.addma.2025.104719.
- [4] F. Hassani, H. Fu, N. Zobeiry, S. Malek, Semi-Auxetic Cellular Laminate: A Novel Lightweight Stiff Material, Composite Structures (under review)

KPC-RAG: A Retrieval-Augmented Generation Chatbot for Democratizing Composites Knowledge

Shayan Fahimi¹, Marcelo Gorrini², Anoush Poursartip² and Casey J. Keulen²

¹ Presenting Author Composites Knowledge Network, The University of British Columbia, Canada, shayan@composites.ubc.ca

² Composites Knowledge Network, The University of British Columbia, Canada

Composites manufacturing relies on a large body of knowledge that is difficult to access, interpret, and apply consistently in practice. Useful guidance is spread across definitions, method documents, troubleshooting notes, and case studies, while its interpretation depends on process context and engineering judgment [1]. This creates a practical barrier for both smaller manufacturers lacking in-house expertise and larger organizations where knowledge is spread across teams and sites. In 2021, the Composites Knowledge Network (CKN) launched a freely available, online knowledge resource referred to as the Knowledge in Practice Centre (KPC) <https://compositeskn.org/KPC/A1> to address these challenges. In this work, we present a retrieval-augmented generation (RAG) chatbot that is grounded in the KPC, with the goal of providing a reliable interface to curated, current, and peer-reviewed composites knowledge beyond what document search or a general-purpose large language model alone can offer

The KPC organizes composites knowledge into clearly defined topics, relationships, and contextual explanations rather than isolated documents or unstructured text [2]. This structure makes KPC data particularly well-suited for LLM retrieval, as it aligns with modern knowledge-grounded approaches that rely on well-defined concepts, traceable sources, and semantic consistency [3]. Rather than answering from internal model memory, the RAG system first retrieves the most relevant material from the KPC articles and generates a response grounded in that curated context. By coupling the chatbot to a living knowledge base, the system can evolve alongside advances in materials, processes, standards, and qualification methods, while maintaining a clear governance model for content validation.

The system pipeline, illustrated in Figure 1, covers two main stages: data ingestion and indexing, followed by the main chat flow and RAG cycle. During ingestion, technical composites content is parsed, sanitized, and chunked into segments with segment overlap, then embedded and stored in a vector index. At query time, the engine retrieves the most semantically similar document chunks and filters them using a similarity cutoff to prevent responses from loosely related material [4]. The finalized prompt, enriched with curated context and domain-specific instructions, is submitted to the general LLM model, configured at a low enough temperature to keep responses factual and deterministic.

The user interface, shown in Figure 2, reflects the same design objective. Beyond the generated answer, the application presents an “Analysis and Sources” panel with a confidence score, source timeline, and ranked references linked back to the underlying KPC resources. This citation-based response strategy allows users to verify information, check whether the source is current, and navigate directly into the original KPC knowledge article. This gives the user an opportunity to further explore static documents that were written and reviewed by a subject matter professional, a feature that improves explainability and is becoming more important in safety-critical and regulated applications.

To evaluate system performance, a benchmark of question-answer items was constructed from the KPC

website. Items were filtered to include only QA and task-style prompts, focusing the benchmark on answer generation quality. Each response was scored on a 1-to-5 scale using GPT-4o as an external judge. The system achieved a mean score of 4.38/5.0 and a median of 5.0/5.0, with more than 85% scoring 4.0 or higher. Performance was stronger on semantic-similarity items (mean 4.52) than exact-match items (mean 4.12), indicating reliable preservation of technical content even when phrasing differed from the reference answer. Lower scores were mostly seen for prompts that needed specific process, geometry, or case-based details. This suggests that future improvements will depend more on better retrieval of detailed information and tighter control of responses.

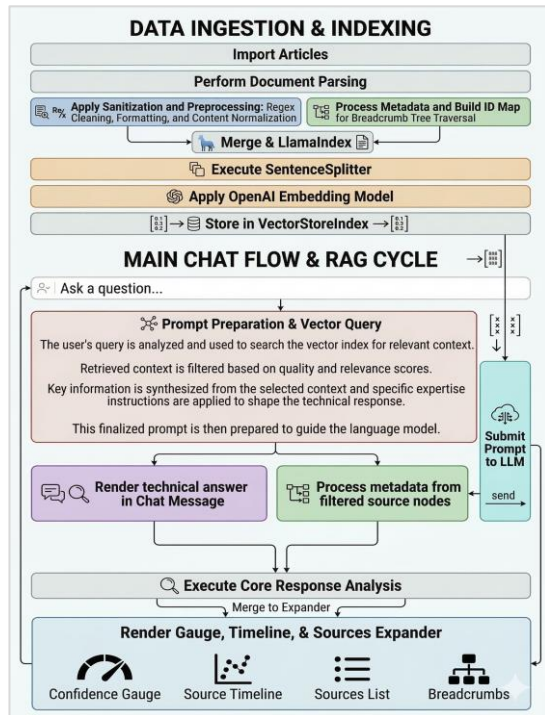


Figure 1: Flowchart of KPC-RAG chatbot

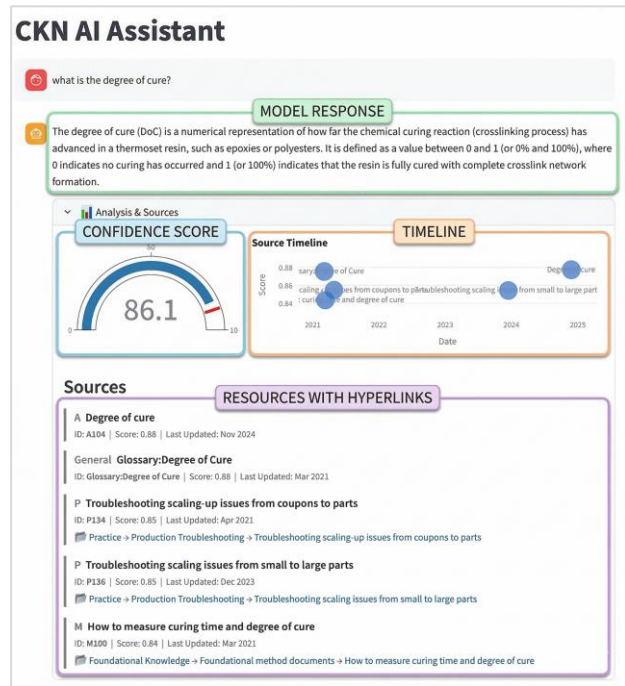


Figure 2: Current application interface and provided information

A key contribution of this work is demonstrating how the same AI system can serve both SMEs and large organizations. For SMEs, the chatbot functions as a knowledge companion. For larger organizations, it acts as an intermediate layer reinforcing consistent terminology and best practices across teams and sites. Critically, KPC content is continuously updated and monitored by subject-matter professionals, directly addressing the common weakness of AI systems coupled to static datasets. The results show that a domain-specific chatbot becomes more useful when tied to a curated knowledge structure offering a practical and responsible path toward AI-supported knowledge access.

References:

- [1] G. Kapoor *et al.*, "Intelligent Manufacturing Support: Specialized LLMs for Composite Material Processing and Equipment Operation," doi: 10.1115/MSEC2025-155920.
- [2] C. Keulen *et al.*, "The Knowledge in Practice Centre: A Resource for Applying Scientific Knowledge to Composites Manufacturing," presented at the CANCOM 2022 - Canadian International Conference on Composite Materials, Fredericton-Moncton, NB, Canada, Aug. 2022.
- [3] P. Lewis *et al.*, "Retrieval-Augmented Generation for Knowledge-Intensive NLP Tasks," in *Advances in Neural Information Processing Systems*, Curran Associates, Inc., 2020.
- [4] Alternates.ai and H. Gupta, "Alternates.ai - AI Agent Marketplace," Alternates.ai. Accessed: Mar. 08, 2026. [Online]. Available: <https://www.alternates.ai/knowledge-hub/articles/building-domain-specific-knowledge-bots-rag-systems>

MACHINE LEARNING-ASSISTED DESIGN OF STOCHASTIC VORONOI LATTICES FOR ENHANCED ENERGY ABSORPTION

M. Thompson¹, H. Yazdani Sarvestani², A. Sohrabi-Kashani², E. Kiyani³, E. Filippi²,
D.A.V. Egmond⁴, M. Rahmat², B. Ashrafi², M. Karttunen^{1,5}

¹Department of Chemistry, The University of Western Ontario, London, ON N6A 5B7, Canada

Presenting Author: ²Aerospace Manufacturing Technologies Centre, National Research Council Canada, 5145 Decelles Avenue, Montreal, QC H3T 2B2, Canada

hamidreza.yazdani@nrc-cnrc.gc.ca

³Department of Applied Mathematics, Brown University, Providence, RI 02912, USA

⁴Advanced Materials Research Facility, Clean Energy Innovation Research Centre, National Research Council Canada, 2620 Speakman Drive, Mississauga, ON L5K 1B4, Canada

⁵Department of Physics and Astronomy, The University of Western Ontario, London, ON N6A 3K7, Canada

Abstract

Lattice materials are widely used in lightweight structural and multifunctional components because they offer high specific stiffness and strength. Classical micromechanics and homogenization approaches provide powerful tools for predicting the effective properties of fiber-reinforced composites and periodic lattices [1,2], but they rely on strong assumptions of regularity and determinism. In contrast, stochastic Voronoi lattices exhibit irregular, non-periodic architectures that can enhance energy absorption and damage tolerance, while making their mechanical behaviour far harder to predict and optimize. This work develops a machine learning (ML)-assisted framework that couples finite element analysis (FEA), data-driven modelling and additive manufacturing to systematically design and optimize stochastic Voronoi lattices for enhanced mechanical performance.

Three-dimensional beam-based Voronoi lattices were generated in nTop within a 25 mm cube at 10% relative density, using 40 seeds connected along cell edges. To continuously tune geometric disorder, we introduce the Relaxation Iteration (RI) parameter, inspired by centroidal Voronoi tessellation. RI controls the number of centroidal relaxation steps applied to the seed distribution, spanning a spectrum from highly stochastic ($RI \approx 0$) to near-Kelvin-like periodic architectures ($RI \geq 2500$). The resulting geometries were discretized using solid tetrahedral elements and analysed under quasi-static compression in ANSYS with a bilinear isotropic hardening model for a vat-photopolymer resin, calibrated from uniaxial tensile tests on 3D-printed dogbone coupons. The simulations provided 54 data points covering total energy absorption, energy absorption to peak load, stiffness, maximum reaction force and displacement at failure as functions of RI.

To fabricate and validate selected designs, Voronoi lattices were printed using LCD-based vat polymerization (PlasCLEAR resin) and tested in compression at 0.1 mm s^{-1} in an MTS frame, with in-situ imaging of the deformation modes. Because the FEA dataset is too small for conventional deep learning, we constructed an augmented dataset by cubic-spline interpolation over $RI \in [0, 3000]$, followed by controlled Gaussian noise injection and random sampling to generate 350 synthetic samples while keeping all original FEA points. Covariance analysis and lag plots confirmed that the augmented dataset preserved the statistical structure and auto-

dependencies of the original data. A multilayer perceptron (MLP) with multiple hidden layers and dropout regularization was then trained to map RI to the five mechanical metrics. The network achieved $R^2 > 0.93$ for all properties on the test set, with low and stable MSE/MAE across 10 independent replicas, indicating good generalization without overfitting.

The trained surrogate model was used to perform scalarized multi-objective optimization targeting (i) maximum energy absorption with minimum stiffness (Max EA/Min ST) and (ii) simultaneous maximization of energy absorption and stiffness (Max EA/Max ST), with and without weighting of EA. All optimal solutions converged to a narrow RI window of ≈ 1500 –2000, corresponding to partially ordered Voronoi topologies that balance structural regularity and beneficial disorder. Relative to an organized Kelvin-like reference lattice, ML-FEA-optimized Voronoi structures exhibit up to 95% higher stiffness and approximately four-fold improvement in energy absorption under compression. Experiments on lattices with RI = 1783 and 1992 confirm the predicted trends: ML-optimized designs achieve $\sim 35\%$ higher peak load, $\sim 40\%$ higher toughness and $\sim 20\%$ higher stiffness compared to the organized architecture, while stochastic non-optimal designs (RI = 139) show premature localized collapse and reduced energy absorption. Deformation contours from FEA agree closely with post-test images, capturing distributed buckling and progressive, rather than catastrophic, failure in optimized lattices.

A comparative map of specific energy absorption versus peak stress indicates that ML-optimized Voronoi lattices outperform a range of conventional periodic lattices, including cubic and octet-truss architectures, at similar or lower relative density. The results highlight RI as a practical scalar descriptor of disorder that links geometry, connectivity and mechanical response, and demonstrate that combining ML with physics-based simulation enables efficient navigation of high-dimensional stochastic design spaces. The proposed ML-FEA–AM framework provides general guidelines for tuning the order–disorder balance in architected materials and is directly extensible to dynamic loading, multi-physics objectives (e.g. thermal management), and generative or reinforcement-learning-based design. This approach opens a route toward next-generation stochastic lattices for energy-absorbing and crash-worthy structures in aerospace, automotive and biomedical applications.

References

- [1] C. C. Chamis, “Simplified composite micromechanics equations for hygral, thermal and mechanical properties,” Ann. Conf. of the Society of the Plastics Industry (SPI) Reinforced Plastics/Composites Inst., NASA-TM-83320, 1983.
- [2] R. Hill, “Elastic properties of reinforced solids: some theoretical principles,” *J. Mech. Phys. Solids*, 11(5), 357–372, 1963.
- [3] L. J. Gibson, M. F. Ashby, *Cellular Solids: Structure and Properties*, 2nd ed., Cambridge University Press, 1997.
- [4] S. P. Lloyd, “Least squares quantization in PCM,” *IEEE Trans. Inf. Theory*, 28(2), 129–137, 1982.
- [5] N. A. Maskery et al., “Mechanical properties of gyroid lattice structures manufactured by selective laser melting,” *Mater. Des.*, 155, 88–98, 2018.
- [6] J. Mueller, K. Shea, “Generalized Voronoi structures: design, fabrication, and experimental validation,” *Acta Mater.*, 165, 485–497, 2019.
- [7] Y. LeCun, Y. Bengio, G. Hinton, “Deep learning,” *Nature*, 521, 436–444, 2015.
- [8] M. Thompson et al., “Machine learning-optimized stochastic Voronoi lattices for enhanced mechanical performance,” *Engineering Applications of Artificial Intelligence*, 160, 111937, 2025.

Physics-Informed Bayesian Gaussian Processes for Accelerated Characterization in Composite Materials: From Formulation to Performance

Navid Zobeiry¹, Paulina Portales Picazo

¹ University of Washington, Seattle, WA 98195, navidz@uw.edu

The stochastic nature of composite materials is rooted in raw material variability and process uncertainties. These effects are compounded by the inherently multiscale structure of composites, through which variability propagates across length scales and ultimately manifests as a distribution of material behaviour. Accordingly, qualification and certification of composite structures require quantifying this stochastic behaviour from formulation and processing to part performance to support physics-based analysis, robust design, and safe certification. This typically requires repeated testing across processing conditions to characterize key process-dependent properties, such as cure kinetics, as well as repeated mechanical testing across multiple material batches under different loading conditions and environmental exposures. Not surprisingly, this experimental burden drives high cost and long schedules, which can slow innovation and limit the adoption of novel composite material systems.

We present a unified physics-informed Bayesian Gaussian Process framework that integrates physics- and chemistry-guided descriptors with probabilistic surrogate modelling and Bayesian inference to capture underlying physics and uncertainty, while accelerating material characterization through targeted, information-rich testing. In addition, the framework enables accelerated design optimization spanning chemical formulation, manufacturing parameters, and part performance.

The schematic of the framework is shown in Figure 1 and is briefly discussed here. First, physics- and chemistry-informed descriptors and encoded target outputs are constructed based on the underlying governing equations of the thermo-chemo-mechanical problem, to anchor learning in physical constraints and promote generalization near the training domain. Second, a probabilistic surrogate model, here Gaussian Process Regression (GPR), is trained on sparse test data, providing both mean predictions and uncertainty quantification. Third, an acquisition function selects the next experimental conditions by balancing exploration and exploitation, either to accelerate optimization or to most efficiently reduce uncertainty. Finally, the targeted experiments are performed, the dataset is updated, and the loop is repeated until a predefined decision-confidence criterion is met.

Here, we demonstrate the application of the framework to reduce experimental work and accelerate optimization in three areas [1-4]. First, for formulation optimization, the framework is applied to aerospace epoxy-amine structural resins to accelerate formulation optimization toward target properties using targeted dynamic mechanical analysis (DMA) measurements of glass transition temperature and rubbery modulus; we further show how limited test data, combined with chemistry-aware priors and descriptors, can substantially reduce the number of iterations required for optimization. Second, for kinetics characterization and process optimization, the method is applied to (i) thermoset composite cure kinetics using differential scanning calorimetry (DSC), (ii) thermoplastic composite crystallization kinetics using polarized microscopy, and (iii) carbon-carbon composite pyrolysis kinetics using thermogravimetric analysis (TGA). In each case, sparse targeted experiments are performed to train kinetics surrogates, which are then used to predict and optimize processing cycles, for example to maximize char yield during pyrolysis. Finally, we demonstrate accelerated fatigue characterization of

short-fibre thermoplastic composites, where a physics-informed Bayesian GPR model uses limited tensile test data to rapidly learn the entire S–N response while quantifying uncertainty using substantially fewer experiments than conventional test matrices.

Collectively, these demonstrations show the capability and efficiency of the framework to speed up testing campaigns while providing uncertainty-aware predictions. Additionally, the resulting probabilistic surrogate models enable risk-informed, qualification-relevant decisions by quantifying confidence at every step of the targeted testing campaign.

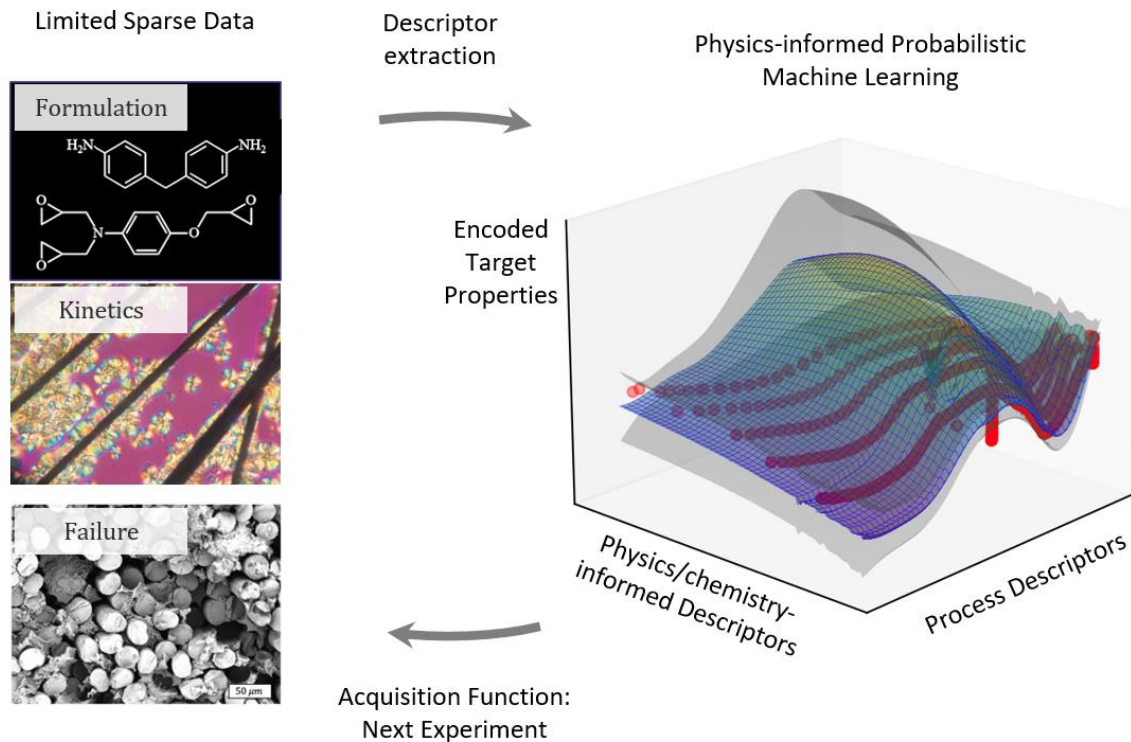


Figure 1. Physics-informed Bayesian GPR loop for accelerated characterization and optimization of composites.

References:

- [1] Schoenholz, C., et al., “Efficient analysis of composites manufacturing using multi-fidelity simulation and probabilistic machine learning.” *Composites Part B: Engineering*, 2024. 280: p. 111499.
- [2] Schoenholz, C. and N. Zobeiry, “An Accelerated Process Optimization Method to Minimize Deformations in Composites Using Theory-guided Probabilistic Machine Learning.” *Composites Part A: Applied Science and Manufacturing*, 2024. 176: p. 107842.
- [3] Wynn, M., & Zobeiry, N. “Investigating the effect of temperature history on crystal morphology of thermoplastic composites using in situ polarized light microscopy and probabilistic machine learning.” *Polymers*, 2022. 15(1), 18.
- [4] Portales Picazo, P., A. Gray, and N. Zobeiry, “Efficient characterization and optimization of pyrolysis in carbon-carbon composites through machine learning.” *Composites Part A: Applied Science and Manufacturing*, 2025. 190: p. 108664.

Rapid Inverse Design of Meso-Architected Composites using Sequence-based Deep Learning

Saral Mittal¹ and B. Gangadhara Prusty¹

¹ ARC Training Centre for Automated Manufacture of Advanced Composites (AMAC),

School of Mechanical & Manufacturing Engineering, UNSW Sydney, NSW 2052, Australia

Presenting author email: g.prusty@unsw.edu.au

Meso-architected composite (MAC) laminates enable tailored structural performance through strategic control of tow placement sequence, facilitated by automated manufacturing technologies such as Automated Fibre Placement (AFP). In this design strategy, controlled variation of tow deposition order during automated placement leads to the formation of a semi woven laminate architecture, as illustrated in Figure 1. Previous investigations involving both low velocity and high velocity impact loading have demonstrated that MAC configurations can exhibit significantly improved damage tolerance compared to conventional non-woven laminates, with reported enhancements of up to 50% in Compression after Impact (CAI) strength [1], [2], [3], [4]. While this expanded design freedom enables access to non-conventional architectures with enhanced mechanical response, it also introduces a highly combinatorial design space that is challenging to explore using traditional parametric or optimisation driven methodologies. Consequently, establishing robust and scalable relationships between meso-scale architecture and macroscopic material properties remains a significant challenge.

Existing optimisation efforts in composite materials have largely been limited to variations in ply orientations and binder tow paths [5], [6], [7], [8]. This restriction arises primarily from the prevailing representation of composite laminates as ply-based stacking sequences, for example [0/90/0/90], which is insufficient to capture the architectural complexity introduced by tow-wise layup strategies. To address this limitation, the present work introduces a novel tow-based representation framework that is better suited to describing meso-architected laminates. Composite architectures are encoded using a sequence-based formulation in which each tow is assigned a unique identifier based on its location and orientation, yielding a discrete sequential description of the laminate architecture, as shown in Figure 2. This representation is aligned with digital manufacturing instructions and eliminates reliance on manually defined geometric descriptors or explicit parameterisation of fibre trajectories. As a result, complex architectures can be compactly described as ordered sequences that are directly compatible with data-driven learning.

The forward relationship between architectural sequences and mechanical properties is modelled using recurrent neural networks based on Long Short-Term Memory (LSTM) architecture. Such architectures enable the learning of non-local interactions between spatially distant tow placements, which play a critical role in governing global laminate behaviour [9], [10]. Once trained, these models provide rapid and accurate forward property prediction across a large design space, significantly reducing dependence on repeated high-fidelity simulations or experimental characterisation.

The sequence-based formulation further enables inverse design through integration with iterative optimisation strategies. The trained neural network is employed as a surrogate forward model within an optimisation loop driven by genetic algorithms or self-learning evolutionary strategies, where candidate

laminate architectures are evaluated and refined across successive generations based on predicted performance, as illustrated in Figure 3. This surrogate-assisted optimisation approach enables efficient navigation of high-dimensional architectural design spaces. Moreover, because manufacturability constraints are embedded within the sequence representation framework, all generated architectures remain compatible with existing AFP infrastructure.

The predictive accuracy of the surrogate LSTM model, insights into recurring architectural features associated with superior performance, and experimental validation of selected optimised configurations will be presented during the conference presentation to demonstrate the effectiveness of the proposed framework. Overall, the proposed framework establishes a unified approach for forward modelling and optimisation-driven inverse design of meso-architected composites, supporting accelerated development of application-specific laminate architectures.

Figures:

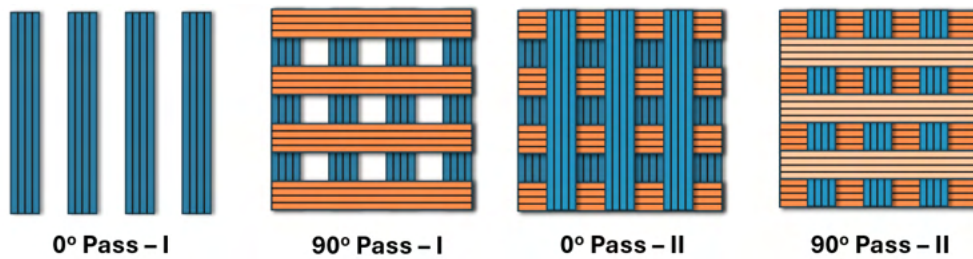


Figure 1: Step-wise layup of a baseline MAC configuration with alternate tow skipping.

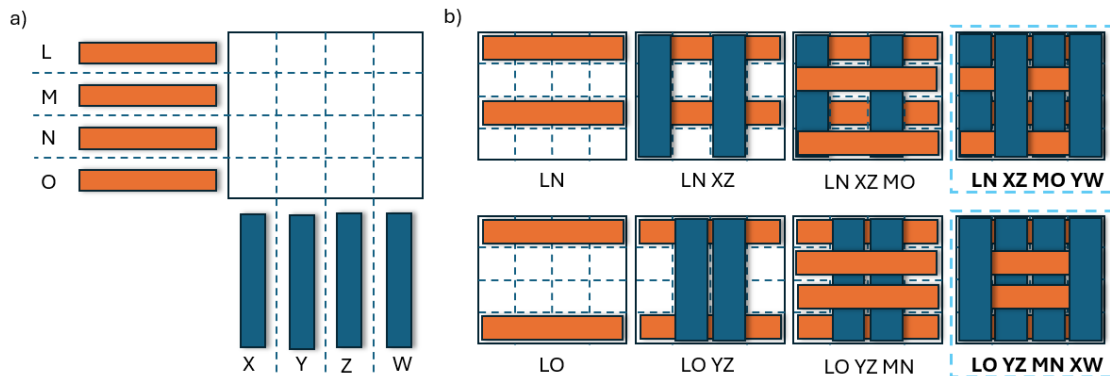


Figure 2: a) Laminate design domain discretised at the tow width scale, showing individual tow placement slots identified by unique labels; b) Sequence based encoding of laminate architectures, represented as an ordered arrangement of individual tows.

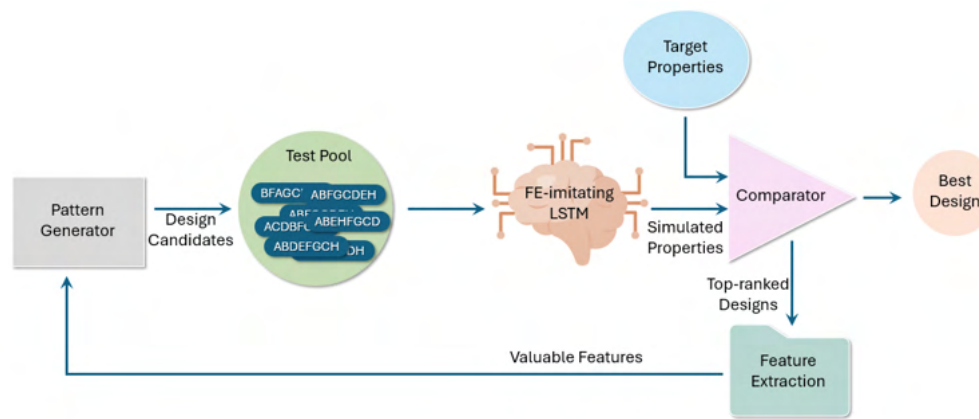


Figure 3: Schematic overview of the proposed automated design framework, highlighting the integration of a neural network-based property prediction model for laminate architecture optimisation.

References:

- [1] C. Vakili Rad *et al.*, “High velocity impact response of hybridized pseudo-woven carbon fiber composite architectures,” *Composites Part B: Engineering*, vol. 203, p. 108478, Dec. 2020, doi: 10.1016/j.compositesb.2020.108478.
- [2] R. Kok *et al.*, “Low velocity impact response of Automated Fiber Placement Advanced Placed Ply composites,” *Composites Science and Technology*, vol. 253, p. 110636, Jul. 2024, doi: 10.1016/j.compscitech.2024.110636.
- [3] K. Kodagali, C. Vakili Rad, S. Sockalingam, Z. Gurdal, and E. Miller, “Low velocity impact and compression-after-impact response of hybrid pseudo-woven meso-architected carbon/epoxy composite laminates manufactured via automated fiber placement,” *Composites Part B: Engineering*, vol. 271, p. 111154, Feb. 2024, doi: 10.1016/j.compositesb.2023.111154.
- [4] M. H. Nagelsmit, “Fibre Placement Architectures for Improved Damage Tolerance,” 2013. doi: 10.4233/UUID:F8C8AD4E-5D52-4BFD-8449-2748BAD26673.
- [5] M. Ansar, W. Xinwei, and Z. Chouwei, “Modeling strategies of 3D woven composites: A review,” *Composite Structures*, vol. 93, no. 8, pp. 1947–1963, Jul. 2011, doi: 10.1016/j.compstruct.2011.03.010.
- [6] L. Brown, F. Gommer, X. Zeng, and A. Long, “Modelling framework for optimum multi-axial 3D woven textile composites,” Sep. 2016.
- [7] X. Zeng, A. Long, I. Ashcroft, and P. Potluri, “Fibre architecture design of 3D woven composite with genetic algorithms: a unit cell based optimisation framework and performance assessment,” Jul. 2015.
- [8] M. T. Herath, B. G. Prusty, A. W. Phillips, and N. St. John, “Structural strength and laminate optimization of self-twisting composite hydrofoils using a Genetic Algorithm,” *Composite Structures*, vol. 176, pp. 359–378, Sep. 2017, doi: 10.1016/j.compstruct.2017.05.012.
- [9] B. Ding, D. Li, and Y. Chen, “A Novel Long Short-Term Memory Based Optimal Strategy for Bio-Inspired Material Design,” *Nanomaterials*, vol. 11, no. 6, p. 1389, Jun. 2021, doi: 10.3390/nano11061389.
- [10] A. J. Lew, K. Jin, and M. J. Buehler, “Designing architected materials for mechanical compression via simulation, deep learning, and experimentation,” *npj Comput Mater*, vol. 9, no. 1, p. 80, May 2023, doi: 10.1038/s41524-023-01036-1.

Session Two

2 AI FOR NON-DESTRUCTIVE TESTING AND STRUCTURAL HEALTH MONITORING

AI-ENABLED METROLOGY FRAMEWORK FOR DAMAGE ASSESSMENT OF HYDROTHERMALLY AGED UNIDIRECTIONAL GLASS-FIBER-REINFORCED THERMOPLASTICS

Jorge Palacios Moreno¹ and Pierre Mertiny¹

¹ Presenting Author, Department of Mechanical Engineering, University of Alberta, Canada,
ajorge@ualberta.ca

Unidirectional glass fiber-reinforced thermoplastic (UGFT) composite tapes are increasingly adopted in structural applications requiring recyclability, toughness, and long-term durability, including thermoplastic composite piping systems operating at elevated temperatures. Despite these advantages, hydrothermal exposure remains a critical challenge. Moisture ingress at high temperature accelerates polymer matrix plasticization and fiber-matrix interfacial degradation, leading to premature damage initiation and reduced load-bearing capacity [1]. Conventional durability assessments rely mainly on post-aging mechanical testing and microscopy, which provide limited insight into damage evolution and are unsuitable for in-service monitoring. Acoustic emission (AE) is a non-destructive technique capable of capturing damage-related elastic waves generated during mechanical loading. However, AE signals are inherently high-dimensional, stochastic, and partially overlapping across damage mechanisms. As a result, traditional threshold-based or single-parameter interpretations lack objectivity and repeatability [2]. Artificial intelligence (AI), particularly unsupervised learning, provides a powerful framework to extract latent structure from complex AE datasets. To ensure scientific rigor and industrial relevance, AI-based approaches must be embedded within a metrology-driven framework that emphasizes traceable measurements, repeatability, uncertainty quantification, and physical validation.

Commercial glass fiber-reinforced polypropylene (GF-PP) unidirectional tapes with a nominal thickness of 0.5 mm and a fiber volume fraction of approximately 60 ± 5 % were investigated. Specimens were aged in deionized water at 95 °C for durations of 1 and 4 weeks. Aging progression was quantified through mass-change measurements conducted according to standardized procedures, providing traceable characterization of moisture uptake behavior. Tensile testing was performed along the fiber direction using standardized methods to ensure traceability of force and displacement measurements. A tensile strength reduction exceeding 25 % relative to the unaged condition was defined as a quantitative threshold for significant degradation. AE monitoring was conducted during tensile loading using sensors with fixed threshold and timing parameters. Rather than analyzing raw waveforms, standardized AE descriptors, including amplitude, duration, energy, rise time, and frequency-based parameters, were treated as quantitative measurement outputs. This descriptor-based strategy improves noise robustness and enables reproducible data-driven analysis [3,4].

Given the multidimensional nature of AE data, principal component analysis (PCA) was applied to reduce redundancy and identify the most informative combinations of descriptors. Across unaged and aged conditions, the first two principal components consistently captured the majority of the variance, enabling low-dimensional representation without significant information loss. From an AI perspective, PCA acts as an implicit feature-selection and weighting mechanism, eliminating subjective parameter ranking and enhancing model transferability. Unsupervised k-means clustering was subsequently applied in the PCA space to classify AE events into statistically distinct groups.

Internal validation metrics, including the Davies-Bouldin and Calinski-Harabasz indices, consistently identified three optimal clusters across all aging conditions. These clusters were associated with matrix cracking, matrix/fiber debonding, and fiber breakage based on their descriptor signatures and frequency content, in agreement with prior AE-based composite damage studies [3,4]. Unlike rule-based classification, the unsupervised approach allows damage mechanisms to emerge directly from the data, representing a key AI-driven advance. To explicitly address algorithmic uncertainty, clustering robustness was quantified using the Adjusted Rand Index (ARI) over repeated simulations. High ARI values approaching unity were obtained for baseline and aged conditions, demonstrating that the clustering results are stable, reproducible, and insensitive to initialization effects or data perturbations. This explicit quantification of AI stability is critical for integrating machine-learning outputs into a metrology-driven assessment framework.

Hydrothermal aging produced a progressive reduction in tensile strength, exceeding the predefined 25 % degradation threshold after prolonged exposure. Mass-change measurements suggest diffusion-controlled moisture uptake, providing a physically consistent basis for interpreting degradation trends. AE analysis showed earlier damage initiation, reduced cumulative AE energy, and shorter signal durations with increasing aging duration, indicating a transition from progressive, energy-dissipative failure toward more brittle behavior. Although fiber breakage remained the dominant damage mechanism in terms of AE hit count across all conditions, this dominance reflects the high fiber volume fraction and longitudinal loading configuration rather than the primary aging mechanism. Aging effects were more sensitively captured through AI-derived metrics such as changes in AE energy distribution, hit duration, and damage onset, which are associated with matrix and interfacial degradation. Optical microscopy provided independent physical validation of the AI-identified damage mechanisms, reinforcing traceability between measured signals and observed microstructural damage.

This study demonstrates that unsupervised AI techniques can be rigorously integrated into a metrology-driven framework for assessing hydrothermal degradation in UGFT composites. By treating AE descriptors as traceable measurement quantities, applying objective dimensionality reduction and clustering, and explicitly quantifying algorithmic stability, the proposed approach moves beyond qualitative AE interpretation. The framework provides a robust link between micro-scale damage evolution and macroscopic mechanical degradation and establishes a transferable foundation for AI-assisted structural health monitoring of thermoplastic composites.

References:

- [1] R. Zhu, X. Li, C. Wu, L. Du, X. Du, T. Tafsirojjaman, "Effect of Hydrothermal Environment on Mechanical Properties and Electrical Response Behavior of Continuous Carbon Fiber/Epoxy Composite Plates," *Polymers*, vol. 14, no. 19, pp. 4072, 2022.
- [2] C. Rubio-González, M. del Pilar de Urquijo-Ventura, J.A. Rodríguez-González, "Damage progression monitoring using self-sensing capability and acoustic emission on glass fiber/epoxy composites and damage classification through principal component analysis," *Compos. B Eng.*, vol. 254, pp. 110608, 2023.
- [3] W. Harizi, S. Chaki, G. Bourse, M. Ourak, "Damage mechanisms assessment of Glass Fiber-Reinforced Polymer (GFRP) composites using multivariable analysis methods applied to acoustic emission data," *Compos. Struct.*, vol. 289, pp. 115470, 2022.
- [4] J. Palacios Moreno, H. Nazaripoor, P. Mertiny, "Damage Mechanism Characterization of Glass Fiber-Reinforced Polymer Composites: A Study Using Acoustic Emission Technique and Unsupervised Machine Learning Algorithms," *J. Compos. Sci.*, vol. 9, pp. 426, 2025.

Identification of Impact Damage in Composite Structures from Sparse Strain Sensor Data using Graph Neural Networks

Christopher Gorsky¹, Raffael Bogenfeld¹ and Tobias Wille¹

¹ German Aerospace Center (DLR), Institute of Lightweight Systems, Department of Structural Mechanics, Germany, christopher.gorsky@dlr.de

The identification of impact damage in composite structures based on sparse sensor data is a fundamentally ill-posed inverse problem. In practical applications, only limited sensor measurements are available and the underlying impact damage is highly localized. This challenge is particularly relevant for large-scale composite structures such as wind turbine blades, where reliable identification of structural anomalies is required for predictive maintenance.

This work presents a machine learning framework for the identification of local structural anomalies in composite structures using Graph Neural Networks (GNNs) (see Fig. 1), which have recently been shown to effectively exploit spatial interdependencies in strain-based SHM [1]. The approach is developed on the basis of a validated finite element (FE) model of a wind turbine blade [2], from which extensive virtual datasets are generated. Instead of explicitly resolving detailed damage mechanisms, local damage effects are represented by localized degradations of effective laminate stiffness properties. These degradations serve as simplified damage representations, allowing the generation of physically consistent strain responses and enabling controlled variation of local damage scenarios.

The structural domain is represented as a graph derived from the FE mesh, preserving spatial topology. This representation enables neighborhood-based learning, which is a key characteristic of graph neural networks [3]. Graph node features include selected strain quantities as well as reconstructed strain information from sparse measurements using gappy Proper Orthogonal Decomposition (gappyPOD) [4]. In this approach, global strain modes are extracted from a large set of simulated strain fields and used to reconstruct physically consistent full-field strain distributions from limited sensor measurements. Regularization is applied to ensure stability under low sensor densities and to suppress noise-sensitive high-frequency components. In addition, engineered features are incorporated to capture spatial context, including distance-based weighting of sensor influence, local strain contrasts, and approximated strain gradients. These features provide explicit spatial context related to sensor locations, thereby improving the robustness of the learning process with sparse sensor data.

The proposed GNN architecture, based on a GraphSAGE formulation, learns to map sparse strain observations to element-wise indicators of structural anomalies by aggregating information from neighboring elements through localized message passing. Using few graph convolution layers with limited neighborhood aggregation enables the model to capture localized damage patterns while avoiding oversmoothing that would otherwise obscure small-scale structural anomalies. Special emphasis is placed on handling extreme class imbalance and the non-uniqueness of the inverse problem. This is addressed through tailored loss functions, feature engineering and the explicit use of spatial relationships between neighboring elements defined by the FE mesh.

Results indicate that the proposed approach is capable of identifying spatially localized damage under sparse sensing conditions. The framework further enables a systematic analysis of the trade-off between sensor density and prediction performance, providing insights into the detectability of damage-related

structural changes and supporting the design of sensor networks for SHM applications. The findings highlight the importance of physically consistent strain reconstruction and sensor-informed feature representations for stable and robust model performance, while also revealing limitations in the detectability of very small stiffness perturbations.

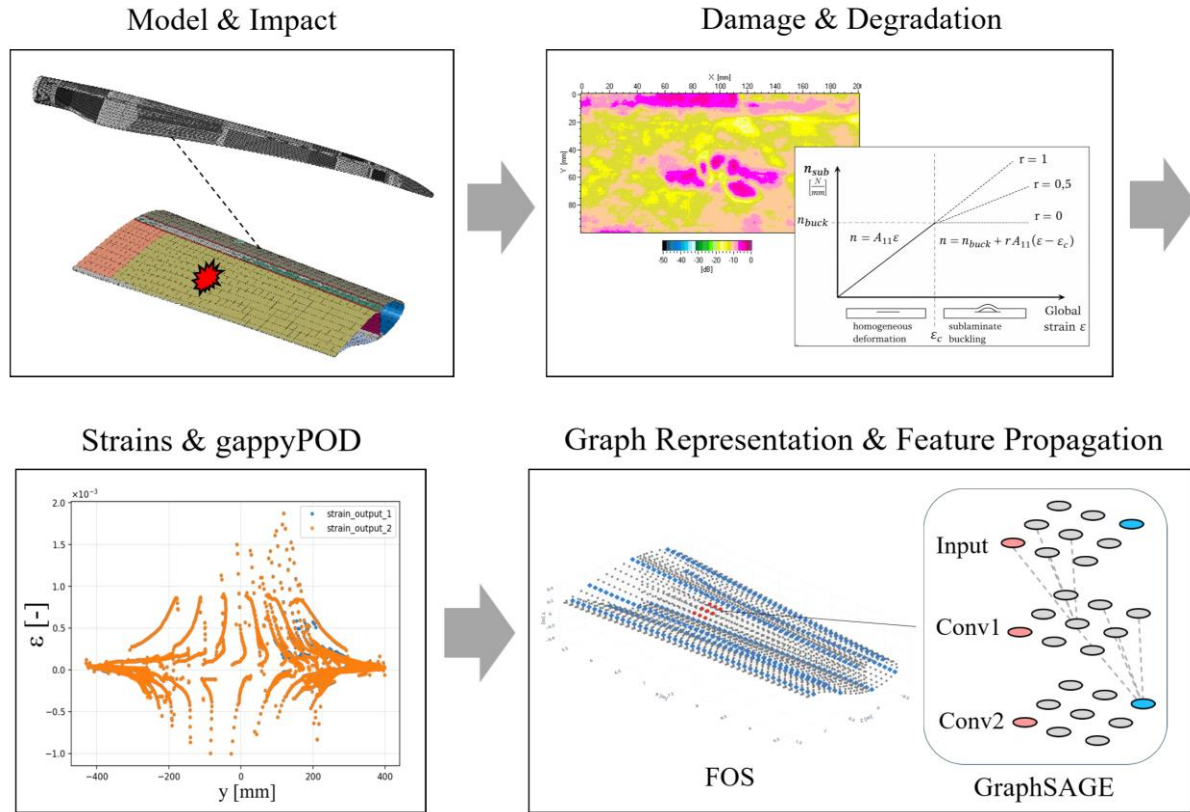


Figure 1: Schematic workflow of the proposed graph-based framework for structural anomaly identification from sparse sensor data.

References:

- [1] G. Stamatelatos, G. Galanopoulos, D. Zarouchas and T. Loutas, “Graph neural networks for SHM: exploiting spatial interdependencies of strain data for diagnostics and prognostics,” *Struct. Health Monit.*, 2025, Art. no. 14759217251386802, doi: 10.1177/14759217251386802.
- [2] C. Willberg, R. Ravi, J. Rieke and F. Heinecke, “Validation of a 20 m wind turbine blade model,” *Energies*, vol. 14, no. 9, 2021, doi: 10.3390/en14092451.
- [3] J. Zhou, G. Cui, Z. Zhang, C. Yang, Z. Liu, L. Wang, C. Li and M. Sun, “Graph neural networks: A review of methods and applications,” *AI Open*, vol. 1, pp. 57–81, 2020, doi: 10.1016/j.aiopen.2021.01.001.
- [4] R. Everson and L. Sirovich, “Karhunen–Loève procedure for gappy data,” *J. Opt. Soc. Am. A*, vol. 12, no. 8, pp. 1657–1664, 1995, doi: 10.1364/JOSAA.12.001657.

Machine Learning Interpretation of Acoustic Emission Signals for Mixed-Mode Damage Detection in Composites

Johannes Reiner¹, Ruben Erives², Xing-Yuan Miao² and Bent F. Sørensen²

¹ School of Engineering, Faculty of Science Engineering and Built Environment, Deakin University, Geelong, Australia, johannes.reiner@deakin.edu.au

² Department of Wind and Energy Systems, Technical University of Denmark, Denmark

Acoustic Emission (AE) has been widely explored as a non-destructive technique to detect damage in composite laminates. The principle is to capture the release of accumulated strain energy at crack tips in the form of elastic waves. Figure 1 shows a typical elastic wave. These waves are often analysed using specific AE parameters such as rise time, duration, count, the Measured Area of the Rectified Signal Envelope (MARSE) to represent energy, and amplitude [1]. In addition, the waveform can be transformed into the frequency domain through Fast Fourier Transforms to identify characteristic frequency events that help distinguish matrix cracking, fibre breakage, delamination, and the severity of these failure modes [1].

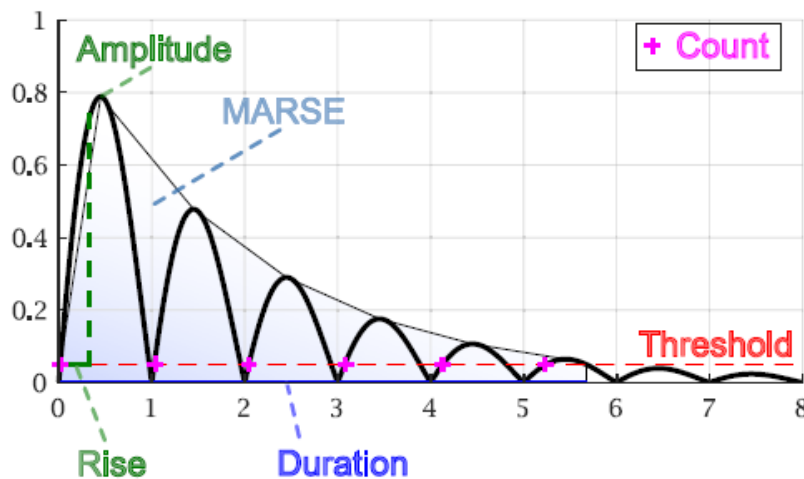


Figure 1 Example of parameters recorded during fracture testing using acoustic emission [2].

Unlike most engineering applications, AE detection during fracture testing produces large and heterogeneous datasets, which motivates the use of Machine Learning (ML) techniques to relate measured AE features to fracture events based on recorded data or observed behaviour [1]. ML offers significant advantages in this context: it has the potential to uncover subtle, nonlinear relationships between features, enable early-stage damage detection, and support near real-time classification of damage mechanisms. Such capabilities are difficult to achieve using traditional human-centred signal processing alone. These strengths are particularly attractive for structural health monitoring of large-scale systems such as on-site operating wind turbines, where AE measurements are not only high-volume but can also be very noisy due to environmental effects, operational loads, and complex wave propagation in composite blades.

However, the successful development of robust ML models depends not only on large and information-rich datasets but also on a thorough understanding of the underlying signal structure, feature correlations, and noise characteristics. Without this foundation, ML models may overfit, misclassify early damage, or become unreliable when deployed in real-world turbine environments.

This study investigates a comprehensive experimental dataset by Erives et al. [3, 4], consisting of double cantilever beam tests on unidirectional glass-fibre composites subjected to eleven distinct mode-mixities, spanning the full range from pure Mode I to pure Mode II fracture. As illustrated in Figure 2, the specimens were loaded with uneven bending moments to promote stable crack propagation across all mode-mixity conditions. For each test, synchronous measurements of AE, applied forces, normal and tangential displacements, as well as fracture energies evaluated via J-integral methods, are available.

We present a structured framework for interrogating and visualising AE features to uncover their relationships with fracture processes, with the goal of establishing a physically informed foundation for downstream ML applications.

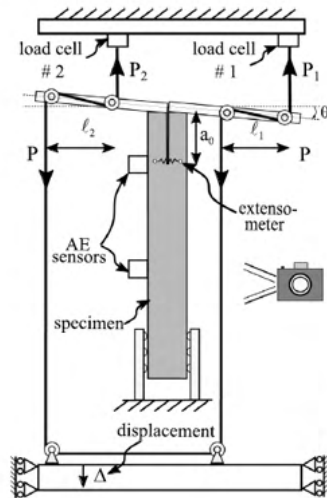


Figure 2 Illustration of double cantilever beam test with uneven bending moments to investigate quasi-static fracture in unidirectional glass-fibre composites [3].

The analysis highlights key AE characteristics corresponding to noise events, crack initiation, and crack propagation, enabling the development of efficient supervised and unsupervised ML approaches tailored to these distinctions. The resulting workflow provides a pathway for integrating advanced signal processing and machine learning into structural health monitoring strategies, supporting earlier and more reliable detection of damage in composite structures.

References:

- [1] Muir, C., Swaminathan, B., Almansour, A.S. et al., “Damage mechanism identification in composites via machine learning and acoustic emission,” *npj Comput Mater*, Vol 7, 95, 2021. <https://doi.org/10.1038/s41524-021-00565-x>.
- [2] A. Mielke, H-H. Benzon, M. McGugan, X. Chen, H. Madsen, K. Branner, T. K.S. Ritschel, “Analysis of damage localization based on acoustic emission data from test of wind turbine blades,” *Measurement*, Vol. 231, 114661, 2024. <https://doi.org/10.1016/j.measurement.2024.114661>.
- [3] R. Erives, B.F. Sørensen, S. Goutianos, “Extraction of mix-mode cohesive laws of a unidirectional composite undergoing delamination with large-scale fibre bridging,” *Composites Part A: Applied Science and Manufacturing*, Vol. 165, 107346, 2023. <https://doi.org/10.1016/j.compositesa.2022.107346>.
- [4] R. Erives, “Dataset of mixed-mode R-curves from DCB-UBM fracture tests of a UD glass/epoxy composite,” *Data in Brief*, Vol. 48, 109076, 2023. <https://doi.org/10.1016/j.dib.2023.109076>.

The Effect of Photo-Quality on Photo-Learning Waviness Segmentation in NCFs

**Umeir Khan^{1*}, Vincent. K. Maes¹, Robert Hughes¹, Jon Wright², Petar Zivkovic²,
Turlough McMahon² and James Kratz¹**

¹ University of Bristol, United Kingdom), *corresponding author email:umeir.khan@bristol.ac.uk

² Airbus UK (United Kingdom)

Deep Learning (DL) Tow Segmentation has enabled a pathway for quantifying in-plane waviness in Non-Crimp Fabric (NCF) preforms from photographs [1] (**Figure 1**) - a process termed *Photo-Learning*. The key challenge is identifying the photo-quality requirements in order to support end-users to adopt the technology for repeatable and robust segmentation of NCF tows.

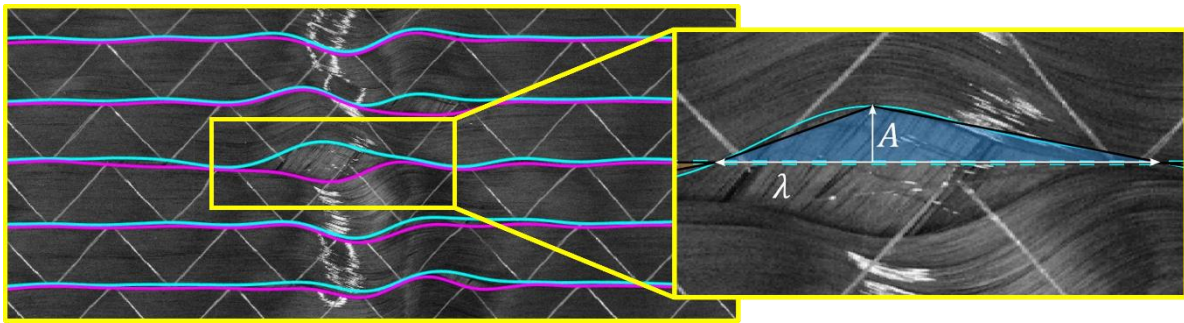


Figure 1: In-plane waviness segmentation of NCF tows for defect severity analysis [1].

This study evaluates several factors of the data-capture (*camera type, imaging environment, part and material features*) that influence the success of Tow Segmentation. These findings aim to inform best-practice for applying Photo-Learning in different imaging settings (**Figure 2**).

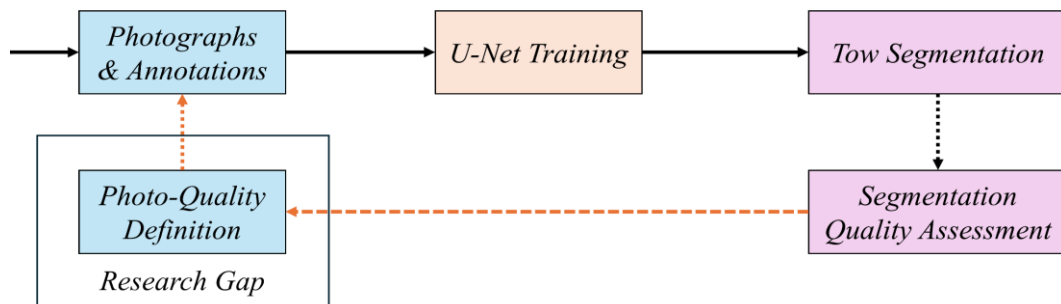


Figure 2: Photo-Learning workflow, via the U-Net architecture [2], with feedback loop that considers input data quality.

Single diaphragm forming of biaxial carbon fibre NCF plies was executed over a complex geometry. The default camera position is normal to the ply surface, therefore, any observed waviness was assumed

to be in-plane. To study the effect of differing photo-capture quality, a range of digital cameras (Sony α 6100, and iPhone 12 Pro Max) with variable settings (*focal length, aperture, lighting intensity and position*) were used. This resulted in photo-datasets of: (1) training / test images, and (2) descriptors (**Figure 3**).

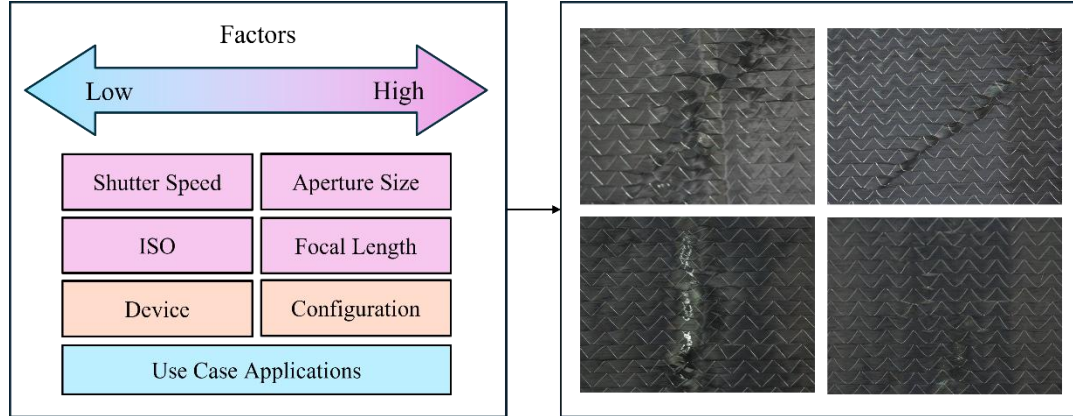


Figure 3: Photo data-capture with factors for defining quality input.

The photo-annotation and training procedures from our previous work [1] was undertaken with segmentation agreement quantified via the Matthews Correlation Coefficient [3]. The photograph sets that produced high MCC scores (≥ 0.80) were qualitatively deemed to be the representative standard for enabling waviness tracing (with a representative example shown in **Figure 4**). These photographs are then used to extract relevant waviness parameters: amplitude A , wavelength λ , and aspect ratio.

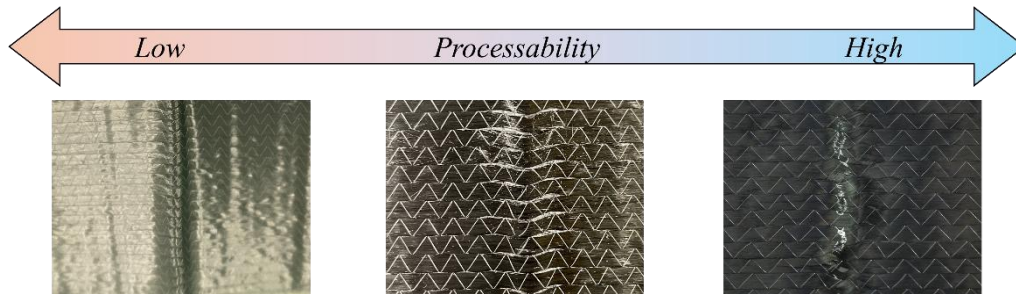


Figure 4: Preliminary Photograph vs. Processability Mapping.

Overall, this study seeks to inform photo-capture guidelines for enabling Tow Segmentation for end-users to adopt. A parameter sweep of photograph variables was explored and correlated to Deep Learning-based segmentation scores. Examples of best-practices and how to reliably obtain high-quality segmentations for waviness quantification is provided.

References:

- [1] U. Khan *et al.*, ‘In-plane waviness parameterisation from in-factory photographs of non-crimp fabrics’, *Composites Part A: Applied Science and Manufacturing*, vol. 193, p. 108822, Jun. 2025, doi: 10.1016/j.compositesa.2025.108822.
- [2] O. Ronneberger, P. Fischer, and T. Brox, ‘U-Net: Convolutional Networks for Biomedical Image Segmentation’, May 18, 2015, *arXiv*: arXiv:1505.04597. doi: 10.48550/arXiv.1505.04597.
- [3] D. Chicco and G. Jurman, ‘The advantages of the Matthews correlation coefficient (MCC) over F1 score and accuracy in binary classification evaluation’, *BMC Genomics*, vol. 21, no. 1, p. 6, Jan. 2020, doi: 10.1186/s12864-019-6413-7.

UNSUPERVISED CLASSIFICATION OF DEFECTS IN AFP PROFILOMETRY SCANS

H. Buhagiar¹, I. Tretiak¹ and B. El Said¹

¹ Bristol Composites Institute, University of Bristol, UK, harvey.buhagiar.2021@bristol.ac.uk

Advances in Automated Fibre Placement (AFP) technology have enabled higher production rates and lower manufacturing induced variability compared to hand lamination, making it the state-of-the-art method of composites manufacturing for high performance applications such as civil airliners. However, manufacturing induced defects remain common, primarily caused by complex tool geometries and poorly optimised material placement [1]. Two particularly severe defect types have been identified in the literature: 'pucker' and 'twist' defects [2]. Pucker defects refer to out-of-plane wrinkles caused by excess tow feeding, while twist defects refer to a tow which has rolled axially 180° due to friction in the tape dispensing head mechanism. Both lead to high stress concentrations and significant reductions in strength [1]. Defect detection is therefore a critical part of the manufacturing process, however manual inspection is estimated to consume up to 50% of total production time, compared to only 20% for material deposition itself [3], making automation of the inspection process a high-impact area for accelerating production rates.

Current AI-based solutions for defect detection in composites can be further automated to save manufacturers time and resources. At present, these systems still require considerable human supervision in the training phase. This supervised training process requires significant effort from the user in generating segmentation masks and annotating training data. In contrast, unsupervised learning methods model the intrinsic statistical structure of the data itself, enabling classification without predefined labels. This makes unsupervised approaches particularly valuable in scenarios where the underlying structure of the data has not been fully characterised. In this paper, we introduce a novel unsupervised method for classifying pristine AFP tapes and pucker and twist defects from laser scan profilometry images, demonstrating 99.5% accuracy in binary defect detection on unseen test data with a dataset of only 97 images and an inference time of 37 milliseconds on standard laptop hardware.

The model proposed in this paper is based on a modification to the Gaussian Mixture Variational Autoencoder (GMVAE) [4]. The GMVAE is a generative model which infers both a continuous latent variable, encoding the content of the image, and a categorical latent variable encoding the class to which the image belongs. The model was trained and evaluated on the AFP defects dataset. Data augmentation through rotation and flipping was leveraged to expand the dataset tenfold, and the generalisability of the model was assessed on a set of test images and through 5-fold cross validation.

The recall score was used to assess the model's ability assign the same label to all instances of each true class. On the test set, the model achieved recall scores of 98.5%, 81.3% and 84.4% for pristine, twist and pucker classes respectively, with corresponding F1 scores of 99.2%, 81.9% and 83.1%. Visualisation of the latent space using t-SNE confirmed that pristine samples are well separated from defective ones, while twist and pucker embeddings show greater overlap, indicated by the lower recall scores for these classes. The proposed model could form part of a reactive, in-situ defect mitigation framework in which the profilometry sensor runs continuously during AFP and upon detection of a defect, triggers appropriate reworking. Pucker defects can be remedied in a fully automated fashion

using Automated Tape Relaying (ATR) [5], while twist defects require manual splicing. Time since deposition is a critical factor determining the effectiveness of reworking both defects, making rapid in-situ detection critical. The 37 ms inference time of our GMVAE model is significantly lower than comparable AFP defect detection systems [6], enabling timely intervention before defects are consolidated into the laminate and become difficult to rework.

This work demonstrates that unsupervised AI methods are a viable and practical route to fully automated defect detection in AFP composites manufacturing, removing the need for labelled training data while maintaining high classification accuracy. Furthermore, we demonstrate that this result is achievable on a small dataset of 97 images, making it feasible for small scale manufacturing operations with limited process data. The model is highly generalisable to unseen test data and can perform quick inference, highlighting defects in-situ, with no defect undetected and a low false positive rate, potentially further accelerating production rates by minimising machine halts for reworking.

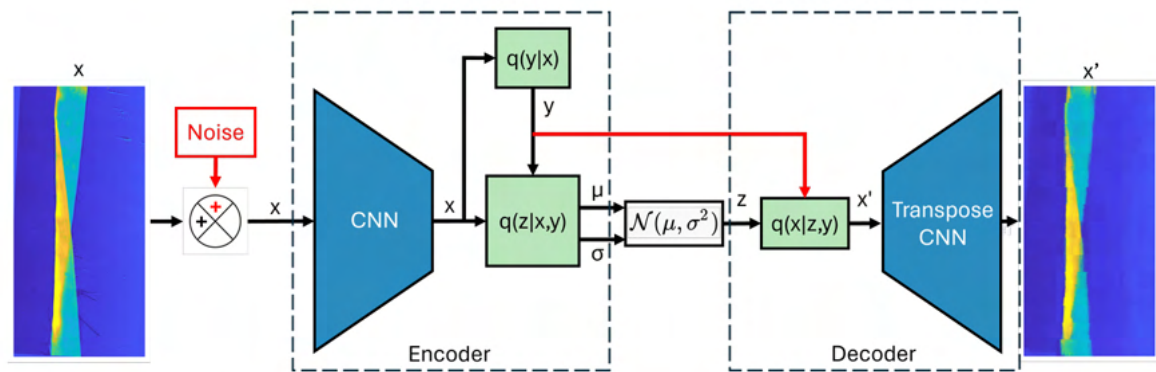


Figure 1: GMVAE architecture with our modifications in red, green blocks represent fully connected neural networks. The input image is a twist defect. The class label, y , is learnt directly.

References

- [1] R. Harik, C. Saidy, S. Williams, Z. Gurdal, B. Grimsley, Automated fiber placement defect identity cards: cause, anticipation, existence, significance, and progression, SAMPE 18 - Long Beach, 2018.
- [2] K. Croft, L. Lessard, D. Pasini, M. Hojjati, J. Chen, A. Yousefpour, Experimental study of the effect of automated fiber placement induced defects on performance of composite laminates, Composites Part A: Applied Science and Manufacturing 42 (2011) 484–491.
- [3] T. Rudberg, J. Cemenska, E. Sherrard, A process for delivering extreme AFP head reliability, in: SAE Technical Paper Series, SAE International, 2019.
- [4] N. Dilokthanakul, P. A. M. Mediano, M. Garnelo, et al., Deep unsupervised clustering with gaussian mixture variational autoencoders, arXiv preprint arXiv:1611.02648 (2016).
- [5] E. Arabul, V. K. Maes, D. H. Nguyen, R. Hughes, J. Kratz, Automated tape relaying to monitor and control first-ply deposition, Composites Part A: Applied Science and Manufacturing 202 (2026) 109469.
- [6] A. Koptelov, B. El Said, I. Tretiak, Enhancing AFP manufacturing with AI: Defects forecasting and classification, Composites Part B: Engineering 304 (2025) 112655.

Session Three

3 MECHANICAL BEHAVIOR AND FAILURE PREDICTION WITH AI

Bayesian Inference on Finite Element Input Parameters to Simulate Variability in Progressive Crush Tests of Composites

Johannes Reiner¹, Reza Vaziri²

¹ School of Engineering, Faculty of Science Engineering and Built Environment, Deakin University, Geelong, Australia, johannes.reiner@deakin.edu.au

² Composites Research Network, Departments of Civil Engineering and Materials Engineering, The University of British Columbia, Vancouver, Canada

Composite materials play a critical role in modern engineering structures, yet their performance is inherently influenced by variations and uncertainties arising from manufacturing defects, material heterogeneity, fibre misalignment, environmental exposure, and evolving damage states. These uncertainties make it challenging to reliably predict their structural integrity, particularly in safety-critical applications. As composite structures become more widespread and are pushed to operate closer to their design limits, there is a growing need for simulation strategies that can not only predict mean responses such as loads, deformation and damage but also explicitly account for uncertainty and provide quantitative, physics-based insight into material behaviour.

During the axial crushing of composite laminates, the global energy dissipation is governed by two dominant macroscopic failure modes: splaying and fragmentation [1]. Reliable simulation and prediction of these mechanisms are crucial for the assessment of crashworthiness and impact-induced failure in aerospace composite substructures. However, performing physics-based finite element (FE) simulations of full-scale composite components under crushing or other severe loading scenarios remains highly challenging [1]. This difficulty stems from inherently complex material behaviour, large deformations, contact interactions, and high computational cost. As a result, many industrial FE models still rely on empirically-tuned input parameters which undermine their physical fidelity and predictive capability.

This study aims to simulate the experimentally observed variations in progressive crush tests of quasi-isotropic IM7/8552 carbon fibre reinforced polymer laminates through FE simulations coupled with uncertainty quantification (UQ) [2, 3]. To simulate the crushing process, we employ a Continuum Damage Mechanics (CDM) framework, which provides a computationally efficient means of representing distributed damage without requiring explicit modelling of individual cracks or delaminations. As illustrated in Figure 1, the computational efficiency of CDM enables the generation of large virtual datasets by systematically varying the FE input parameters.

Because UQ procedures typically require tens of thousands of model evaluations, machine-learning-based surrogate models are employed to achieve the necessary computational speed-up [4, 5]. To design efficient surrogate models, a thorough understanding of the simulated response variability is required. A global sensitivity analysis identifies the most influential FE input parameters, which are then used as the basis for surrogate modelling [6]. Gaussian process regression is applied to establish a relationship between the three most sensitive FE parameters and the specific energy absorption (SEA) obtained from the FE simulations. Subsequently, Markov Chain Monte Carlo (MCMC) is used to infer distributions of these parameters such that the simulated response matches the experimentally measured variations from flat-coupon crush tests.

These posterior parameter distributions are then applied to a different geometry, a composite tube (see Figure 1), to investigate the transferability of the inferred uncertainties. The results demonstrate that the combined experimental–computational framework not only captures the natural variability inherent in composite materials but also successfully extrapolates these findings to new structural configurations. This highlights the potential of UQ-enhanced CDM models and surrogate-assisted simulation workflows for improving the robustness and reliability of crashworthiness predictions in composite structures.

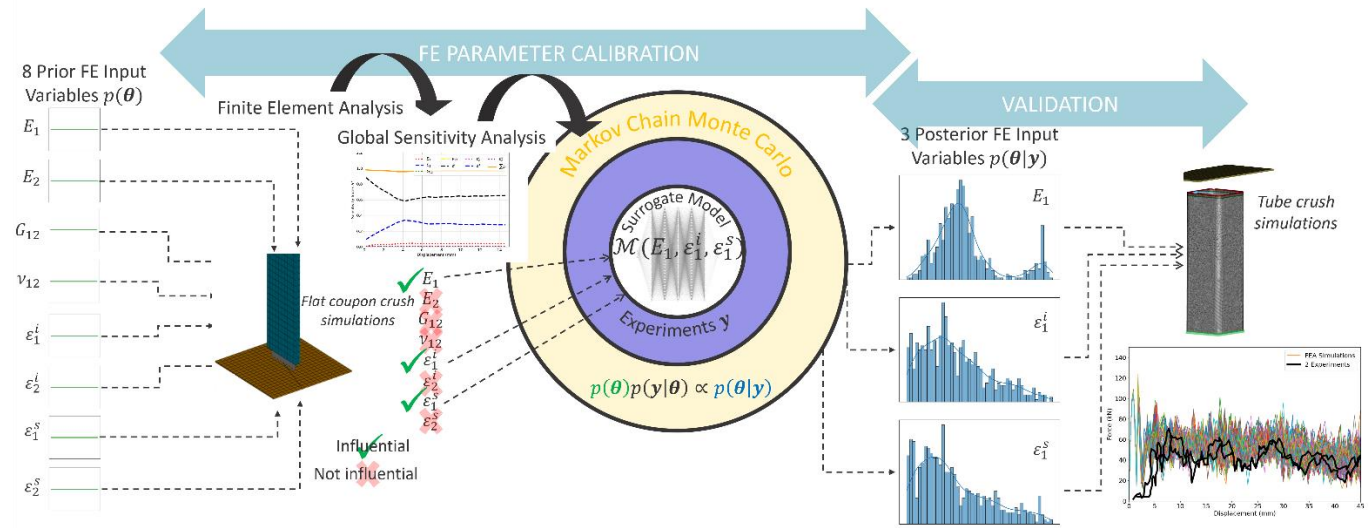


Figure 1 Schematic representation of the computational–experimental workflow developed to quantitatively predict variability in the crushing behaviour of carbon-fibre composite laminates, adapted from [3].

References:

- [1] Reiner J., Feser T., Waimer M., Poursartip A., Voggenreiter H., and Vaziri R. “Axial crush simulation of composites using continuum damage mechanics: FE software and material model independent considerations.” *Composites Part B: Engineering*, 225:109284, 2021.
- [2] Reiner J., Linden N., Vaziri R., Zobeiry N., and Kramer B. “Bayesian parameter estimation for the inclusion of uncertainty in progressive damage simulation of composites.” *Composite Structures*, page 117257, 2023.
- [3] Reiner J. “A multi-analysis framework for uncertainty quantification and data driven simulation of design allowables in laminated composites.” *Composites Science and Technology*, 261:111030, 2025.
- [4] Zobeiry N., Reiner J., and Vaziri R. “Theory-Guided Machine Learning for Damage Characterization of Composites.” *Composite Structures*, 246:112407, 2020.
- [5] Reiner J., Vaziri R., and Zobeiry N. “Machine learning assisted characterisation and simulation of compressive damage in composite laminates.” *Composite Structures*, page 114290, 2021.
- [6] Reiner J. “Higher-order sensitivity analyses to understand the role of FE input parameters on the simulation of composites in progressive fracture tests.” *Composite Structures*, 351:118585, 2025.

Data-Efficient Transfer Learning Framework for Digital Allowables of Open-Hole Compression Strength of Composite Laminates

Xin Liu^{1,2}, Sung Park³ and Nav Muraliraj³

¹Mechanical and Aerospace Engineering Department, University of Texas at Arlington, USA.
xin.liu@uta.edu

²Institute for Predictive Performance Methodologies, University of Texas at Arlington Research Institute, USA.

³Aeronautics Systems, Northrop Grumman Corporation, USA.

Abstract: Composite materials are widely used in modern aircraft due to their high stiffness/strength-to-weight ratio. However, before a new composite material or manufacturing method can be used, engineers must create material allowables, which are statistically determined, conservative limits for a material's strength for given confidence interval [1]. Currently, these allowables require a large number of physical tests with many layups, loading conditions, and environmental conditions. This process is slow, expensive, and often takes years to complete. As a result, it has become a significant barrier to introducing new materials with improved design for responding new needs quickly. Recent development in machine learning (ML) offers a promising cost-effective alternative. Instead of relying only on physical tests, ML models can learn from experimental and simulation data, and can help predict material strengths, estimate uncertainties, and support the creation of "digital allowables" that reduce the amount of physical testing required. However, one of the most pressing challenges in ML-assisted composites modeling is data scarcity. In industry practice, the available datasets for new material systems are very limited which significantly affects the insertion of such materials. Yet, advanced ML models like neural networks (NN) usually require far larger datasets to achieve high predictive accuracy and generalization. This mismatch has been a major barrier to the practical adoption of ML in modeling and design of composite materials and structures. To address this gap, the paper will propose a data-efficient, transfer learning ML framework that can leverage efficient simulation data and uncertainty quantification to produce trustworthy predictions with substantially fewer experimental data. The proposed computational framework has the potential to significantly reduce testing cost and time, accelerate certification workflows, and support faster, evidence-based design decisions.

In this paper, we will focus on the prediction of open-hole compression (OHC) strength with quantified uncertainty. Figure 1 illustrates the proposed hybrid simulation-experiment transfer learning framework. In Step 1, a multilayer perceptron (MLP) NN model is trained using efficient simulation data generated from classical laminate theory (CLT) coupled with failure initiation criterion. Note that this baseline surrogate aims to learn the global trends between design parameter θ (i.e., laminate layup) and the simulated compression strength, providing a fast and inexpensive estimation. In Step 2, sparse experimental data are introduced to correct systematic bias between simulations and experimental measurements. This is achieved by developing a Gaussian process (GP) model to learn the residual error $g_{GP}(\theta, y_{sim}(\theta))$ between simulation and experiment. The g_{GP} offers both mean prediction (μ_{GP}) and variance (σ_{GP}^2). The experimental scatter (i.e., coupon-to-coupon variability) is computed through the variance σ_{coupon}^2 based on experimental data. Finally, in Step 3, the baseline prediction and GP correction are synthesized to obtain the final hybrid prediction $y_{pred} = y_{sim} + \mu_{GP}$. The total predictive uncertainty is computed as $\sigma_{total}^2 = \sigma_{coupon}^2 + \sigma_{GP}^2$, which will provide a fully probabilistic prediction suitable for design and allowable determination under limited experimental data.

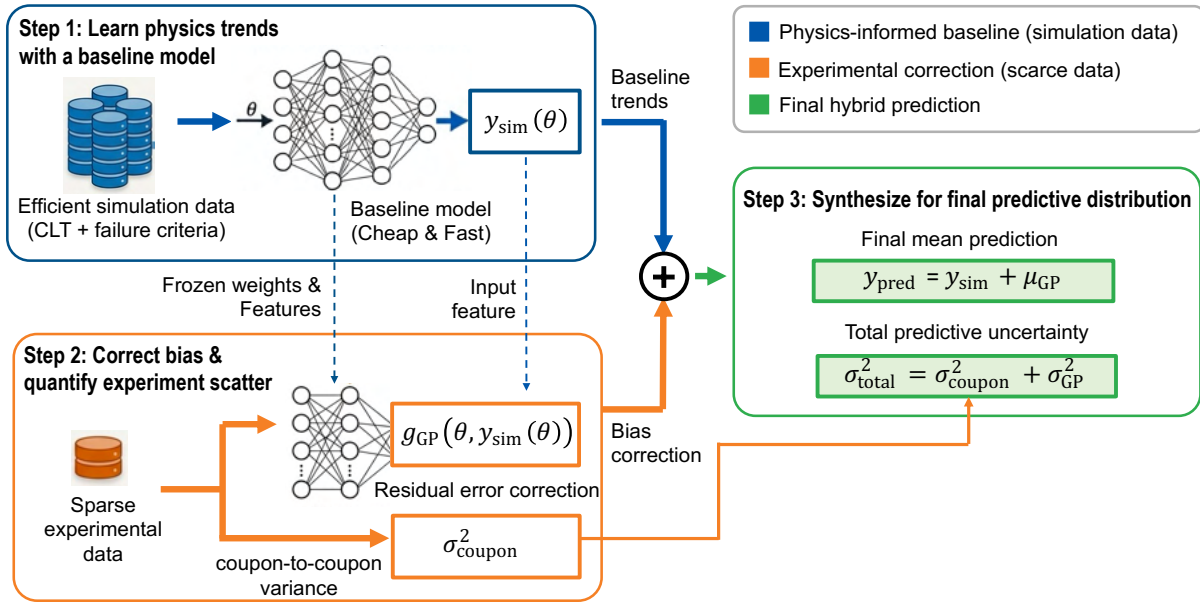


Figure 1: Hybrid simulation-experiment transfer learning framework

A synthetic benchmark problem was developed to demonstrate the feasibility of the proposed framework. As shown in Figure 2, the baseline model (blue curve) captures only the global trend of the underlying true response (red dashed curve). The model is trained using 20 scattered OHC data points. While the baseline prediction exhibits noticeable bias, the proposed neural network model augmented with a GP head successfully corrects this discrepancy and shows good agreement with the true model, with the associated 95% confidence interval accurately capturing the predictive uncertainty.

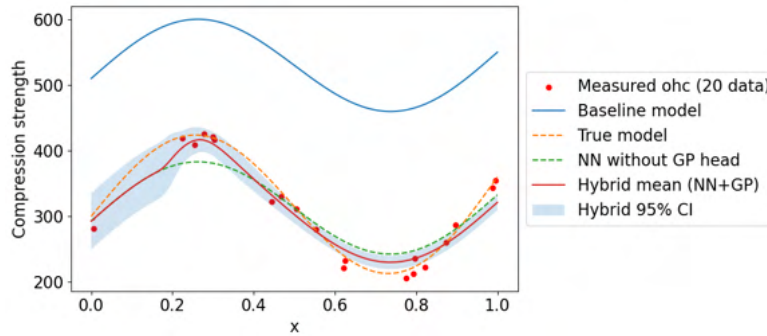


Figure 2: A synthetic model to demonstrate the feasibility. Baseline model: $y_{\text{sim}} = 510 + 80 \sin(2\pi x) + 40x$. True model: $y_{\text{pred}} = 300 + 120 \sin(2\pi x) + 60x^2$

The proposed computational framework and models will 1) reduce the need for extensive physical testing and costly high-fidelity simulations, and 2) guide future OHC experiments through GP-based uncertainty quantification, prioritizing the most informative OHC tests. By identifying where new data are truly needed, the approach enables a more strategic and efficient testing plan. Together, these capabilities will provide a powerful computational toolset for the development of digital allowables. These advances will shorten development cycles, lower certification costs, and support more rapid and confident decision-making in composite airframe design and qualification.

References:

- [1] R. Cumbo, A. Baroni, A. Ricciardi, S. Corvaglia, “Design allowables of composite laminates: A review”, *Journal of Composite Materials*, 56 (2022) 3617–3634.

Deep learning and multi-scale strategies for failure modelling of composite structures with complex material architectures

**Aewis K. W. Hii¹, Ruggero Filippone, Stephen R. Hallett,
Alberto Pirrera and Bassam El Said**

¹ Bristol Composites Institute, University of Bristol, United Kingdom, aewis.hii@bristol.ac.uk

Composite materials are becoming more complex architecturally to meet the weight and performance requirements across the aerospace, automotive, wind energy and defence sectors. Rapid virtual design and optimisation of structural components remains computationally challenging due to the multi-scale nature of the material geometry and underlying damage phenomena. We present a deep learning and multi-scale strategy to enable efficient structural failure modelling of composites with complex material architecture. There are two parts to the framework. Firstly, computational homogenisation is used to create the boundary value problems that link the fine and coarse scale models. Secondly, physics-informed neural networks are used to create surrogate material models across the length-scales from pre-computed material response databases.

The macroscopic length-scale is modelled using shell finite elements for computational efficiency. Their constitutive relations, e.g. ABD and transverse shear stiffness matrices as well as the force and moment resultants are obtained through second-order homogenisation of high-fidelity mesoscopic models [1]. Data-driven modelling of materials such as thick laminates (with hundreds of layers) or textile composites is challenging due to the large number of degrees of freedom in unit cells that span the full thickness, which significantly slows down the data generation process. This can be resolved by introducing an additional lower scale, where the local material geometry is further abstracted into a sub-meso scale that provides the constitutive relations at the upper length-scale through first-order homogenisation. For instance, the sub-mesoscopic unit cells would contain ply-by-ply model of the sub-laminates for thick laminates; and they would contain detailed discretisation of the yarn/matrix geometry for textile composites. This FE³ strategy, as shown in Figure 1, allows for significant speedup in creating the training data needed for the surrogate macroscopic material model. To enable efficient modelling of textile composites unit cells, this work features a conformal meshing algorithm to enable high quality meshing of yarn geometry and insertion of cohesive elements between yarn/matrix interfaces to model debonding.

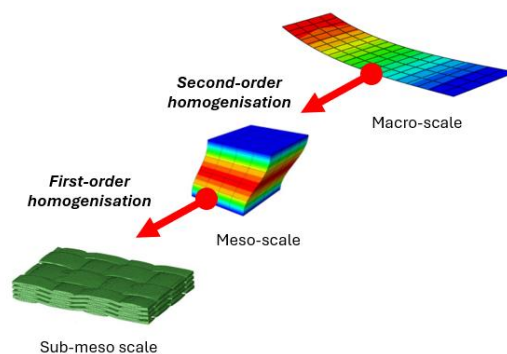


Figure 1: FE³ setup for the analysis of textile composites, using shell elements at the macro-scale, and solid elements at the meso- and sub-meso scales.

There are two key challenges in creating the surrogate material models. Firstly, in an implicit static/dynamic solver, the material stiffness tensors need to be provided in the training database. The added computational costs are non-trivial as the extraction of these tensors require additional perturbation and homogenisation steps. The second challenge is that neural networks lack physical basis in the model predictions despite being able to provide accurate fit to a database. Here, we present a physics-informed deep learning framework to resolve these challenges. In this framework, only strains, strain energy and stresses (resultants) are required for the training data, completely bypassing the need to sample material stiffness tensors. The network encodes the physical relationship between strain energy and stresses by penalising the loss functions in two-fold: firstly, the first gradient of the strain energy output is made equivalent to the stress outputs [2]; secondly, the second gradient of the strain energy output is made equivalent to first gradient of the stress outputs – the material stiffness tensors are evaluated in the output layer using an average of the two. Such a setup creates a model whose outputs are self-regulating and energetically consistent, all whilst allowing for material stiffness tensors to be learned directly during training. Furthermore, the surrogate material outputs, e.g. resultants and material stiffness tensors are now explicitly linked to the slopes of the strain energy landscape. In addition, Riemannian manifolds are used to constrain the model outputs so to preserve the underlying geometry of the material stiffness tensors [3]. This is achieved by using affine-invariant Riemannian metric in the loss functions and including eigen- and Cholesky decomposition in the output layer.

This work benchmarks the accuracy of the FE^3 modelling approach through comparisons with direct numerical simulations for both thick laminates and textile composites. The model setup details for specific application to composites are also discussed, e.g. how to select to capture the rapid change in material response during brittle failure whilst enabling higher-order automatic differentiation of the outputs, how to handle batch normalisation to achieve a consistent automatic differentiation when there is a significant difference in the magnitude of in-plane and out-of-plane stress responses. Lastly, the improvement in model performance and computational costs from using the physics-informed deep learning model is demonstrated through comparison with a rudimentary neural network trained on a stiffness-based database.

References:

- [1] A.K.W. Hii and B. El Said, A kinematically consistent second-order computational homogenisation framework for thick shell models, *Computer Methods in Applied Mechanics and Engineering*, Volume 398, 2022.
- [2] M. El Fallaki Idrissi, F. Praud, F. Meraghni, F. Chinesta, G. Chatzigeorgiou, Multiscale Thermodynamics-Informed Neural Networks (MuTINN) towards fast and frugal inelastic computation of woven composite structures, *Journal of the Mechanics and Physics of Solids*, Volume 186, 2024.
- [3] K. Xu, D. Z. Huang, E. Darve, Learning constitutive relations using symmetric positive definite neural networks, *Journal of Computational Physics*, Volume 428, 2021.

Explainable Physics-Informed Machine Learning for Mechanical Property Prediction and Formulation Design of Recycled Polymer Composites

Oumayma T., Tajir^{1*}, Saïd E., Elkoun^{1*}, and Tawfik M., Masrour²

¹ Center for Innovation in Technological Eco-Design (CITE), Department of Mechanical Engineering, University of Sherbrooke, 2500 University Boulevard, Sherbrooke, QC J1K 2R1, Canada

*oumayma.tajir@usherbrooke.ca *said.elkoun@usherbrooke.ca

² Artificial Intelligence for Engineering Sciences Research Team (AIASI), Department of Mathematics and Computer Science, Moulay Ismail University, Meknes, Morocco

Abstract:

Mechanical recycling of post-consumer polymer-based materials, including both unreinforced polymers and fiber-reinforced composites, represents a critical challenge for sustainable circular economy development. Industrial-scale recycled systems exhibit profound compositional heterogeneity, progressive material degradation across multiple recycling cycles, and complex thermal-mechanical processing histories that severely limit accurate property prediction [1,2]. Current machine learning approaches treat material composition as independent features, failing to capture the physical interactions governing material behavior [3,4]. Furthermore, purely data-driven black-box models lack the interpretability required by materials engineers for confident design decisions and process control.

This work introduces an innovative, physics-informed machine learning framework designed to bridge materials science principles with data-driven predictive modeling across polymer-based systems. The core methodological contribution lies in systematic integration of physics directly into feature engineering architecture rather than constraining the model itself. The framework incorporates: (1) mixing-rule baselines encoding composition and material interactions as reference features; (2) entropy-based blend structure descriptors characterizing formulation complexity through information-theoretic indices; (3) rheological material indices capturing material-specific processing behavior; and (4) processing condition variables encoding manufacturing effects. This physics-aware feature architecture encodes compositional interactions and material constitutive knowledge without constraining machine learning model selection, establishing a principled, generalizable approach applicable across material systems.

The framework compares multiple machine learning and deep learning models to identify optimal prediction strategies for various mechanical properties (e.g., tensile strength, melt flow index (MFI), impact resistance) and formulation scenarios. Models are trained and validated using rigorous cross-validation on comprehensive industrial datasets with diverse formulations and processing conditions.

To ensure practical utility, we apply a comprehensive, model-agnostic explainability framework. SHAP [5] and permutation importance identify dominant material and processing drivers, while dependence and conditional expectation analyses reveal nonlinear composition–property interactions and critical thresholds [6]. This ensures model transparency, physical interpretability, and reliable expert validation prior to deployment.

The framework is systematically validated on both unreinforced polymers (large-scale industrial datasets) and fiber-reinforced composites (exploratory formulations), demonstrating the physics-informed approach's applicability across diverse material systems.

Physics-informed features enhance model robustness across algorithms by reducing overfitting and improving generalization to new formulation spaces. Features remain deeply physically interpretable, enabling materials engineers to validate results against established principles and understand model decisions across different material complexities.

This scalable methodology enables reliable property prediction and formulation optimization for recycled polymer composites, supporting sustainable materials development, process control, and data-driven manufacturing strategies critical for circular economy advancement. The framework further supports formulation design by screening candidate compositions under processing constraints to meet target mechanical performance.

References:

- [1] A. Alassali, C. Picuno, Z. K. Chong, J. Guo, R. Maletz, and K. Kuchta, "Towards higher quality of recycled plastics: Limitations from the material's perspective," *Sustainability*, vol. 13, no. 23, p. 13266, 2021.
- [2] N. Andraju, G. W. Curtzwiler, Y. Ji, E. Kozliak, and P. Ranganathan, "Machine-learning-based predictions of polymer and postconsumer recycled polymer properties: A comprehensive review," *ACS Applied Materials & Interfaces*, vol. 14, pp. 42771–42790, 2022.
- [3] M. M. Cencer, J. S. Moore, and R. S. Assary, "Machine learning for polymeric materials: an introduction," *Polymer International*, vol. 71, no. 5, pp. 537–542, 2022.
- [4] L. Gao, J. Lin, L. Wang, and L. Du, "Machine learning-assisted design of advanced polymeric materials," *Accounts of Materials Research*, vol. 5, pp. 571–584, 2024.
- [5] S. M. Lundberg and S.-I. Lee, "A unified approach to interpreting model predictions," in *Proceedings of the 31st International Conference on Neural Information Processing Systems (NeurIPS)*, pp. 4768–4777, 2017.
- [6] A. Goldstein, A. Kapelner, J. Bleich, and E. Pitkin, "Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation," *Journal of Computational and Graphical Statistics*, vol. 24, no. 1, pp. 44–65, 2015.

Graph Transformers for Effective Prediction of Progressive Failure Evolution in Composite Structures

Luca Patrignani, Silvestre T. Pinho

Department of Aeronautics, Imperial College London, Exhibition Rd, South Kensington, London
SW7 2AZ, UK

The aviation industry's CO₂ emissions present a critical challenge for sustainability, driving the adoption of novel aircraft configurations and alternative fuels [1]. This paradigm shift demands high-performance predictive models for full-scale aircraft structures.

While Finite Element Analysis (FEA) remains the trusted approach for solving mechanics problems, it struggles with scalability and computational efficiency [2]. Machine Learning offers accelerations to structural simulations. However, traditional Convolutional Neural Networks fail on unstructured domains due to their reliance on regular grids, making them unsuitable for complex geometries [3]. Graph Neural Networks (GNNs) address these limitations by processing data on graphs [4], inherently capturing physical interactions through mesh connectivity whilst remaining resolution-independent [5].

Despite their advantages, standard GNN architectures face challenges when modelling damage evolution. Over-smoothing during message passing limits long-range information propagation, whilst progressive damage accumulation exhibits dual dynamics: gradual, spatially correlated growth and sudden catastrophic fracture events. Capturing both regimes within a unified autoregressive framework remains an open challenge.

We present a Graph Transformer methodology that addresses these limitations through three key innovations (Figure 1). First, we implement a frequency-controlled local-global attention mechanism that bridges neighbourhood connectivity with global domain awareness, enabling feature propagation across unstructured meshes without over-smoothing. Second, we introduce a discontinuity-capturing module that detects catastrophic failure events through spatial gradient and temporal rate analysis, routing high-rate damage regions through regime-specific decoders. Third, we incorporate Markov state transitions to explicitly model irreversible damage progression.

Our framework integrates seamlessly with commercial finite element workflows through an automated FEM-to-GNN pipeline and effectively predicts damage propagation across unseen configurations. We show various examples with clear aerospace relevance, including open-hole CFRP laminate plates, which can be simulated in just 0.32% of the time of a corresponding conventional FE simulation, while remaining resolution-independent. At the conference, we will show additional examples, including larger structural applications.

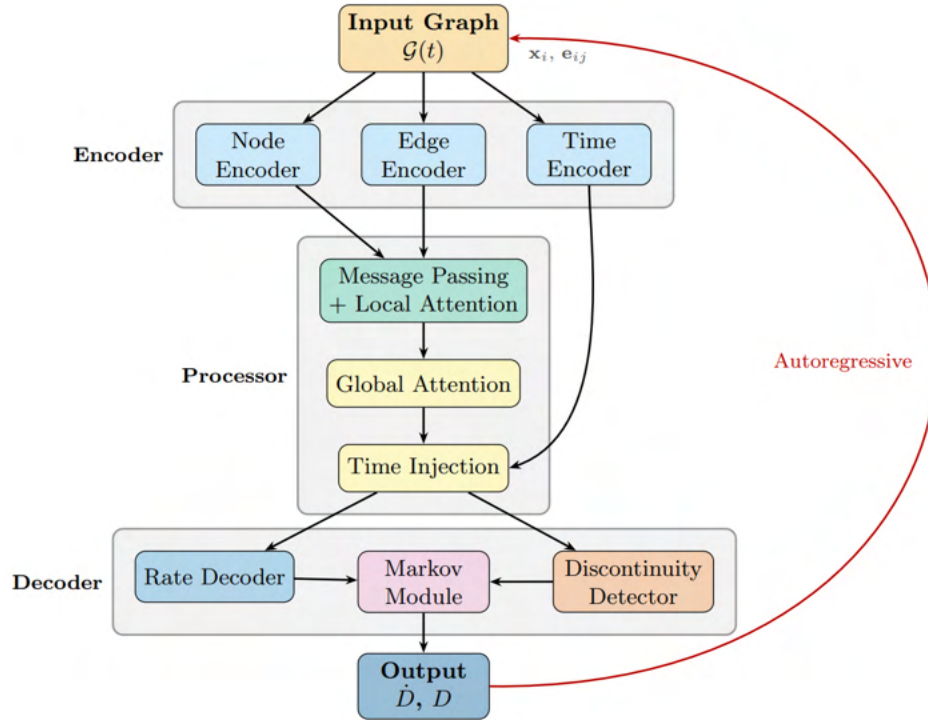


Figure 1: Architecture of the proposed Graph Transformer model showing the autoregressive damage prediction pipeline.

References:

- [1] Lee, David S., et al. "The contribution of global aviation to anthropogenic climate forcing for 2000 to 2018." *Atmospheric environment* 244 (2021): 117834.
- [2] Pinho, S. T., Matos, M., Costa, R. O. S. S., Ibbotson, A., and Ostergaard, M. "Enabling Multiscale Analysis of Very Large Composite Structures." 8th ECCOMAS Thematic Conference on the Mechanical Response of Composites, 2021, DOI: 10.23967/composites.2021.123.
- [3] Rezasefat, M. and Hogan, J.D., 2023. A finite element-convolutional neural network model (FE-CNN) for stress field analysis around arbitrary inclusions. *Machine Learning: Science and Technology*, 4(4), p.045052.
- [4] Scarselli, Franco, Marco Gori, Ah Chung Tsoi, Markus Hagenbuchner, and Gabriele Monfardini. "The graph neural network model." *IEEE transactions on neural networks* 20, no. 1 (2008): 61-80.
- [5] Patrignani, Luca, and Silvestre T. Pinho. "Graph neural networks with hybrid local-global attention for effective prediction of mechanical response in structures." *Computer Methods in Applied Mechanics and Engineering* 452 (2026): 118753.

IMPACT DAMAGE PREDICTION OF COMPOSITE LAMINATES USING MACHINE LEARNING

Meysam Rahmat¹, Zohreh Asaee¹

¹ Aerospace Research Centre, National Research Council Canada, Ottawa, ON K1A 0R6, Canada

Meysam.rahmat@nrc-cnrc.gc.ca

Evaluation and prediction of impact damage in composite materials are important for applications such as the aerospace industry. The extent and severity of damage depend on several factors, including impactor mass and velocity, laminate material and architecture, as well as ply properties (e.g., areal density and thickness). The complex relationship between these parameters and the extent of the damage often calls for comprehensive experimental investigations. For example, evaluation of residual strength of material through standardized compression after impact tests entails different damage levels (such as barely visible), and these damage levels on a particular laminate can only be achieved via trial-and-error efforts of impacting dummy trial specimens at different impact energy levels and observing the extent of the damage. The sheer number and complex relations of influencing parameters on impact damage make these tests very case dependent and, therefore, a good candidate to be studied by machine learning (ML). Thus, a limited but strategically designed set of experiments spanning representative combinations of impact conditions and laminate configurations can be used to generate paired input-output data for supervised learning. The ML model can be trained to learn the complex relationship from input parameters (e.g., the impact energy and laminate properties) to output quantities that characterize the extent of impact damage. The trained model can be evaluated on experimental results to assess predictive accuracy.

It should be noted that the size of the test matrix, even for a given material system, is nearly infinite, when considering the number of laminate plies and orientation, shapes and sizes of the impactor, as well as energy and velocity of impact; so, the ML model has to simulate a vast design space with as much training-data that the project can provide. A practical, yet ambitious, approach is to correlate the damage level with a set of input parameters that truly characterize a laminate; similar to how stress and strain define the material performance regardless of loading case and geometry. In the same way, the performance of material for a given impactor at a particular velocity can be characterized.

Drop tower impact tests characterize a laminate at a certain impact energy, which is a combination of impact velocity and impactor mass. During the test, the laminate absorbs energy and slows down the impactor while deforming elastically (through bending) and plastically (through damage). Hence, the impact energy for each test is constant but the impact velocity changes with time from the moment of impact. In contrast, a servo-hydraulic high-speed load frame (HSLF) is capable of inflicting damage at a constant velocity by overcoming the laminate resistance through supplying the required hydraulic pressure to the actuators as commanded by a closed loop controller [1]. Thus, the HSLF simulates impact of the laminate with an impactor with finite velocity but effectively infinite inertia (i.e., mass). As a result, all plies in the laminate fail at the impact velocity, which remains constant during the test. Therefore, a given laminate (or ply) under dynamic puncture loads (Figure 1-left) can be characterized at different, but constant, velocities as shown in Figure 1-right.

Owing to the boundary conditions, the puncture test generates some degree of bending in the specimen, which inherently creates the tensile-compressive stress field through the thickness. This stress field may

influence the failure mode in some of the plies. When the laminate puncture (or penetration) deformation is decoupled from bending deformation, it indicates the location of the front line of the impactor or the extent of penetration through the laminate. If the impact velocity as a function of time is known (via maximum damage energy absorption of the ply or through ML training), from load-displacement curves at different velocities (obtained from HSLF tests), the load-displacement curve of the laminate under constant energy impact (drop tower impact tests) can be predicted (Figure 2).

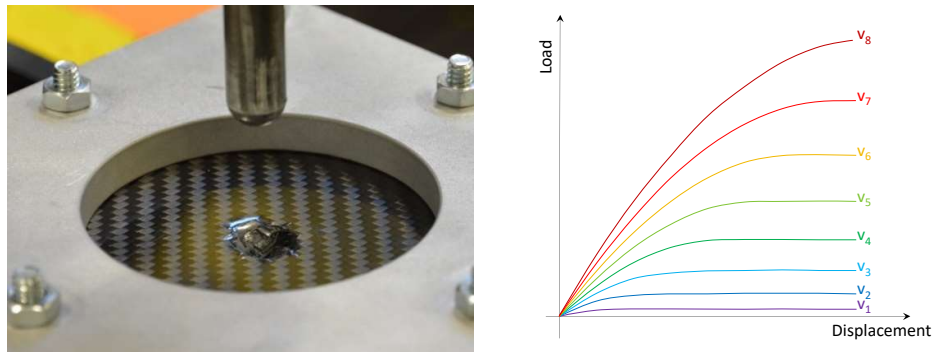


Figure 1: Puncture test fixture and an example of a laminate tested by drop tower impactor (or HSLF) (left), schematic of load-displacement curves at different impact velocities obtained from HSLF (right).

The experimental data presented in this work are obtained from Carbon-PEI laminates. Different impactor shapes and sizes are mounted on the HSLF and drop tower impactor, and velocities from quasi-static to 7 m/s are tested. These data are then used to train an ML model that learns the load-displacement response at various impact velocities (solid lines in Figure 2-left). The drop tower tests are used for ML training to learn the response of the laminate under constant energy impact. Then the impact damage and load-displacement curve of a new energy level are predicted by the ML model (dashed line in Figure 2-left) and compared to experiment, which was not used during ML training. Further investigation can incorporate more input parameters into the ML model and expand its prediction capabilities. Successful prediction of the complex response of composite laminates under impact loads demonstrates the potential of ML to support data-driven prediction of complex problems in the composite world.

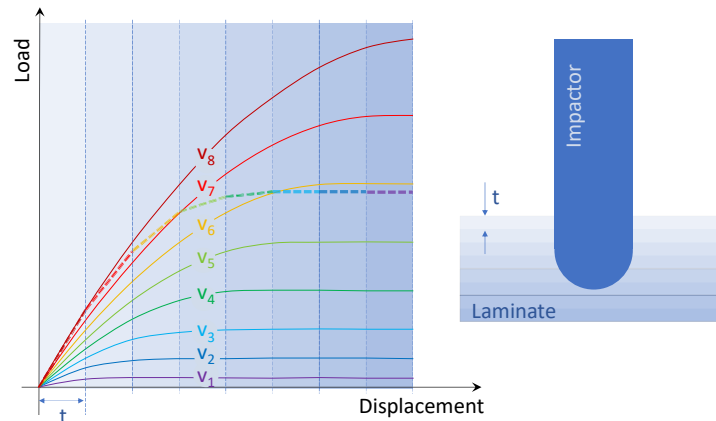


Figure 2: Schematic of load-displacement curves (left) for HSLF tests (solid lines), and drop tower impact (dashed line); schematic of composite laminate impact with ply thickness t .

References:

- [1] M. Rahmat, "Dynamic mechanical characterization of aluminum: analysis of strain-rate-dependent behavior," *Mech Time-Depend Mater*, vol. 23, pp. 385–405, 2019.

MODELING SHORT-FIBER REINFORCED COMPOSITES WITH ROTATION-FREE PARAMETRIC DMN

Huidi Ji¹, Tianyi Li²

¹ **Huidi Ji** (Dassault Systèmes Americas Corp, USA), hjj@3ds.com

² Tianyi Li (Dassault Systèmes, France)

Deep material network (DMN) has recently emerged as a data-driven surrogate model for heterogeneous materials [1]. Based on linear elastic training data generated by high-fidelity computational homogenization (FE-RVE simulation, for example), DMN is capable of predicting their elastic and inelastic behaviors with high accuracy. DMN learns the morphological characterizations of the microstructure by the homogenized effective stiffness tensor $\bar{\mathbf{c}}$ and the stiffness of the constituents $\mathbf{c}_1$ and $\mathbf{c}_2$. The effective stiffness tensor is usually computed using a high-fidelity homogenization method such as the FE-RVE method. The coefficients of DMN are computed by minimizing the difference between the DMN and the FE-RVE predictions.

We have recently presented a parametric DMN model for fiber-reinforced composites with a varying parameterized microstructure [3] based on the work of rotation-free DMN [2]. As shown in Figure 1, a single-layer feedforward neural network is used to account for the dependence of DMN fitting parameters on the microstructural characteristics such as the fiber volume fraction, aspect ratio and orientation. Micromechanical constraints are prescribed both on the parametric architecture and the outputs of this new neural network. Offline training is performed by minimizing a loss function that aggregates solely the linear elastic homogenization data generated across various morphologies.

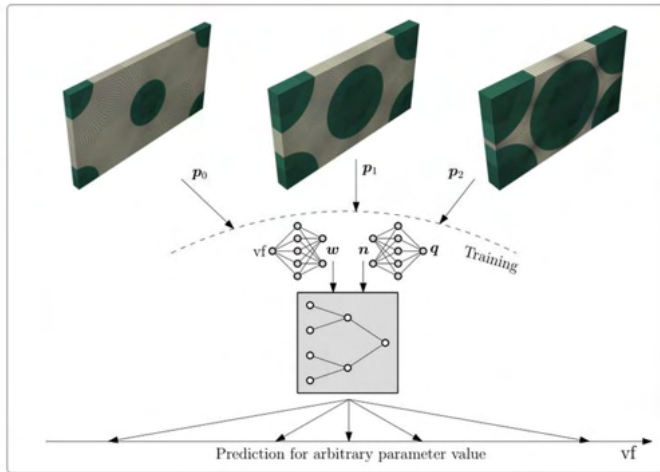


Figure 1: Parametric DMN trained with FE-RVEs of various volume fractions

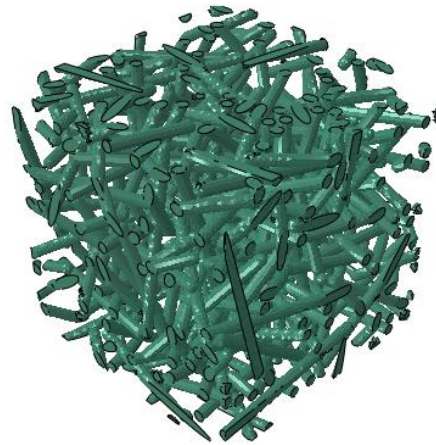


Figure 2: randomly distributed short-fiber reinforced composite

In this talk, we focus on the application of DMN on the modelling of short-fiber reinforced composites as shown in figure 2. Offline training is performed using FE-RVE models varying the fiber size and orientation. The effect of the sample size on the prediction of DMN is studied. We also compare the DMN results with the mean-field homogenization (MFH) method. The DMN results are more accurate when significant variation of the stress field is observed in the FE-RVE results.

References:

- [1] Liu, Z., C.T. Wu, "Exploring the 3D architectures of deep material network in data-driven multiscale mechanics", Journal of the Mechanics and Physics of Solids, vol. 127 20-46, 2019.
- [2] Gajek, S., M. Schneider, and T. Böhlke, "On the micromechanics of deep material networks," Journal of the Mechanics and Physics of Solids, vol. 242, 2020.
- [3] T. Li, "Micromechanics-informed parametric deep material network for physics behavior prediction of heterogeneous materials with a varying morphology, Computer Methods in Applied Mechanics and Engineering", 419, 116687, 2024.
- [4] DS Support Knowledge Base, "Deep Material Network Model for Abaqus/Standard", <https://support.3ds.com/knowledge-base/?q=docid:QA00000420397>, 2025

PHYSICS INFORMED NEURAL NETWORKS FOR THE MICROMECHANICAL ANALYSIS OF COMPOSITE AND STRUCTURAL METAMATERIALS

Yunfa Zhang^{1*}, Liying Jiang² and Ali Yousefpour¹

¹ Aerospace Research Centre, National Research Council Canada, Canada

*Yunfa.Zhang@nrc-cnrc.gc.ca

² Department of Mechanical and Materials Engineering, Western University, Canada

Due to their high stiffness and strength to weight ratios, advanced composite materials and emerging structural metamaterials offer great potentials for lightweight applications in aerospace and defence industries. However, the macroscopic mechanical properties of these materials depend on their micro-configurations including inhomogeneity and complex internal structures which require significant effort of meshing and simulation during a computational process such as the finite element analysis [1]. Although finite element methods (FEM) have been successfully employed in many applications, there are a number of open challenges including multiscale analyses, inverse problems, and uncertainty quantifications [2]. An alternate approach to conventional finite element method is the artificial neural networks (ANN) [3] which usually need large datasets for effective training. The introduction of the physics informed neural networks (PINN) provides an efficient approach for solving micromechanical problems employing smaller and well-defined datasets determined by the governing equations and corresponding initial and boundary conditions. A brief review of applications of PINN in various fields of continuum mechanics can be found in [3].

The present study focuses on the application of PINN in the micromechanical analysis of fiber-reinforced composites and structural metamaterials. Firstly, to facilitate the analysis of bi-material composites, a back-propagated (B-P) neural network with two material sub-networks (dedicated to the fiber and matrix, respectively) was established and the unit cell of a boron/aluminum composite was analysed under both normal and shear loading. Secondly, a neural network capable of performing micromechanical analysis of an auxetic metamaterial (made from a metal sheet with rectangular perforations [1]) was established with an extra layer for input data scaling for the analysis of parametric models. Figure 1 illustrates the schematic configuration of the PINN established.

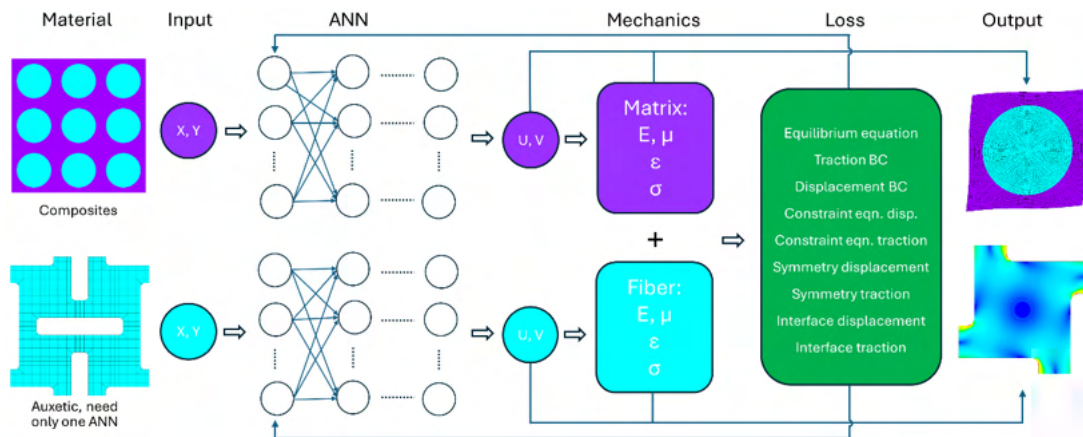


Figure 1. The PINN framework for micromechanical analysis.

All the loss items cited in the “Loss” block (Figure 1) should be accounted for to ensure the convergence of the PINN training process. In particular, the loss related to the traction and displacement continuity across the interface of the composites and the loss related to the periodic and symmetric boundary conditions are properly formulated and implemented in the PINN.

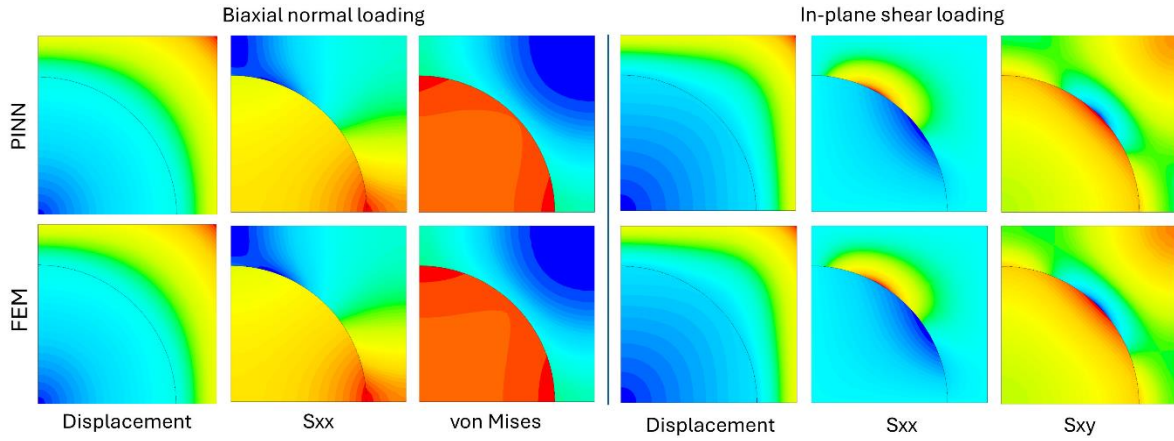


Figure 2. Comparison of PINN and FEM results.

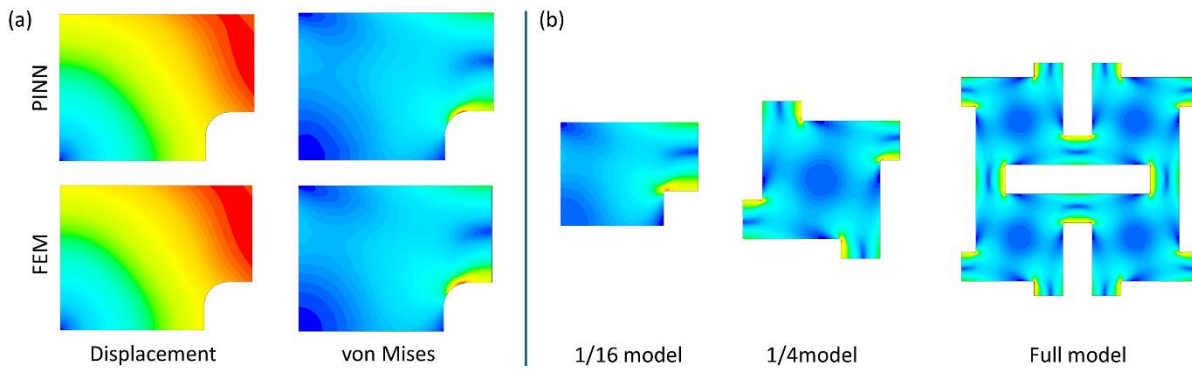


Figure 3. (a) Comparison of PINN and FEM results. (b) Symmetric mapping of the results [1].

The PINN predicted results are compared with those obtained from the finite element analysis (ANSYS) using identical grids. Figure 2 represents the results comparison for the boron/aluminum composites. It is observed that under both the biaxial normal loading and the in-plane shear loading, the two results are very close. Figure 3(a) shows the comparison of the results for the 2D auxetic material and the two results are very close too. Finally, it is noted that, for all the analyses in this study, symmetrically reduced models are employed for the sake of computational efficiency. For the auxetic metamaterial, for instance, a 1/16 model is employed considering the multifaceted symmetries presented. As demonstrated in Figure 3(b), the results for the full-sized model can be easily mapped from the reduced model, see details in [1].

References:

- [1] Y. Zhang, L. Jiang, A. Yousefpour. "Finite Element Analysis of Thermoelastic Properties of Metamaterials with Multifaceted Symmetries." In Mechanical and Aerospace Engineering, pp. 43-51. IOS Press, 2026.
- [2] S. David Müzel, E.P. Bonhin, N.M. Guimarães, E.S. Guidi. "Application of the finite element method in the analysis of composite materials: A review." Polymers 12, no. 4 (2020): 818.
- [3] A. Henkes, H. Wessels, R. Mahnken. "Physics informed neural networks for continuum micromechanics." Computer Methods in Applied Mechanics and Engineering 393 (2022): 114790.

REINFORCEMENT LEARNING-DRIVEN IMPACT ENERGY OPTIMIZATION USING TRANSFORMER-BASED SURROGATE MODELING FOR MULTI-MODAL DAMAGE PREDICTION IN CFRP/GFRP LAMINATES

Bal Krishna Raj Vijeta¹, G. Narayana Naik²

¹ Department of Aerospace Engineering, Indian Institute of Science, India, balraj@iisc.ac.in

² Department of Aerospace Engineering, Indian Institute of Science, India

Low-velocity impact loading in laminated composite structures produces complex and interacting damage mechanisms, including fiber and matrix failures under tension and compression, whose evolution governs energy absorption and residual strength. Understanding and optimizing such impact responses remain central challenges in composite structural design [1]. However, high-fidelity finite element simulations required to capture spatio-temporal damage progression are computationally expensive, limiting their direct use for design exploration.

To address this limitation, a hybrid **physics-informed** artificial intelligence framework combining surrogate modeling and reinforcement learning is proposed. First, a Transformer–CNN architecture based on attention mechanisms [2] is trained to learn the time-series evolution of four physically distinct damage variables, namely fiber tension, fiber compression, matrix tension, and matrix compression. The trained network accurately predicts full-field damage sequences across varying material systems and impact energies while reducing computational cost by several orders of magnitude. The surrogate thereby serves as a fast virtual environment for efficient design optimization. The use of physics-consistent surrogate modeling aligns with recent advances in computational mechanics [3].

Subsequently, the impact design problem is formulated as a reinforcement learning task. A policy network trained using Proximal Policy Optimization (PPO) [4] interacts with the surrogate to select impact energy levels. A physics-aware reward function balances energy absorption against weighted multi-modal damage severity, with material-dependent penalties reflecting dominant fracture mechanisms in unidirectional and cross-ply laminates. A safety-constrained formulation further ensures identification of the maximum sustainable impact energy while maintaining damage below acceptable limits.

The proposed framework transforms damage prediction into a closed-loop design optimization problem and enables automated discovery of material-dependent safe operating regimes. Results demonstrate that the learned policies consistently identify optimal energy thresholds and provide interpretable insights into laminate impact tolerance. The methodology offers a scalable pathway toward intelligent, data-driven design of impact-resistant composite structures.

Keywords: Composite laminates; Low-velocity impact; Damage progression; Transformer networks; Surrogate modeling; Reinforcement learning; Proximal Policy Optimization; Design optimization.

References:

- [1] S. Abrate, *Impact on Composite Structures*, Cambridge University Press, 1998.
- [2] A. Vaswani et al., “Attention is all you need,” *Advances in Neural Information Processing Systems*, 2017.

- [3] M. Raissi, P. Perdikaris and G. E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear PDEs," *Journal of Computational Physics*, vol. 378, pp. 686–707, 2019.
- [4] J. Schulman et al., "Proximal policy optimization algorithms," arXiv:1707.06347, 2017.

Robustness Analysis of Data-Driven Impact Localization Models in the Presence of Experimental Uncertainty

Emanuel von Cramon-Taubadel¹, Martin Becker² and Philipp Weißgraeber³

¹ Presenting Author, Chair of Lightweight Design, University Rostock, Germany,
Email: emanuel.cramon-taubadel@uni-rostock.de

² Hessian.AI - Deep Decision Support Systems, University Marburg, Germany

³ Chair of Lightweight Design, University Rostock

Fiber-reinforced polymer composites provide high specific strength, stiffness, and corrosion resistance, making them attractive for weight-critical structures. However, their anisotropic and heterogeneous nature makes them susceptible to complex failure mechanisms. These can result from barely visible impact damage (BVID) induced by low-energy impacts, which can significantly reduce residual strength while remaining difficult to detect [1].

Conventional acoustic emission (AE)–based structural health monitoring (SHM) systems rely on high-fidelity piezoelectric sensors and time-difference-of-arrival localization [2], requiring dense sensor networks, precise synchronization, and extensive calibration. These constraints limit scalability and cost efficiency for large-area applications. Advances in low-cost digital micro-electro-mechanical systems (MEMS) sensors provide a promising alternative for distributed impact monitoring. Prior investigations have demonstrated the feasibility of MEMS-based sensing for impact detection in composite structures when used in conjunction with machine learning [3]. However, systematic evaluation of robustness, sensitivity to environmental and operational variability, and suitability for damage classification tasks remains limited.

This study experimentally evaluates digital MEMS accelerometers for impact detection in composite laminates. Using a fully automated testbed, we examine diverse impact scenarios with controlled environmental and structural variations to assess prediction performance and robustness under varying boundary conditions. We present a regression convolutional neural network (CNN) that improves results from previously used classification CNN architectures. To address limited labeled data, we apply transfer learning and reduce the required training data by 88% with only a 2% decrease in localization accuracy relative to a fully trained model. Additionally, we use explainable AI methods to enhance model transparency by identifying physically relevant signal features influencing predictions.

The results demonstrate that MEMS-based sensing, combined with data-efficient learning and interpretability frameworks, represents a scalable and economically viable approach for distributed monitoring of impacts in composite structures.

References:

- [1] J. Jang, I.Y. Lee, Y.B. Park, “Impact response analysis and Physics-Informed damage classification of sandwich composites using electrical resistance-based self-sensing”, Composites Part A: Applied Science and Manufacturing, Volume 190, 2025
- [2] S.A. Zargar and F.G. Yuan. “Impact diagnosis in stiffened structural panels using a deep learning approach”. Structural Health Monitoring. 2020; 20(2):681-691
- [3] A.M. Damm, C. Spitzmüller, A. T. S. Raichle, A. Bühler, P. Weißgraeber, P. Middendorf. “Deep learning for impact detection in composite plates with sparsely integrated sensors”. Smart Materials and Structures, 29(12):125014, October 2020.

Using Explainable Machine Learning to Support the Modeling Strategies of Composite Structures

M. Petrolo¹, G. Candita¹, A. Pagani¹, E. Carrera¹ and A. Racionero Sánchez-Majano²

¹MUL2 Lab, Department of Mechanical and Aerospace Engineering, Politecnico di Torino, Italy,
marco.petrolo@polito.it

²Department of Aerospace Engineering, Universidad Carlos III de Madrid - UC3M, Spain

The proper modeling of composite structures aims to minimize computational overhead without compromising accuracy. When finite elements are used, modeling requires selecting the structural theory, element type, and mesh; these choices depend on the problem features, e.g., the type of analysis, the outputs of interest, the material system, and others. The aim of the present work is to use Explainable Machine Learning methods to provide guidelines for the proper modeling of composite structures, with a focus on the choice of the set of generalized variables, i.e., the model's degrees of freedom.

One-dimensional (1D) structural theories with higher-order displacement fields are implemented using the Carrera Unified Formulation (CUF) [1], which enables systematic multi-fidelity analyses by varying the order of the kinematic expansion [2]. In this work, the evaluated theories range from first- to fourth-order models, with the full fourth-order theory adopted as the reference.

$$\begin{aligned} u_x &= u_{x1} + xu_{x2} + zu_{x3} + x^2u_{x4} + xzu_{x5} + z^2u_{x6} + \dots + xz^3u_{x14} + z^4u_{x15} \\ u_y &= u_{y1} + xu_{y2} + zu_{y3} + x^2u_{y4} + xzu_{y5} + z^2u_{y6} + \dots + xz^3u_{y14} + z^4u_{y15} \\ u_z &= u_{z1} + xu_{z2} + zu_{z3} + x^2u_{z4} + xzu_{z5} + z^2u_{z6} + \dots + xz^3u_{z14} + z^4u_{z15} \end{aligned} \quad (1)$$

The classical Timoshenko theory is a special case of the expansion that uses five of the 45 degrees of freedom. A Neural Network (NN) [3,4] is trained on input features representing generalized variables [5], material properties, and geometry to predict the accuracy of structural theories for a given problem. Explainable ML [6] tools based on SHapley Additive exPlanations (SHAP) [7] are then used to quantify the contribution of each generalized variable and problem feature to the predicted error, enabling identification of the most influential terms.

Preliminary results focus on a three-layer laminated beam $[0^\circ/90^\circ/0^\circ]$, clamped-free, made of an orthotropic material with $E_L = 250 \text{ GPa}$, $E_T = 10 \text{ GPa}$, $\nu_L = \nu_T = 0.33$, $G_L = 5 \text{ GPa}$, $G_T = 2 \text{ GPa}$, $\rho = 2700 \text{ kg/m}^3$, $L/h = 50$. Figure 1 reports, on a logarithmic scale, the errors associated with the best structural theories as their degrees of freedom change. Errors were computed on the first ten natural frequencies. These curves are referred to as Best Theory Diagrams (BTD) [8], as they show the best achievable accuracy for a given number of DOF. The 15-DOF model is the full fourth-order theory of Eq. 1; the actual number of DOF is 45, but the three components of a given expansion term are either activated or deactivated simultaneously, and, therefore, the number of expansion terms is reported. The 21-DOF and 12-DOF theories are highlighted as the best combinations of 21 and 12 generalized variables, respectively, i.e., those that maximize accuracy. The results from a full FEM analysis and those obtained by a Deep Neural Network are compared and a perfect match was found. Table 1 reports all the best theories with black triangles indicating active terms. The SHAP analysis includes Feature Importance bar plots, see Fig. 2, and Beeswarm plots, see Fig. 3. In both cases, generalized variables are reported along one axis and SHAP values (ϕ) along the other, representing each variable's contribution to the predicted error. The bar plot shows the average absolute SHAP value $|\bar{\phi}|$, providing a direct measure of variable importance. The Beeswarm plot displays the distribution of SHAP values across all structural theories, with red points indicating active terms and blue points inactive ones. This analysis provides insight into how generalized variables influence accuracy. Figures 4 and 5 show, respectively, the effects of changing the lamination $[0^\circ/0^\circ/90^\circ]$ and the slenderness, $L/h = 10$. Assessing the influence of generalized variables on the dynamic response of composite beams supports the extraction of the most relevant terms, facilitating the construction of efficient reduced-order models with minimal complexity and high accuracy.

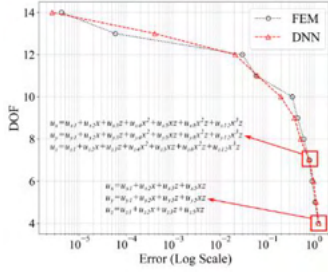


Figure 1: BTD of the $[0^\circ/90^\circ/0^\circ]$ laminated beam with $L/h=50$

DOF	const.	x	z	x^2	xz	z^2	x^3	x^2z	xz^2	z^3	x^4	x^3z	x^2z^2	xz^3	z^4	$\%E_{AVG}$
14	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	2.642E-06
13	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	4.069E-04
12	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	2.090E-02
11	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	6.277E-02
10	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	1.969E-01
9	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	3.844E-01
8	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	5.193E-01
7	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	7.905E-01
6	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	9.858E-01
5	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	1.115E+00
4	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	▲	1.268E+00

Table 1: Best theories of the $[0^\circ/90^\circ/0^\circ]$ laminated beam with $L/h=50$ evaluated by DNN

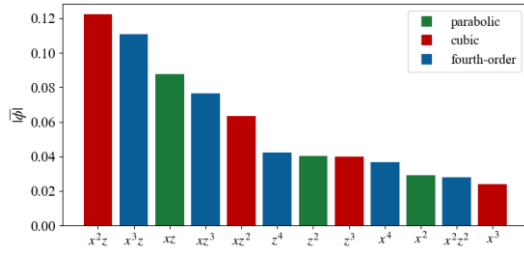


Figure 2: Generalized variables influence bar plot for the $[0^\circ/90^\circ/0^\circ]$ laminated beam with $L/h=50$

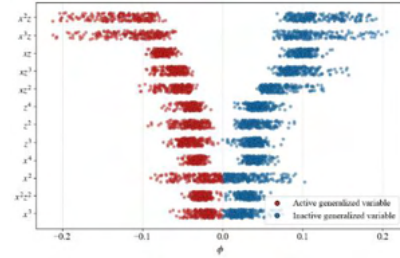


Figure 3: Generalized variables beeswarm plot for the $[0^\circ/90^\circ/0^\circ]$ laminated beam with $L/h=50$

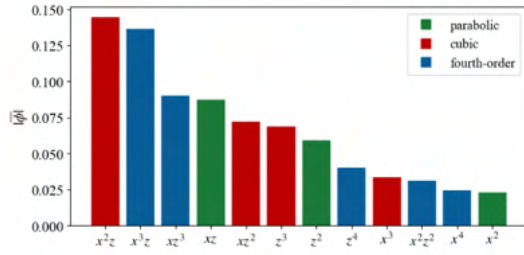


Figure 4: Generalized variables influence bar plot for the $[0^\circ/0^\circ/90^\circ]$ laminated beam with $L/h=50$

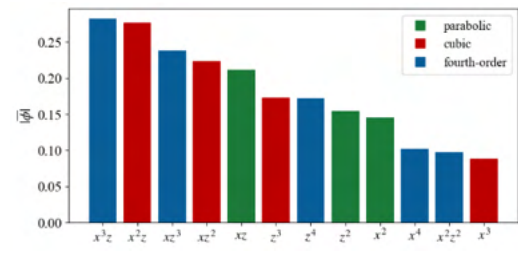


Figure 5: Generalized variables beeswarm plot for the $[0^\circ/90^\circ/0^\circ]$ laminated beam with $L/h=10$

References

- [1] E. Carrera, M. Cinefra, M. Petrolo, and E. Zappino, "Finite element analysis of structures through unified formulation." John Wiley & Sons, 2014.
- [2] E. Carrera and M. Petrolo, "On the effectiveness of higher-order terms in refined beam theories." Journal of Applied Mechanics, 78(2):021013, 11 2010.
- [3] Sarker, I. H. "Machine learning: Algorithms, real-world applications and research directions." SN Computer Science Vol. 2 No. 3 (2021): p. 160.
- [4] B. Z. Cunha, A.-M. Zine S. Foulard M. Ichchou, C. Droz. "A review of machine learning methods applied to structural dynamics and vibroacoustic." Mechanical Systems and Signal Processing Vol. 200 (2023): p. 110535
- [5] M. Petrolo, A. Pagani, E. Carrera, G. Candita, P. Iannotti, "Mapping beam cross-section features to higher-order generalized variables using machine learning." Thin-Walled Structures, Vol. 218, Part C (2026), 114108
- [6] M. Lundberg and S.-I. Lee. "A Unified Approach to Interpreting Model Predictions." Advances in Neural Information Processing Systems Vol. 30 (2017)
- [7] P. Linardatos, S. Kotsiantis, V. Papastefanopoulos. "Explainable AI: A review of machine learning interpretability methods." Entropy Vol. 23 No. 1 (2020): p. 18
- [8] M. Petrolo, P. Iannotti, "Best Theory Diagrams for Laminated Composite Shells Based on Failure Indexes". Aerotec. Missili Spaz. 102, 199–218 (2023)

Session Four

4 DATA-DRIVE SURROGATE MODELS AND ACCELERATED SIMULATIONS

AI-Enabled Composite Textiles within the UPWARS Sustainable Innovation Framework

**Mohammad S. Rouhi¹, Qunyue Liang², Sandra-Meriem Mokli², Ming-Jun Zhang³,
Ahmed Mehaoua⁴, Erik Marklund¹, Sofiane Guessasma²**

¹ RISE Research Institutes of Sweden (Dept. Sustainable Material Systems, Unit Composite Technology, Sweden), mohammad.rouhi@ri.se

² INRAE, Research unit BIA, Nantes, France

³ CNAM, Conservatoire National des arts et metiers, Paris, France

⁴ Centre Borelli UMR 9010, Université Paris Cité, France

The UPWEARS project funded by Horizon Europe develops a new generation of sustainable e-textiles based on flax/hemp fibres and lignin-derived matrices, whose intrinsic natural variability and hierarchical structure pose major challenges for predictive modelling. At the fibre, yarn, and fabric levels, high-fidelity FE models can be used to capture the multi-physics behaviour—mechanical, thermal, hygrothermal—of natural-fibre-based systems. These finite element (FE) models can become computationally demanding, particularly when their size reaches on the order of millions of degrees of freedom [1-2]. In this work, we present an integrated multiscale modelling and AI framework combining physics-based FE simulations with artificial neural networks (ANNs) to replace costly 3D FE simulations for predicting yarn-level mechanical responses and provide reliable performance prediction for fibre, yarn, and fabric across the scales [3]. These developments form the backbone of a physics-informed learning strategy: simulation data from FE are used to train surrogate models that approximate the FE response while dramatically reducing computational cost.

The developed workflow integrates experimental data based on 2D /3D imaging and mechanical testing for fibres and rovings with a semi-analytical homogenisation framework to derive effective fibre properties. These homogenised properties are then used alongside a ABAQUS Python/C++ scripts approach for generating idealised yarn geometries using cooperative models, enabling systematic and reproducible model construction while avoiding fibre overlap [4]. Building on these yarn-level models, the workflow further extends to the development of idealised fabric-level geometries, providing a coherent multiscale modelling foundation from fibres to textiles.

The specifications considered for yarn consists of random number of transversely isotropic fibres arranged in a circular cross-section, 10 mm in length, with an S-pitch twist. Instead of running full FE simulations, synthetic datasets were generated to capture variations in fibre radius, modulus, applied load, and orientation vectors. These datasets were used to train an ANN model, to correlate the geometrical and intrinsic fibre properties to the yarn performance (predict axial stress, axial strain, stiffness, and failure load). The integration of physics-informed constraints ensures consistency with fundamental mechanics, improving generalization and interpretability. Preliminary results demonstrate that the ANN model can achieve near-perfect accuracy for stress and strain predictions while reducing computational time by several orders of magnitude. This approach enables rapid design space exploration and optimization for complex yarn structures, paving the way for scalable and efficient virtual testing in textile engineering.

References

- [1] Delphine Quereilhac, Emmanuel De Luycker, Sofiane Guessasma, Marwa Abida, Jonathan Perrin, Timm Weitkamp, Alain Bourmaud, Pierre Ouagne, “Synchrotron X-ray microtomography and finite element modelling to uncover flax fibre defect’s role in tensile performances”, *Composites Part A: Applied Science and Manufacturing*, Volume 184, September 2024, 108276, <https://doi.org/10.1016/j.compositesa.2024.108276>
- [2] Abderrahmane Ayadi, Hedi Nouri, Sofiane Guessasma, Frederic Roger, “Determination of orthotropic properties of glass fibre reinforced thermoplastics using X-ray tomography and multiscale finite element computation”, *Composite Structures*, Volume 136, February 2016, Pages 635-649, <https://doi.org/10.1016/j.compstruct.2015.10.041>
- [3] S. Guessasma, D.H. Bassir, “Identification of mechanical properties of biopolymer composites sensitive to interface effect using hybrid approach”, *Mechanics of Materials*, Volume 42, Issue 3, March 2010, Pages 344-353, <https://doi.org/10.1016/j.mechmat.2009.12.001>
- [4] S. Guessasma and M. Oyen, “Virtual design of electrospun-like gelatin scaffolds: the effect of three-dimensional fibre orientation on elasticity behaviour”, *Journal of Soft Matter*, Issue 2, 2016, <https://doi.org/10.1039/C5SM02342D>

AI-Enabled Multiscale ICME Workflow for Injection-Molded Composites in LS-DYNA

Arash Kargar-Estahbanati¹, Haoyan Wei² and Sunil Acharya³

¹ Synopsys, Inc., 1007 Church Street, Suite 250 Evanston, IL 60201 USA, akargar@synopsys.com

² Synopsys, Inc., 7374 Las Positas Rd, Livermore, CA 94551 USA

³ Synopsys, Inc., 220 Valley Creek Blvd Exton, PA 19341 USA

Accurate prediction of mechanical performance in injection-molded fiber-reinforced composites requires explicit consideration of manufacturing-induced microstructures, including heterogeneous fiber orientation and volume fraction distributions. In this work, we develop and implement an AI-enhanced multiscale simulation workflow in LS-DYNA through the material model *MAT_303 (*MAT_DMN_COMPOSITE_FRC) [1]. We integrate injection molding simulation, macro-scale material calibration using MCalibration, and nonlinear structural analysis within an Integrated Computational Materials Engineering (ICME) framework [2].

We combine process simulation, microstructure mapping, and a Deep Material Network (DMN)-based multiscale material model [3] to efficiently predict anisotropic and history-dependent composite responses at the structural level. This ICME workflow enables the mapping of fiber orientation and volume fraction data from molding simulations onto structural meshes to create locally adapted multiscale material models. To minimize computational overhead, MCalibration is adopted based on experimental data to identify constituent material parameters, particularly matrix plasticity behavior, thereby significantly reducing calibration effort compared to conventional anisotropic composite models.

We validate the proposed workflow using injection-molded short-fiber-reinforced thermoplastic specimens and demonstrate accurate prediction of stiffness and stress-strain responses across multiple loading orientations, even when calibrated using minimal experimental data. By evaluating the model in both tensile and drop test applications, we further show that it accurately captures deformation and equivalent plastic strain distributions at the component level. Overall, the workflow enables reliable, computationally efficient, and process-aware virtual testing of composite components while supporting structural design optimization and manufacturing process improvement within a unified CAE environment.

References:

- [1] LS-DYNA Keyword User's Manual, Ansys Inc., 2024. [Online]. Available: <https://lsdyna.ansys.com/manuals/>
- [2] J. Allison, D. Backman, and L. Christodoulou, "Integrated computational materials engineering: a new paradigm for the global materials profession," JOM, vol. 58, no. 11, pp. 25–27, 2006.
- [3] H. Wei, C. T. Wu, W. Hu, T. H. Su, H. Oura, M. Nishi, T. Naito, S. Chung, and L. Shen. "LS-DYNA machine learning-based multiscale method for nonlinear modeling of short fiber-reinforced composites." Journal of Engineering Mechanics, 149(3), 04023003, 2023

Bayesian Calibration and Uncertainty Quantification to Support Bonded Composite Textile Modeling with Limited Data

Matthew L. Kirby, Erin C. DeCarlo, Marcus L. Stanfield, and David S. Riha

Mechanical Engineering Division, Southwest Research Institute, USA, matthew.kirby@swri.org

Bonded composites are increasingly being used in aircraft structures to reduce weight and improve performance. However, certification of these structures following a traditional “building block” testing approach is typically onerous and costly and still only yields limited data at the component level [1,2]. A recent program funded by the United States Air Force Research Laboratory titled Organic matrix composite (OMC) Process-to-Performance, Evaluation, Research and Analysis (OPPERA) developed physics-based models of bonded composite pi-preform joints (referred to simply as pi-joints) to reduce risk and testing costs during certification [3,4,5,6]. The idea is to use the physics-based models to augment the certification test data, especially at the component level, ultimately enriching what is typically a “data poor” problem.

Artificial intelligence/machine learning (AI/ML) approaches are used in this research in two aspects:

(1) Due to uncertainty in the material properties, adhesive fracture properties, and pi-joint geometry, the physics-based models of the pi-joint (*i.e.*, homogenized parametric finite element models) require calibration to predict the mechanical response of the pi-preform joint with confidence. Since this is a “data poor” problem, meaning that there is a limited number of pi-preform joint experiments with which to calibrate the model, some conventional AI/ML approaches that require a “data rich” environment are not suitable. Thus, we employed a Bayesian model calibration approach, originally presented in [7], to quantify and reduce uncertainty in model input parameters with limited experimental data. Bayesian methods are ideal for non-deterministic solutions in which data is limited and support incorporation of engineering judgement based on knowledge of physical phenomena, as opposed to “blindly” fitting data.

(2) Gaussian process (GP) regression [8] was also used to make Bayesian calibration tractable. A distinct advantage of GP surrogate models is that they are formulated to predict both the mean and the variance of the response, making them ideal for uncertainty quantification. Bayesian calibration relies on hundreds of thousands of Markov chain Monte Carlo (MCMC) samples to explore the data likelihood across the calibration parameter space and build the posterior distributions of the calibration parameters. Each MCMC sample equates to multiple pi-joint model simulations, depending on the number of responses that are being calibrated simultaneously and sample acceptance ratios. The nominal wall-clock simulation time for the parametric pi-joint model is between 10 and 20 minutes [7]. Therefore, it is not feasible to perform Bayesian calibration with the physics-based models directly in the MCMC sampling loop. GP regression models were first trained as surrogate models to replace physics-based simulations in the MCMC sampling loop during Bayesian calibration. To train the GP surrogate models, we used 125 random samples of the physics-based parametric pi-joint model via Latin hypercube sampling (LHS) [9] for a space-filling design of random variables.

In more detail, the physics-based pi-joint model that will be discussed in this presentation is a parametric finite element model of the pi-joint in Abaqus that employs homogenized, orthotropic elastic properties

to model the pi-preform and composite laminate skin and web response. The adhesive used to bond the pi-preform to the stringer (*i.e.*, skin) and stiffener (*i.e.*, web) is modeled with isotropic elastic properties and damage initiation and progression (*i.e.*, disbond) are simulated via cohesive surfaces. The bilinear cohesive zone model parameters governing adhesive disbond and the pi-preform mechanical properties were the primary calibration parameters. Additional calibration parameters included the pi-preform base thickness, which was challenging to measure experimentally (*i.e.*, difficult to determine where the adhesive ends and the pi-preform base begins), and some of the uncertain skin and web laminate properties. In total, there were twelve calibration parameters in this study. These parameters were calibrated based on experimental data from traditional pi-joint certification test configurations (*i.e.*, web tension pull-off and lateral side bend).

Force-displacement curves for two pull-off and two lateral bend tests were used for calibration data. The specific characteristics of these force-displacement curves that were used as calibration data were the slope of the linear regime (referred to as “stiffness”) and the failure load (the maximum load prior to the first appreciable load drop in the force-displacement curve). Note that Bayesian methods can be employed to calibrate and reflect uncertainty in underdetermined systems, such as the case presented here (*i.e.*, four experiments versus twelve calibration parameters). After calibration, the most likely value for the twelve calibration parameters (referred to as “best fit” parameters) based on the posterior distribution from Bayesian calibration were used in the physics-based model to verify that the calibrated model prediction agreed with the calibration data. Comparing the model predictions to the experimental data for pull-off and lateral bend showed that the absolute error between the predicted and experimental failure load was <6% (*i.e.*, 3.06% absolute error for pull-off failure load and 5.97% for lateral bend). Additionally, the stiffness predictions were within 2.25% of the experimental stiffness values (*i.e.*, 0.23% absolute error for pull-off and 2.05% for lateral bend).

Three combined loading test configurations were used for model validation. The combined loading experiments involved rotating the pi-joint at discrete angles to change the orientation of the applied load relative to the pi-joint. These tests allowed for different combinations of pull-off and lateral bend loading, in which a 0° orientation corresponds to a pure pull-off loading configuration and a 90° orientation corresponds to a pure lateral bend loading configuration. The force-displacement curves for two combined loading tests at an angle of 20°, two at an angle of 45°, and two at an angle of 70°, for a total of six tests, were used for validation data. Validation was performed using the “best fit” parameters calibrated from the pure pull-off and pure lateral bend experiments in the physics-based model to predict the combined loading experiments. The results showed that the failure load predictions were in good agreement with the experiments – the absolute error in the predicted combined loading failure load response was within 9% of the experiments. However, the pi-joint model had more difficulty predicting the stiffness. The absolute error in the predicted stiffness for the 45° and 70° combined loading tests was 12.7% and 6.57%, respectively. The model response was significantly stiffer than the 20° combined loading response from experiments with an absolute error of 183%, revealing gaps in our understanding and/or experimental data. Further investigation is required to determine if this discrepancy is due to error in the experiments or challenges modeling the transition between Mode II and Mode I failure in the model. This study provides a reminder that the models are only as good as the data. As a result of including physics-based models in our AI/ML calibration approach, we were able to identify this gap in our understanding, and the physics-based predictions give guidance on how to improve the models.

In conclusion, this study provides an approach for using AI/ML models to support physics-based model development for enriching datasets in bonded composites. The approach is certification-based and has transferability across joint geometries and adaptability to other bonded composite configurations, which could ultimately be used to reduce risk and cost during the certification process. The approach is highlighted by the use of Bayesian inference to quantify and reduce uncertainty in model parameters in scenarios where data is limited, such as component level certification for bonded composite structures. In general, the authors of this study are in favor of approaches that leverage the strengths of both physics-based and AI/ML modeling approaches when possible and find that these approaches are more

generalizable, have better extrapolation capabilities, and require less training data than pure AI/ML approaches.

References:

- [1] Marshal, P., Rezai, A.: "Use of composites in aerostructures", Newsletter of the European Society for Composite Materials (ESCM), issue 3, May (2000)
- [2] Soutis, C.: Fibre reinforced composites in aircraft construction. *Prog Aerosp Sci* **41**(2), 143–151 (2005)
- [3] Riha, D. S., Kirby, M. L., Stanfield, M. L., Bhamidipati, V., Popelar, C. F., Zhou, E., Forghani, A., Iarve, E. V., Hoos, K. H., Adluru, H. K., Ballard, M. K., Selvarathinam, A. S., and Mollenhauer, D. "Organic Matrix Composites Process-to-Performance, Evaluation, Research and Analysis (OPPERA)," *AIAA SCITECH 2023 Forum*. 2023, p. 2424.
- [4] Riha, D. S., Kirby, M. L., Stanfield, M. L., Bhamidipati, V., Popelar, C. F., Zhou, E., Forghani, A., Iarve, E. V., Hoos, K. H., Selvarathinam, A. S., Mollenhauer, D., and H. K., Ballard. "Results and Findings from the Organic Matrix Composites Process-to-Performance, Evaluation, Research and Analysis (OPPERA) Program," *AIAA SCITECH 2025 Forum*. 2025, p. 2521.
- [5] Stanfield, M., Kirby, M., DeCarlo, E., Popelar, C., Riha, D. (2025). Bayesian Calibration and Uncertainty Quantification of Cohesive Zone Parameters at an Adhesively Bonded Textile and Fabric Interface. In: Zobeiry, N., Liu, X. (eds) *Design and Analysis of Composites*. ASC 2024. Proceedings of the American Society for Composites Annual Technical Conferences. Springer, Cham.
https://doi.org/10.1007/978-3-032-01730-7_6
- [6] Kirby M., DeCarlo E., Stanfield M., Popelar C., Riha D. "Verification, Validation, and Uncertainty Quantification of a Parametric Model for the Structural Response of Bonded 3D Textile Pi-Preform Joints." *In 40th ASC Technical Conference*, Dayton, OH, 2025.
- [7] Kirby, M., Stanfield, M., DeCarlo, E. C., and Riha, D. "Development and Calibration of a Model for Predicting the Structural Response of Bonded Composite Pi-joints," *AIAA SCITECH 2023 Forum*. 2023, p. 2422.
- [8] Williams, C.K. and C.E. Rasmussen, *Gaussian processes for machine learning*. Vol. 2. 2006: MIT press Cambridge, MA.
- [9] Santner, T. J., Williams, B. J., Notz, W. I., and Williams, B. J. *The design and analysis of computer experiments*: Springer, 2003.

Data-Efficient Virtual Materials Twin for Ternary Short Fiber-Magnetic Particle Polymer Composites via AI-Calibrated Microstructure-Based FEA

Yingnan Wang¹ and Pierre Mertiny¹

¹ Department of Mechanical Engineering, University of Alberta, Canada

Presenting author: Yingnan Wang, yingnan1@ualberta.ca

Hybrid polymer composites reinforced by both short fibers and particulate fillers enable multifunctional performance but remain challenging to model due to pronounced microstructural heterogeneity, spatial variability in filler alignment, and complex multi-phase interactions at high filler contents. Short glass fiber reinforced, magnetically loaded polymer (SFRMP) composites developed for electromechanical applications exemplify this challenge. Microstructure-based finite element analysis (FEA) constructed from individual scanning electron microscopy (SEM) fields of view (FoVs) often yields scattered effective properties, while bulk experiments exhibit comparatively stable macroscopic responses. Consequently, selecting a single “representative” SEM FoV is inherently subjective and limits predictive robustness.

To address this limitation, a ‘data-efficient virtual materials twin’ framework is proposed that couples AI-based multi-FoV fusion with microstructure-based FEA, enabling formulation-level representativeness under limited microstructural sampling (Fig. 1). The AI component adopts a set-based learning strategy, in which multiple SEM FoVs are aggregated in an order-invariant manner to extract robust microstructural descriptors at the formulation level [1]. These descriptors are then embedded into computationally efficient microstructure-based representative volume elements (RVEs) and calibrated against experimental measurements using physics-based simulation, with uncertainty-aware calibration enabled through surrogate modeling concepts.

The material system considered is a ternary composite consisting of isotropic NdFeB magnetic particles, short glass fibers, and an epoxy matrix. All formulations are designed with a fixed total filler content of 50 vol%, while the particle-to-fiber ratio is varied across five formulations labeled P65–P85, where the label denotes the NdFeB particle weight percentage in the composite. Among these, P75 (75 wt% NdFeB particles; 35.9/14.1/50 vol% particles/fibers/matrix) is selected as an anchor case for model learning and calibration.

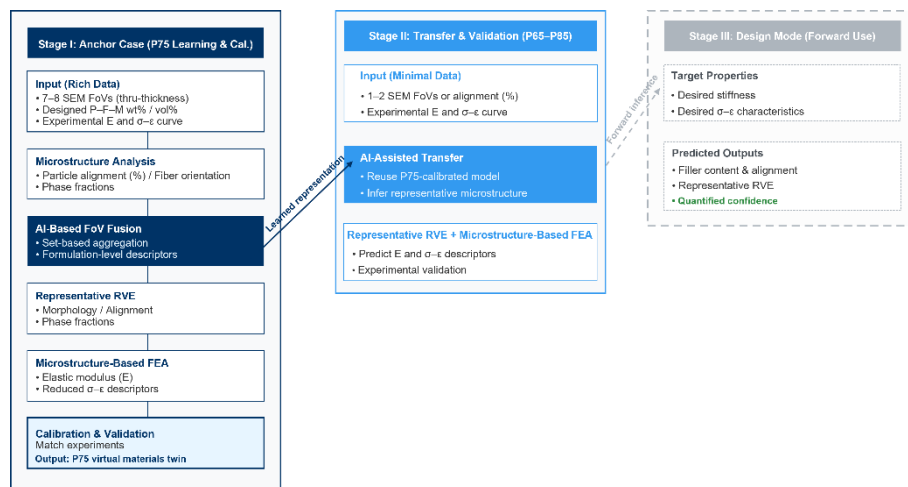


Figure 1. AI-enhanced microstructure-based FEA workflow: P75 anchor-case learning and calibration using multi-FoV SEM and experiments, transfer to P65–P85 using minimal new microstructural input, and forward design mode for property-targeted material design.

Stage I: Anchor case learning and calibration (P75)

For P75, rich input data are provided, including seven to eight SEM FoVs taken from through-thickness sections, designed phase fractions, and experimental mechanical measurements comprising elastic modulus and a representative stress-strain curve. Each SEM FoV is analyzed to quantify particle alignment percentage, fiber orientation, and phase fractions. Rather than treating FoVs independently, AI-based set aggregation is employed to fuse multiple FoVs into formulation-level microstructural descriptors, thereby reducing sensitivity to local heterogeneity and subjective FoV selection [1]. From these descriptors, a representative RVE suitable for microstructure-based FEA is generated and evaluated using a physically consistent simulation framework. A calibration loop is applied to match simulated elastic modulus and reduced stress-strain descriptors to experimental results, yielding a validated P75 virtual materials twin. This stage builds directly on the authors' prior experimental and stochastic FEA investigations of magnetic particle polymer composites [2] and processing-relevant epoxy systems [3].

Stage II: Transfer and validation (P65–P85)

To assess generalization, the calibrated P75 model is transferred to four additional formulations (P65, P70, P80, and P85). For each formulation, only minimal new input data are required, either one to two SEM FoVs or measured alignment percentages, together with experimental elastic modulus and a representative stress-strain curve. The framework reuses the P75-calibrated representation to infer a representative microstructure and construct a corresponding RVE. Microstructure-based FEA is then performed to predict elastic modulus and reduced stress-strain descriptors, which are validated against experimental measurements. Where appropriate, adaptive sampling strategies inspired by Bayesian optimization may be employed to efficiently refine predictions while minimizing computational cost [4].

Stage III: Design mode (forward use)

Finally, the validated framework enables a forward design mode, in which target mechanical properties (e.g., desired stiffness and stress-strain characteristics) are mapped to feasible design variables within the same material family. The model outputs recommended filler contents and alignment characteristics, together with a representative RVE and quantified confidence. This capability supports data-efficient exploration and design of highly heterogeneous ternary composites for electromechanical applications. Overall, the proposed framework seeks to replace subjective FoV selection with AI-driven multi-FoV fusion, preserve physical fidelity through microstructure-based FEA calibrated to experiments, and enable low-effort transfer across related formulations. By explicitly linking microstructural descriptors, representative RVEs, and experimental response, the approach aims to advance practical virtual materials twin development for complex hybrid polymer composites.

References:

- [1] M. Zaheer, S. Kottur, S. Ravanbakhsh, B. Poczos, R. Salakhutdinov, and A. Smola, "Deep Sets," *Advances in Neural Information Processing Systems*, vol. 30, pp. 3391–3401, 2017.
- [2] Y. Wang, H. Ahmadi Moghaddam, J. Palacios Moreno, and P. Mertiny, "Magnetic Filler Polymer Composites—Morphology Characterization and Experimental and Stochastic Finite Element Analyses of Mechanical Properties," *Polymers*, vol. 15, no. 13, p. 2897, 2023.
- [3] Y. Wang and P. Mertiny, "Mechanical and Thermal Properties of Epoxy Resin upon Addition of Low-Viscosity Modifier," *Polymers*, vol. 16, no. 17, p. 2403, 2024.
- [4] M. Balandat, B. Karrer, D. R. Jiang, S. Daulton, B. Letham, A. G. Wilson, and E. Bakshy, "BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization," *Advances in Neural Information Processing Systems*, vol. 33, pp. 21524–21538, 2020.

Development of Probabilistic Surrogate Model for Uncertainty Quantification in Low Velocity Impact (LVI) of Caron/Epoxy Woven Composites

Sanghyun Yoo¹, Mathieu Vinot¹, Nathalie Toso¹ and Heinz Voggenreiter¹

¹ Institute of Structures and Design, German Aerospace Center (DLR), Germany,
Sanghyun.Yoo@dlr.de

² Innovation Center for Small Aircraft Technologies (INK), German Aerospace Center (DLR),
Germany

The design and certification of aero-composite structures rely on the test pyramid, also known as the building block approach. This process currently depends on experimental-based statistical test evidence such as material allowables [1]. Thus, the test pyramid necessitates costly and time-consuming experimental test campaigns up to the full-scale structure. To accelerate the certification process of fibre reinforced polymer (FRP) composite structures, there is growing interest in the aerospace industry for integrating machine learning (ML) models, which can shorten development cycles. For example, surrogate models can replace computationally expensive finite element (FE) simulations with an inverse inference model [2,3]. However, standard surrogate models often fail to capture inherent data variability in the context of the test pyramid. This highlights the need for implementing probabilistic methods that acknowledge real-world variations.

To address these growing needs, this study reports a framework to develop a probabilistic surrogate model that connects the coupon level to the sub-element level of the test pyramid. This study uses low velocity impact (LVI) testing as a case study since understanding of impact damages such as barely visible impact damage (BVID) is crucial in certification process to ensure the performance and safety of composite structures [4]. In this study, material properties measured at the coupon level are used for constructing a material card of FE simulation as input features, while the results of impact simulations are served as the target parameters. By establishing correlations between different length scales within the test pyramid, we aim to reduce the reliance on experimental tests conducted at coupon level.

Fig. 1 presents the overview of a probabilistic surrogate modelling approach that utilises Bayesian Neural Networks (BNNs) via Monte Carlo (MC) Dropout and Gaussian Process Regression (GPR). This framework not only predicts the energy absorption behaviour of CFRP under impact but also quantifies the uncertainty associated with the predictions. Various mechanical tests at the coupon level are performed to generate a LS-DYNA® material card, *MAT_ENHANCED_COMPOSITE_DAMAGE*. Subsequently, experimental impact testing is conducted in accordance with ASTM D7136/D7136M to validate the impact FE simulation.

The first step in training a surrogate model involves generating a comprehensive dataset that encompasses the design space of interest. To build a robust surrogate model, Latin Hypercube Sampling (LHS) is implemented to cover the multidimensional parameter space efficiently. This ensures that the entire range of each parameter is sampled, significantly improving the convergence rate of the surrogate model compared to random sampling. In the second step, the contribution of each parameter to the model prediction is investigated using SHapley Additive exPlanations (SHAP) [5] to quantify and determine the importance of each parameter on the prediction for model interpretability. Finally, the

surrogate model based on BNN and the GPR model are trained with the reduced input parameters based on their importance. The results from the trained surrogate model enable an accurate prediction of the impact residual energy at reduced time-to-prediction. The output generated by the surrogate model is a distribution rather than a single deterministic prediction. Additionally, the uncertainty within the model helps assess the confidence of the predictions. The comparative study between the BNNs and the GPR models indicates that performance significantly depends on the size of the training dataset.

This work represents a first step toward developing a data-driven approach that decrease the reliance on physical experimental testing through probabilistic surrogate modelling. The proposed surrogate model is capable of accurately predicting the impact of residual energy with associated uncertainty. The identified uncertainty can be incorporated into decision-making processes, especially in the early stage of developing composite structures like evaluating operational applicability. Consequently, predictions that include uncertainty can help identify suitable material candidates while reducing the number of required experiments. Furthermore, this work paves the way for a scalable approach for the reduction of the computational time required to obtain the impact residual energy for composite laminates.

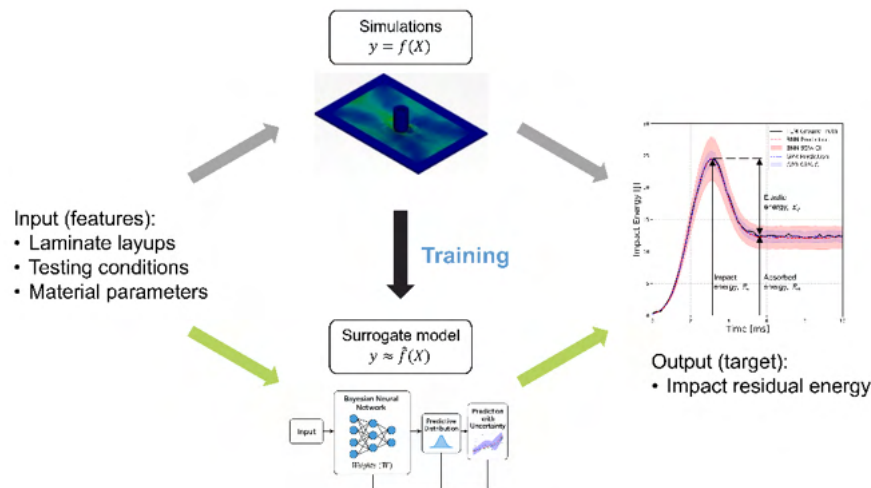


Figure 1: The overview of a probabilistic surrogate modelling.

References:

- [1] Cumbo R, Baroni A, Ricciardi A, et al. Design allowables of composite laminates: A review. *Journal of Composite Materials*. 2022;56(23):3617-3634.
- [2] Arndt C, Crusenberry C, Heng B, et al. Reduced-Dimension Surrogate Modeling to Characterize the Damage Tolerance of Composite/Metal Structures. *Modelling*. 2023;4(4):485-514.
- [3] Sakaridis E, Karathanasopoulos N, Mohr D. Machine-learning based prediction of crash response of tubular structures. *International Journal of Impact Engineering*. 2022;166:104240.
- [4] SUBPART A — GENERAL, AMC 20-29 Composite Aircraft Structure. European Aviation Safety Agency (EASA).
- [5] Lundberg SM, Lee S-I. A Unified Approach to Interpreting Model Predictions. *Advances in Neural Information Processing Systems*. 2017;30.

A Novel Output Space Sampling Method for Bayesian Modelling of Composites

Runze Li¹, Mário Miranda² and Silvestre T. Pinho³

¹ Presenting Author, Department of Aeronautics, Imperial College London, UK,
runze.li@imperial.ac.uk

² Department of Aeronautics, Imperial College London, UK

³ Department of Aeronautics, Imperial College London, UK

Machine learning has emerged as a powerful paradigm for predicting and designing composite structures by learning complex mappings from geometric parameters and layup configurations to mechanical responses. However, composite layup modelling poses a fundamental challenge for data-driven learning due to its high dimensionality, variable-length structure, and discrete nature. Practical carbon fiber reinforced polymer (CFRP) components may contain dozens to hundreds of plies, rendering exhaustive sampling of the input space infeasible and severely limiting the scalability of conventional supervised learning approaches.

In this work, we introduce a Bayesian learning framework for fast and probabilistic prediction of composite failure behaviour that explicitly addresses the curse of dimensionality in structured layup representations. Rather than approximating the full layup–response mapping, the proposed model directly learns the failure probability distribution of composite structures, enabling uncertainty-aware estimation of upper and lower bounds of failure indices prior to any downstream layup optimization.

To further improve data efficiency, we propose a novel output-space sampling strategy that systematically generates representative layups conditioned on diverse failure responses. By shifting the sampling process from the high-dimensional input space to the response space, the method effectively captures the full spectrum of possible failure behaviours and provides informative training signals for Bayesian inference.

The proposed framework is validated on open-hole compression benchmarks, with failure indices evaluated using the LaRC05 criteria. A comprehensive dataset spanning multiple geometries and layup configurations is constructed, and a heteroscedastic variational Bayesian last-layer model is employed for predictive uncertainty quantification. Results demonstrate that the proposed approach achieves accurate, robust, and data-efficient probabilistic predictions of composite failure indices across varying geometries and loading conditions, highlighting its potential as an uncertainty-aware AI framework for the design and optimization of advanced composite structures.

MACHINE LEARNING-BASED MULTISCALE MODELLING OF COMPOSITE LAMINATES FOR EFFICIENT STRUCTURAL SIMULATIONS

Radouan BOUALLALA¹ and Carlos González^{1,2}

¹IMDEA Materials Institute, Getafe, Madrid, Spain

²Dpt. Materials Science, Universidad Politécnica de Madrid, Madrid, Spain

Accurate prediction of the structural response of composite laminates requires capturing mesoscale mechanisms such as inter-ply stress redistribution, matrix nonlinearities, and progressive damage evolution [1-2], which are typically neglected in classical laminate theory and standard shell formulations. These simplified approaches assume homogenized constitutive behaviour at the ply level and often fail to represent the complex interactions between plies that govern the overall laminate response under multiaxial loading conditions. Although explicitly modelling the laminate stacking sequence using three-dimensional solid finite elements can capture these mechanisms, such an approach becomes computationally prohibitive for large-scale structural simulations due to the high number of degrees of freedom and the small element sizes required through the laminate thickness.

To address this limitation, this work proposes a multiscale surrogate modelling strategy that transfers the mechanical response of composite laminates from the mesoscale [3,4] to the structural scale. The central idea is to learn the effective constitutive behaviour of a laminate representative volume element (RVE) and embed this learned response into shell elements used in structural analyses. In this way, the surrogate model acts as a data-driven constitutive law capable of reproducing the nonlinear and path-dependent behaviour of the laminate while maintaining the computational efficiency of shell-based structural models.

The proposed methodology follows a two-stage offline–online computational framework. In the offline stage, a periodic RVE representing the laminate stacking sequence was constructed using three-dimensional solid finite elements. Periodic boundary conditions were applied to ensure energetic consistency and represent the behaviour of an infinite laminate subjected to macroscopic loading. To efficiently explore the strain space and generate a representative training dataset, multiaxial strain paths were applied to the RVE using a Latin Hypercube Sampling (LHS) strategy. This sampling technique ensures a uniform coverage of the multidimensional strain domain while minimizing the number of required simulations. The numerical simulations were performed using an explicit finite element formulation coupled with a previously developed VUMAT constitutive model in Abaqus Explicit capable of describing the nonlinear and damage behaviour of the composite constituents. During these simulations, histories of generalized strains and corresponding internal forces were extracted from the RVE. These data constitute a high-fidelity dataset describing the mesoscale mechanical response of the laminate under a wide range of loading conditions.

The resulting dataset was used to train a recurrent neural network (RNN) surrogate model that learns the path-dependent mapping between strain histories and force responses. The use of recurrent architectures allows the surrogate model to incorporate temporal dependencies and internal state evolution, which are essential to represent the history-dependent behaviour characteristic of laminated composites, including stiffness degradation and nonlinear response under cyclic or non-proportional loading paths.

The trained network was validated against independent strain paths not included in the training dataset to evaluate its generalization capability and predictive accuracy. In the online stage, the trained surrogate model is integrated into the structural finite element framework to define the constitutive behaviour of shell sections. During the structural simulation, the neural network receives the generalized strain history of each shell integration point and predicts the corresponding force resultants, effectively reproducing the mesoscale laminate response without explicitly resolving the laminate through the thickness. This approach enables the efficient simulation of large-scale composite structures while retaining the fidelity of mesoscale modelling.

The proposed multiscale framework therefore provides a computationally efficient alternative to fully resolved laminate simulations and opens new possibilities for integrating high-fidelity mesoscale physics into structural-scale analyses through machine learning-based surrogate constitutive models.

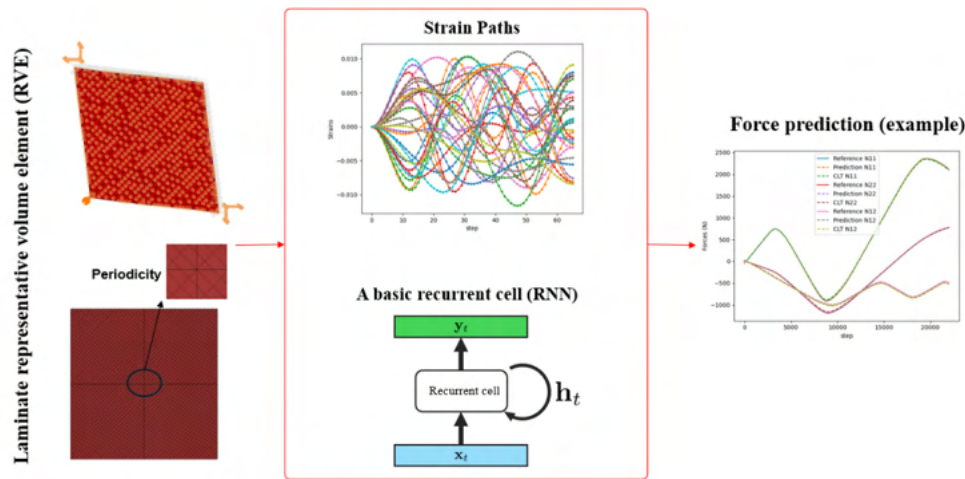


Figure 1. Multiscale surrogate modelling framework proposed in this work. In the offline stage, a laminate representative volume element (RVE) is simulated under multiaxial strain paths to generate a dataset used to train a recurrent neural network surrogate model. In the online stage, the trained model is embedded into shell elements to reproduce the laminate constitutive response during structural simulations.

- [1] González, C., Vilatela, J. J., Molina-Aldareguía, J. M., Lopes, C. S., Llorca, J. Structural composites for multifunctional applications: Current challenges and future trends. *Progress in Materials Science* 89 (2017) 194–251.
- [2] Llorca, J., González, C., Molina-Aldareguía, J. M., Segurado, J., et al. Multiscale modeling of composite materials: a roadmap towards virtual testing. *Advanced Materials*, 23, 2011, pp. 5130–5147.
- [3] Lopes, C. S., González, C., Falco, O., Naya, F., Llorca, J. Multiscale virtual testing: the roadmap to efficient design of composites for damage resistance and tolerance. *Aerospace Science and Technology* 46 (2015) 424–432.
- [4] Mocerino, D., Zarzoso, M., Sket, F., Molina-Aldareguía, J. M., González, C. A Machine Learning Boosted Data Reduction Methodology for Translaminar Fracture of Structural Composites. *Applied Composite Materials* 31 (2024) 1833–1848.

Machine Learning-Enabled Bayesian Inference for Constituent Hydrogen Permeabilities in Polymer Composites

#Mustafa Okumus¹, Łukasz Figiel^{1,2}

¹ IINM, WMG, University of Warwick, Coventry, CV4 7AL, UK, mustafa.okumus@warwick.ac.uk

² Warwick Centre for Predictive Modelling, University of Warwick, Coventry, CV4 7AL, UK

Reliable modelling of hydrogen permeation in fibre-reinforced polymer composites is essential for the safe design of hydrogen storage and transport infrastructure. However, the hydrogen permeabilities of the *in-situ* matrix, carbon fibres and fibre–matrix interphase cannot be measured directly under *in-situ* conditions and therefore remain significant sources of uncertainty [1].

This work presents a fully Bayesian machine learning framework that integrates stochastic three-dimensional Representative Volume Element (RVE) simulations, Gaussian Process (GP) surrogate modelling and hydrogen permeation experiments to infer constituent hydrogen permeabilities from composite-scale experimental measurements. Hydrogen permeation tests are first conducted on both carbon fibre-reinforced MTC510 epoxy laminates and the corresponding neat epoxy. The neat polymer measurements provide experimentally informed prior information for the *in-situ* matrix permeability, while composite permeation measurements define the observations used for Bayesian inference. The RVE forward model explicitly accounts for fibre orientation, fibre-rich and polymer-rich regions, and a distinct fibre–matrix interphase based on experimentally characterised microstructural statistics.

Unlike conventional surrogate-assisted Bayesian approaches, the proposed framework formulates the likelihood using the GP marginal likelihood of an augmented dataset comprising offline RVE simulations and experimental observations. This enables simultaneous inference of both the unknown constituent permeabilities and the GP hyperparameters, resulting in simultaneous construction of the GP emulator and calibration of the unknown material parameters within a unified Bayesian Inference framework. This fully Bayesian formulation naturally accounts for forward-model stochasticity and experimental measurement noise, together with epistemic uncertainty arising from the finite set of forward-model evaluations and uncertainty in the covariance function hyperparameters. Consequently, the posterior distribution provides a more realistic quantification of predictive uncertainty and typically yields wider credible intervals than plug-in approaches [2, 3]

The proposed framework successfully identifies physically meaningful constituent permeabilities from limited experimental observations. The inferred *in-situ* matrix permeability remains close to the experimentally informed neat epoxy value, whereas the fibre–matrix interphase is inferred to possess an effective hydrogen permeability approximately three times lower than the surrounding matrix, indicating that local fibre-induced modifications significantly influence hydrogen transport. The posterior distribution of the carbon fibre permeability contracts towards very low values, consistent with the highly impermeable nature of carbon fibres. Furthermore, posterior predictive simulations accurately reproduce the experimentally measured composite permeability. The corresponding prior and posterior distributions (Fig. 1) demonstrate substantial reductions in parameter uncertainty and reveal correlations between constituent permeabilities and GP hyperparameters through Bayesian updating.

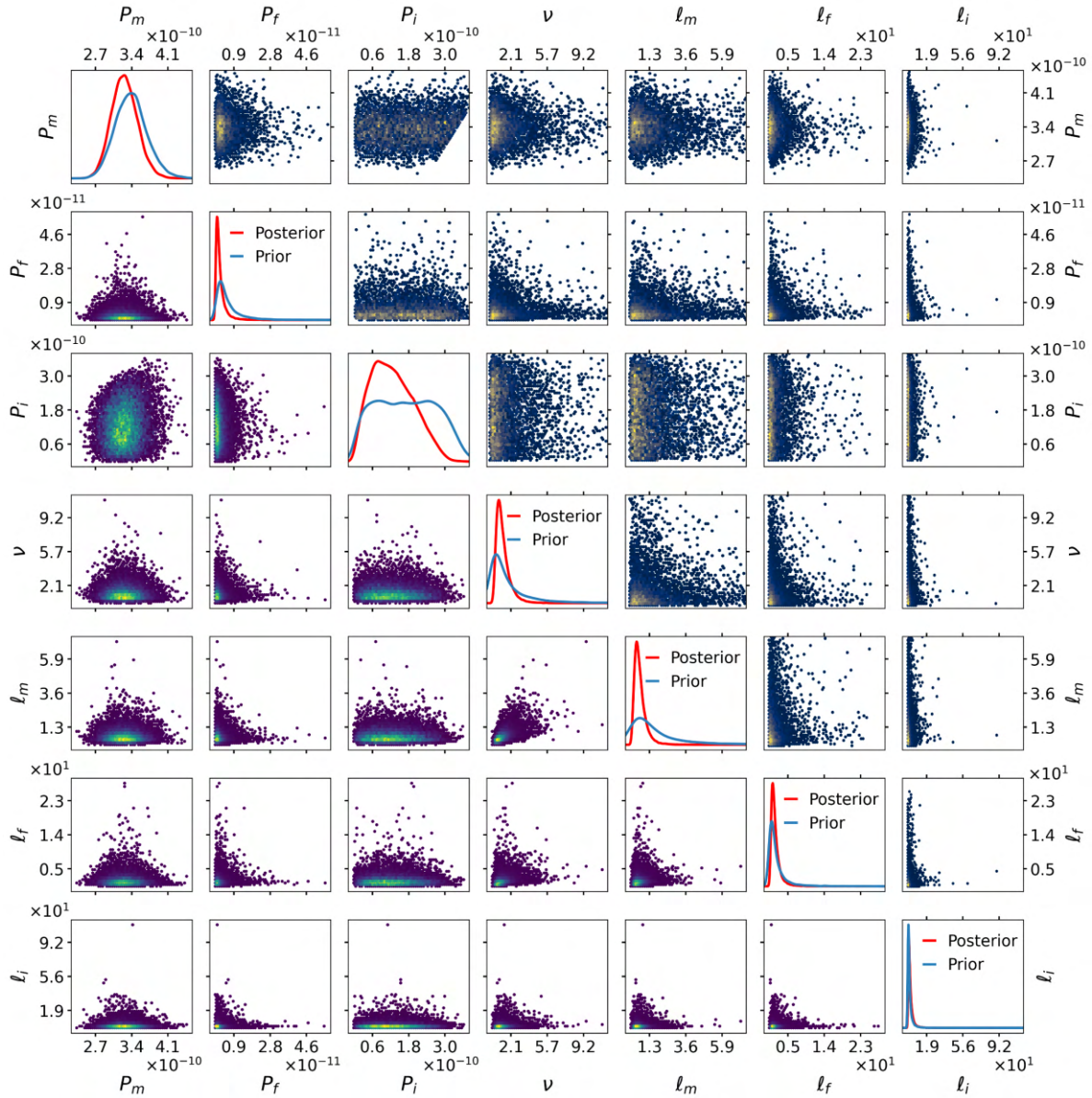


Figure 1: Prior and posterior distributions of the inferred constituent hydrogen permeabilities and Gaussian Process hyperparameters. Here, P_m , P_f , and P_i denote the in-situ matrix, fibre, and fibre–matrix interphase permeabilities, respectively; ν is the GP signal variance; and ℓ_m , ℓ_f , and ℓ_i are the GP characteristic length scales associated with the matrix, fibre, and interphase permeability dimensions. Diagonal panels compare the marginal prior and posterior distributions, while the lower-left off-diagonal panels show pairwise joint posteriors.

References:

- [1] M. Okumuş, F. Janssen and Ł. Figiel, "Modelling and experimental study of hydrogen permeation in polymer composites," *Compos. Part A Appl. Sci. Manuf.*, vol. 199, 109213, 2025.
- [2] A. Angus, M. Okumuş and Ł. Figiel, "Bayesian modelling approach to hydrogen permeation in fibre-reinforced polymer composites," *Compos. Part C Open Access*, vol. 18, 100630, 2025.
- [3] I. Bilonis and N. Zabaras, "Solution of inverse problems with limited forward solver evaluations: A Bayesian perspective," *Inverse Probl.*, vol. 30, no. 1, 015004, 2014.

Physics-led generation of missing data for effective use of AI/ML

Harika Tankasala¹, Giuseppe Romano¹, Nehir Kandemir¹ and Edoardo Rusconi^{1,2}

¹ Data Products, Synopsys, United Kingdom, harika.tankasala@synopsys.com

² School of Engineering, University of Warwick, United Kingdom

Problem & Context

AI/ML methods in materials engineering rely on the availability of high-quality, representative data. In practice, however, the most critical properties are often missing, difficult to measure, or inconsistent across sources. This creates a gap where purely data-driven approaches struggle to generalise and where predictions may become unreliable.

This challenge is particularly evident in composite laminas. Finite-element simulations require the full three-dimensional elastic tensor, yet supplier datasheets typically report only in-plane properties. Through-thickness moduli, shear moduli, and Poisson's ratios are often absent or uncertain. Engineers are therefore forced to choose between (i) full homogenisation using representative volume elements (RVEs), which is accurate but computationally expensive [1], (ii) classical micromechanics models such as Mori-Tanaka or Halpin-Tsai [1], which are efficient but rely on idealised assumptions, or (iii) empirical lookups, which are simple but lack transferability.

Approach

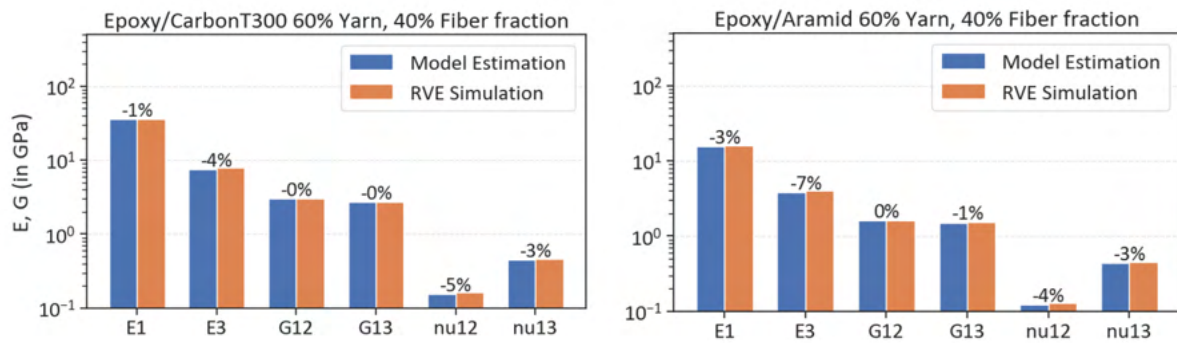
This work argues that physics-led modelling is a necessary foundation for AI/ML in data-sparse regimes. We present a reduced-order framework that reconstructs the full elastic tensor of composite laminas from a minimal set of physically meaningful inputs: constituent properties expressed through stiffness ratios and a small number of architecture descriptors.

The framework is implemented as a two-stage upscaling. At the fiber-to-yarn level, standard mixture-type expressions are retained as the base kinematics and enriched with interaction factors that encode load transfer and constraint. At the yarn-to-lamina level, weave transfer factors capture architecture-driven kinematics such as yarn rotation, crimp, and crossover constraint. These factors are calibrated once using RVE simulations over a constrained, physically meaningful design space and are reused across material systems without per-system fitting. The approach aligns with broader developments in multiscale modelling of composites [3], while remaining intentionally reduced in form.

Results

Across both unidirectional and woven laminas, the framework reproduces RVE trends for stiffness components while maintaining mechanically consistent Poisson's ratios. It captures the transition from mixture-dominated behaviour in unidirectional systems to kinematics-dominated behaviour in woven architectures.

Within the calibrated operating envelope, prediction errors for stiffness components remain within the variability observed across RVE realisations, while computational cost is reduced by orders of magnitude compared to full homogenisation. The resulting models provide simulation-ready elastic tensors suitable for early-stage design.



Model accuracy for representative plain weave lamina systems.

Conclusions & Significance

This work shows that a physics-led approach can generate the missing data needed to make AI/ML methods usable. Rather than learning directly from limited datasets, the framework encodes the governing mechanisms explicitly and uses high-fidelity simulations only for calibration.

Physics-led reduced-order models can therefore serve as a foundation for AI/ML, improving both robustness and interpretability. This perspective is consistent with emerging directions in physics-informed machine learning [4]. More broadly, it provides a practical pathway for combining physics and data in materials modelling, enabling trustworthy predictions where data alone is insufficient.

References

- [1] Geers, M. G. D., Kouznetsova, V. G., & Brekelmans, W. A. M. (2010). Multi-scale computational homogenization: Trends and challenges. *Journal of Computational and Applied Mathematics*, 234(7), 2175–2182.
- [2] Mori, T., & Tanaka, K. (1973). Average stress in matrix and average elastic energy of materials with misfitting inclusions. *Acta Metallurgica*, 21(5), 571–574.
- [3] Wan, L., Ismail, Y., Sheng, Y., Ye, J., & Yang, D. (2023). A review on micromechanical modelling of progressive failure in unidirectional fibre-reinforced composites. *Composites Part C: Open Access*, 10, 100348.
- [4] Karniadakis, G. E., et al. (2021). Physics-informed machine learning. *Nature Reviews Physics*, 3, 422–440.

Uncertainty Characterization of Thermal Shock Performance of Aerospace Composites with Physics-Informed Neural Networks

Juhyeong Lee¹, Scott Millen² and Xiaodong Xu³

¹ Department of Mechanical and Aerospace Engineering, Utah State University, USA
juhyeong.lee@usu.edu

² School of Mechanical and Aerospace Engineering, Queen's University Belfast, Northern Ireland, UK

³ Centre for Aeronautics, Faculty of Engineering and Applied Sciences, Cranfield University, Cranfield, UK

High-temperature protection of carbon fiber reinforced polymer (CFRP) composites remains a critical challenge due to the susceptibility of the polymer matrix to thermal degradation. While thin ceramic thermal barrier coatings (TBCs) can mitigate surface heating of the underlying CFRP, experimental characterization of TBC-CFRP systems under thermal shock conditions is time-consuming, costly, and inherently stochastic, thereby limiting the number of design variations that can be practically tested. Conventional computational models (*i.e.*, finite element models) often require high fidelity, fine meshing, and repeated runs for different coating thicknesses or boundary conditions, making comprehensive parametric studies impractical. To address these practical challenges, this work proposes a coupled physics-informed neural network (PINN) and Bayesian optimization (BO) framework that can characterize rapid exploration of TBC design parameters while incorporating optional experimental datasets into predictions. In the framework, PINNs numerically solve the governing physics of nonlinear heat conduction with temperature-dependent properties, reducing reliance on extensive simulations or exhaustive thermal shock testing. BO systematically identifies uncertainties associated with thermal shock tests (*i.e.*, flame characteristics). This work aims to bridge the underlying physics with experimental (and further extension to material) uncertainties, providing an efficient and flexible platform for designing thermally resilient CFRP composites.

The PINN [1, 2] is developed to predict transient temperature distributions in CFRP and TBC-CFRP materials, incorporating both room-temperature and temperature-dependent, orthotropic thermal diffusivities. Boundary conditions are defined based on conventional thermal shock experiments, with the initial temperature set to room temperature and Dirichlet (temperature) boundaries imposed on the TBC side at a peak temperature of 500°C (as a reference in this work), with optional inclusion of convective cooling. The Dirichlet boundary condition on the TBC surface is imposed as a Gaussian temperature distribution, generating a circular heating footprint whose intensity decays radially from the center, with the spatial parameters calibrated from thermal shock test measurements. The governing nonlinear heat conduction equations and boundary conditions are embedded directly into the network loss function, enabling the PINN to enforce physical laws without reliance on training data. BO is implemented alongside the PINN to systematically quantify uncertainties associated with thermal shock boundary conditions, focusing specifically on Gaussian heat source parameters, including flame radius, shape-decaying coefficient, and other experimentally relevant thermal loading characteristics. BO iteratively explores the uncertainty space to identify parameter combinations that best reproduce the predicted thermal response, enabling robust calibration of thermal shock test parameters. The coupled PINN-BO framework (Fig. 1) provides a predictive and flexible design platform for TBC-CFRP materials under extreme thermal loading, linking physics-based estimates with experimental uncertainty quantification.

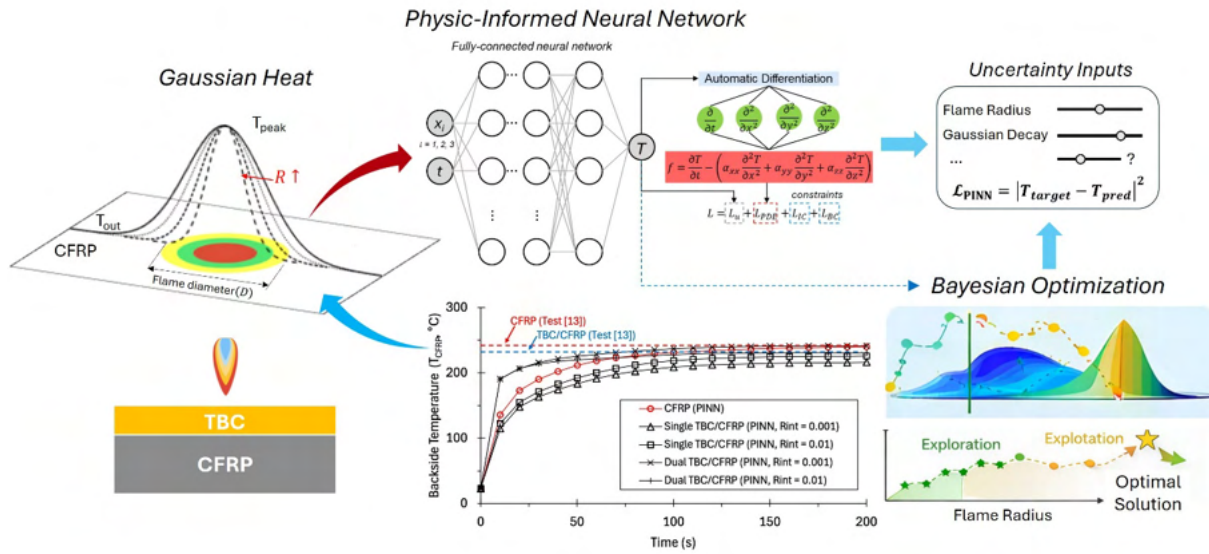


Figure 1. Coupled PINN-BO framework for thermal shock modeling of TBC–CFRP composites.

References:

- [1] Lee, J., Kim, H., & Lee, M. W. (2025). Paradigm shift in the design of thermal barrier coatings for fiber-reinforced composites using physics-informed neural networks. *Advanced Composite Materials* (under revision).
- [2] Dabell, J., Millen, S., Xu, X., & Lee, J. (2026). Physics-informed neural networks for predicting lightning damage in CFRP composites. *Proceedings of the 18th European Symposium on Impact and Shock Structures (ESIA18) - ISSI2026 International Conference*, Glasgow, UK (accepted).

Session Five

5 AI AND STATISTICAL METHODS FOR PROCESS MODELLING OF COMPOSITES

Bayesian Optimization of Non-Gaussian Process-Induced Deformations in Aerospace Composites

Kendall A. Johnson¹, Huilong Fu¹, Rowan M. Preedy¹, Jackson W. Scharf¹, and Navid Zobeiry¹

¹ Presenting Author Department of Materials Science and Engineering, University of Washington, USA, kaj1402@uw.edu

Material and process variability in aerospace composites can lead to process-induced deformations (PIDs) that complicate assembly and require costly shimming or rework. While deterministic process simulations are commonly used to predict deformation, they often neglect the inherent variability in material properties and processing conditions. Building on our recent work, combined stochastic process modelling and probabilistic machine learning have shown success in discovering the dominant contributors to deformation variability. Global sensitivity analysis of stochastic finite element simulations demonstrated that cure cycle parameters are among the dominant contributors to the variance of maximum assembly gap (Δz) [1] (Fig.1). These findings motivated a targeted experimental investigation to determine whether the predicted variability, and its underlying distribution, is observed in manufactured parts.

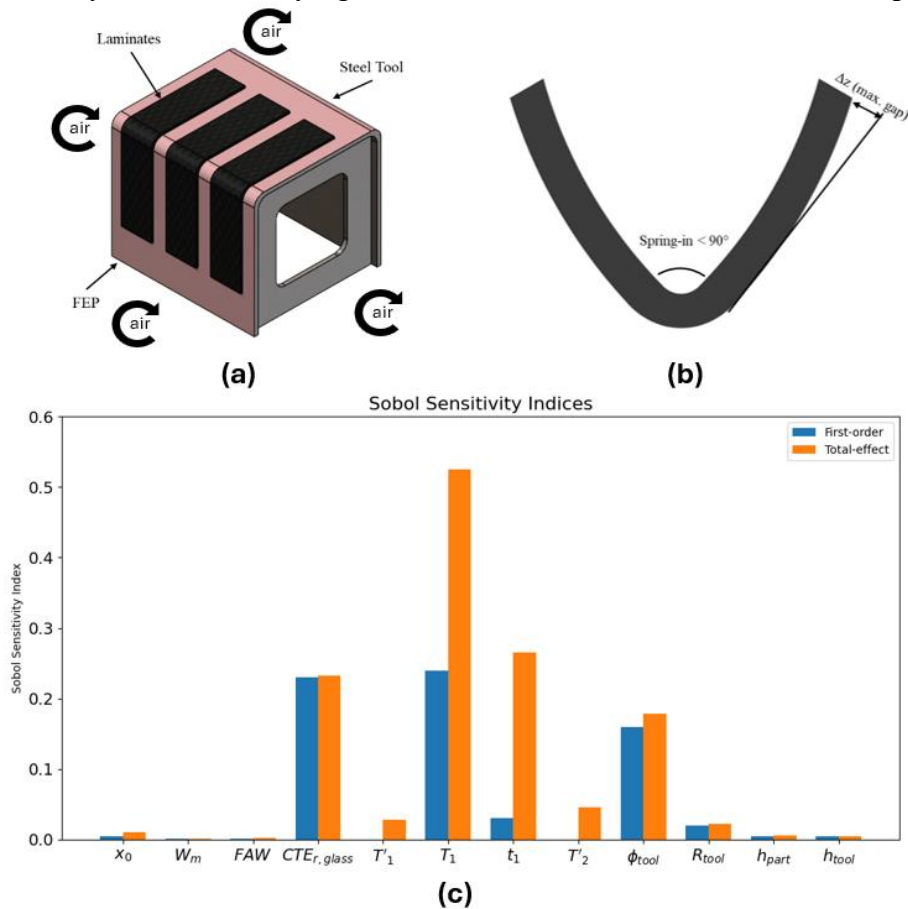


Figure 1: (a) L-shaped parts on steel tooling with airflow surrounding during curing. (b) Demolded part after curing with PIDs. (c) Global sensitivity analysis showing the contribution of process parameters to the variance of Δz [1].

A series of L-shaped composite parts were manufactured using a fixed laminate configuration while varying cure cycle parameters. Measurements of the resulting maximum gap revealed non-Gaussian statistical distributions, deviating from the normality assumptions typically used in surrogate modelling [2]. To separate operator effects from process-intrinsic parameters, a controlled baseline build was performed in which identical parts were fabricated by two different operators under identical processing conditions. Statistical analysis showed that both operators produced skewed distributions (Fig. 2), indicating that the non-Gaussian behaviour is intrinsic to the process rather than operator-dependent variability.

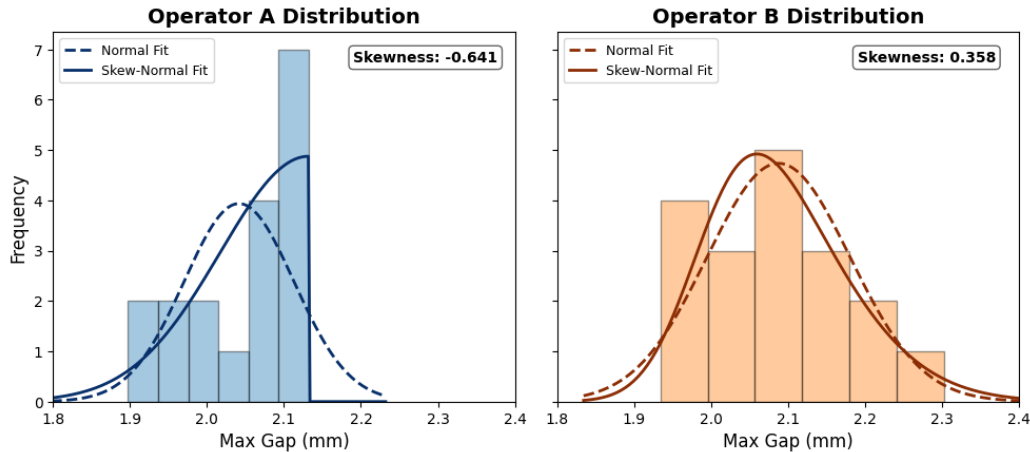


Figure 2: Experimental distributions of maximum gap measurements from manufactured L-shaped composite parts [3].

To incorporate this behaviour into predictive modelling, a warped heteroscedastic Gaussian Process surrogate was developed to account for both the non-Gaussian output distributions and input-dependent variance. Bayesian Optimization using the BoTorch [4] framework was then applied to efficiently explore the cure-cycle design space and identify processing conditions that minimize deformation while accounting for the observed uncertainty structure. By explicitly modelling non-Gaussian experimental variability, the framework enables more statistically consistent Gaussian Process Regression models and improves the reliability of surrogate-based optimization for aerospace composites manufacturing processes.

References:

- [1] H. Fu, K. A. Johnson, and N. Zobeiry, “Uncertainty Quantification in Advanced Aerospace Composite Manufacturing Through Stochastic Finite Element Analysis and Probabilistic Machine Learning,” *Proceedings of the American Society for Composites (ASC) 2024 Conference*, 2024.
- [2] C. Schoenholz, E. Zappino, M. Petrolo, and N. Zobeiry, “Efficient analysis of composites manufacturing using multi-fidelity simulation and probabilistic machine learning,” *Compos. B Eng.*, vol. 280, p. 111499, Jul. 2024, doi: 10.1016/j.compositesb.2024.111499.
- [3] K. A. Johnson, R. M. Preedy, and N. Zobeiry, “A data-efficient machine learning framework for uncertainty quantification of assembly gap in aerospace composites,” *accepted for presentation at the SAMPE 2026 conference*, 2026.
- [4] M. Balandat *et al.*, “BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization,” Dec. 2020.

GENERATIVE MATERIAL CARDS FOR PROCESS SIMULATION

Goran Fernlund^{1,2}, Alireza Forghani¹ and Alberto Mussali¹

¹ Convergent Manufacturing Technologies, Canada (goran.fernlund@convergent.ca)

² Materials Engineering, The University of British Columbia, Canada

Material cards, used in high-fidelity simulations are commonly constructed from extensive experimental data and are represented as mathematical equations or tabulated response surfaces over relevant state variables [1]. Generating material cards is currently a largely manual and time-intensive process because of the experimental testing required.

The goal with this work was to develop fast data driven methods to generate approximate material cards for materials where there is yet any direct experimental data, using knowledge of the behaviour of related materials and fundamental material science. This paper presents a probabilistic generative framework for constructing material cards using hierarchical Bayesian modelling and functional dimension reduction.

For each material in the existing material card library a response surface is first discretized on a common state-variable grid and transformed to ensure positivity and to stabilize variance. Principal component analysis (PCA) is then used to obtain a low-dimensional latent representation of surface variability across materials. The resulting latent scores are modelled using a hierarchical Bayesian regression framework, enabling partial pooling across material classes. This structure allows materials with limited data to borrow statistical strength from related classes while preserving systematic class-dependent differences.

The proposed model provides a full posterior predictive distribution for new material cards conditioned on material class and material descriptors. This yields not only a mean predicted response surface but also spatially resolved uncertainty estimates across the entire state-variable domain.

The framework enables data-efficient generation of physically consistent material cards, supports uncertainty quantification for downstream simulations, and provides a statistically principled pathway for incorporating new materials into existing material databases. The approach is general and applicable to a wide range of constitutive modelling contexts.

The generated approximate material cards can be used for quick exploratory analysis and simulation, and to provide insight via Bayesian optimization of how and where to generate the most effective experimental data to increase the fidelity of the material card.

References:

[1] G. Fernlund, K. Gordnian, O. Fernlund, and A. Poursartip, "Machine Learning Enhanced Material Models for Composites Process Simulation," in *Proc. SAMPE 2024 Conf. & Exhibition, Long Beach, CA, USA, May 20–23, 2024*, doi:10.33599/nasampe/s.24.0070.

Machine Learning Surrogate-Assisted Optimization of Cure Cycles in Multi-Material Thermoset Composite Systems

Alberto Mussali¹, Kamyar Gordnian¹, Aidan Floyd¹, Anthony Floyd¹, Alastair McKee¹, Alireza Forghani¹, Yuxiang Wang², Goran Fernlund^{1,3} and Anoush Poursartip^{1,3}

1 Convergent Manufacturing Technologies
403-6190 Agronomy Road,
Vancouver, BC, Canada V6T 1Z3
alberto.mussali@convergent.ca

2 GE Vernova
Jan Duikerweg 15 C, Heerhugowaard, 1703 DH, the Netherlands

3 Composites Research Network, Department of Materials Engineering,
The University of British Columbia
3950 Stores Road,
Vancouver, BC, Canada V6T 1Z4

Cure cycle optimization for thermoset composite structures is essential for reducing manufacturing cycle time, lowering energy consumption, and mitigating cure-induced defects such as excessive exotherm and residual stress. For large, geometrically complex parts, such as wind turbine blades, aero-structures, and other multi-material laminates, cure schedule design remains predominantly empirical. High-fidelity process simulations based on coupled heat transfer and cure kinetics can, in principle, support systematic optimization, but they are too computationally expensive to be embedded directly in iterative search or broader digital process planning workflows. This limits the systematic exploration of alternative cure strategies, particularly in industrial settings where cure modelling is not yet routine.

This work proposes a machine-learning surrogate-based framework for efficient cure cycle optimization of multi-material thermoset composite parts, with emphasis on large wind turbine blade components as a representative application. The framework targets generic one-dimensional through-thickness stacks that may include multiple laminate fabrics and cores and is intended to be applicable to other sectors (e.g., aerospace) that rely on thick, multi-material composite lay-ups. The key idea is to replace repeated high-fidelity simulations within the optimization loop by a data-driven surrogate trained on a large, Sobol-sampled synthetic dataset generated using the commercial process modelling tools like ORCA, RAVEN and COMPRO from Convergent Manufacturing Technologies. The resulting surrogate enables rapid, low-cost exploration of cure schedules while respecting material- and process-specific constraints, thus providing a practical route for introducing systematic cure optimization into design and manufacturing practice in domains where process modelling has historically been underutilized.

The considered process configuration is a heated-mould cure of an infused, fully impregnated laminate stack, representing a very long blade-like component. The part is processed under vacuum bag, with a mould heated by a PID-controlled system and the optional use of manually applied insulation blankets on the top surface. The thermal boundary conditions include ambient and initial temperatures for the laminate and tooling, convective heat transfer coefficients at the top and bottom surfaces (with distinct values for blanket and non-blanket conditions), and timing parameters describing the application and removal of the insulation blankets. The tooling thickness is also considered, with fixed PID and power parameters.

The material stack is resolved into up to five distinct curing material systems sharing a two-part epoxy-like infusion resin, in addition to non-curing core materials. For each curing material, the feature set includes layer thickness, fibre volume fraction, and initial degree of cure. The core is characterized by its thickness and basic impregnation descriptors, enabling the workflow to represent core infusion effects when relevant.

The cure schedule is parameterized by up to three thermal ramp-dwell segments applied via the heated tool. For each segment, the ramp rate, target dwell temperature, and dwell duration are included as design variables, subject to bounds reflecting equipment limitations and material guidelines. Blanket usage is represented by the timing of its placement and removal relative to the cure cycle, and additional engineered features capture the normalized timing of these events. TGML-type features are further introduced to nonlinearly transform certain process parameters into forms that are more amenable to learning complex dependencies between cycle design and cure outcomes.

A large synthetic dataset, on the order of 10^5 simulations, is generated by Sobol sampling over the multidimensional input space defined by ambient and initial temperatures, boundary condition parameters, tool and material properties, and cure cycle design variables. The sampling ranges are selected to cover representative conditions for multi-material wind blade regions while remaining compatible with the underlying resin system and equipment constraints. For each sampled point, the one-dimensional transient thermal-cure response is computed using Convergent Manufacturing Technologies ORCA framework; and key scalar outputs are extracted, including total cure cycle time, minimum degree of cure within the laminate, maximum part temperature, and other cure state metrics of interest. This synthetic dataset forms the basis for training the surrogate models.

The surrogate itself is implemented as a set of feedforward neural network (MLP), trained in a multi-output configuration for all target quantities. Hyperparameters (e.g., network depth, width, activation functions, and regularization parameters) are tuned via Bayesian optimization, and model performance is assessed using a 70/30 train/test split combined with k-fold cross-validation ($k = 5$) to guard against overfitting and to quantify generalization across the high-dimensional input space.

The surrogate models are embedded in a global optimization routine whose primary objective is to minimize total cure cycle time subject to physics- and manufacturing-informed constraints. The design variables include ramp rates, dwell temperatures and durations, the number and placement of thermal dwells, and the number and timing of insulation blanket applications. Constraints enforce a minimum degree of cure exceeding a prescribed design threshold, upper bounds on maximum part temperature (to control exotherm and degradation risks), and limits on allowable ramp rates, dwell temperatures, and equipment loads (e.g., maximum tool power).

The optimization is carried out using the ANN surrogates as fast evaluators, which reduces the cost of exploring the design space by approximately one to two orders of magnitude compared with a naive approach in which each candidate cure schedule is evaluated directly by high-fidelity simulation. Candidate optima identified by the surrogate-based search are subsequently validated a posteriori using full RAVEN simulations; any candidate that fails the high-fidelity constraint checks (e.g., due to local surrogate inaccuracy) is rejected and can inform further refinement of the surrogate or optimization setup.

The proposed surrogate-based framework offers a computationally tractable and industrially relevant path toward systematic cure cycle design for complex thermoset composite parts. It provides a practical route to modernizing cure design in industries, such as wind energy, where process modelling has traditionally been underexploited.

ROUGHNESS DESCRIPTORS DISCOVERY DRIVEN BY THE PREPEG TAPES CONSOLIDATION PROCESS

Anais Barasinski¹, Camilo Cruz¹, Sebastian Rodriguez², Jad Mounayer², Mikhael Tannous² and Francisco Chinesta²

¹ ICA, IMT Albi, Albi, France

² PIMM, Arte et Métiers Institute of Technology, Paris, France Francisco.Chinesta@ensam.eu

Tapes surface roughness determines the time evolution of the degree of intimate contact -DIC- required for ensuring the molecular diffusion and the associated tapes consolidation.

To evaluate the DIC evolution measured rough surfaces are compressed numerically, at constant velocity or constant applied compression force.

When proceeding at constant compression rate, the surface evolution is almost governed by the material incompressibility, whereas the associated compression force relies on the thermo-dependent rheology.

When proceeding at constant compression force the thermo-dependent rheology plays a central role and the compression rate follows the momentum balance.

Rheology can be described from a TIF model, that is, from a transversally isotropic fluid model, inextensible in the fiber direction or slightly extensible in presence of fibers undulation. However, such a rheological model ignores second order physical mechanisms occurring at the roughness level, and particularly important when addressing consolidation.

Thus, from collected data during compression, the TIF rheology can be improved by discovering the extra-variables involved in the rheological model by using advanced machine learning techniques, and then, trying to provide a physical interpretation of them by invoking adequate procedures, as for instance Bayesian machines or symbolic regression.

Different simulation techniques can be envisaged for solving the non-Newtonian fluid flow, operating on the measured surfaces, the later described by using wavelets, or from a grid-based VOF (volume of fluid) particularly suitable for cellular automata based efficient simulations.

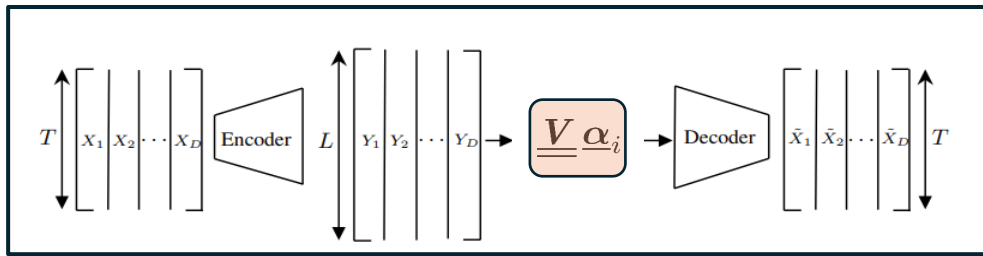
Concerning the surface roughness, usual characterization relies on the use of statistical and/or geometrical descriptors, that even if they could represent the roughness, they are disconnected from the physics occurring at the interface where consolidation occurs and involved in engineering predictions.

Recent machine learning technologies, particularly the ones based on the use of auto-encoders, enable connecting their latent space with a series of extra parameters (related to the material and processing conditions) to jointly infer the physics-based quantities of interest, as for instance the time evolution of the DIC.

For providing a valuable response, we propose a novel procedure based on the use of a powerful autoencoder, the so-called RRAE (rank reduction autoencoder) [1] with a linear vector latent space, enforced by applying a PCA (principal component analysis) at the latent space level during the encoder-decoder training.

The resulting PCA modes can be enforced to represent any existing “a priori” knowledge, for instance valuable statistical descriptors, complemented with the ones required for inference purposes (classification or regression), and finally for those needed to ensure the profiles representation after decoding.

The RRAE architecture is described in the figure below, where the alpha-descriptors are discovered from the input data (roughness) to optimally approximate it, but they can be also enforced to be the ones describing the first-order physics-based quantities of interest via regression, as for instance the DIC evolution in consolidation modeling and simulation.



To prove the potential of the proposed methodology, different tapes are measured by using a profilometer and then simulated to evaluate the associated DIC time evolution. Both data, roughness and DIC time evolution, consist of the input data of two RRAE, whose latent spaces are connected by using a MLP (multi-layer perceptron). The three neural architectures (the two RRAEs and the MLP) are trained simultaneously.

The subsequent trained model is then able to infer the DIC time evolution for any roughness profile data, enabling determining the right roughness for ensuring an adequate processability (material and process by design).

References:

- [1] J. Mounayer, S. Rodriguez, C. Ghnatios, C. Farhat, F. Chinesta, Rank reduction autoencoders, <https://arxiv.org/html/2405.13980v1>, 2025

Three-Dimensional Kinetically Enriched Homogenisation for AI-Assisted Consolidation Analysis of Discontinuous Composites

Maria Onoufriou¹, Jonathan P.-H. Belnoue², Alyn D. N. James² and Malin Åkermo¹

¹ Material & Structural Mechanics, KTH Royal Institute of Technology, Sweden, mariaon@kth.se

² School of Civil, Aerospace and Design Engineering, University of Bristol, United Kingdom

Tow-based discontinuous composites exhibit a stochastic and locally anisotropic architecture arising from the random deposition of short fibre tows. During consolidation, applied heat and pressure induce tow rearrangement, resin redistribution and densification, creating strong coupling between evolving microstructure and macroscopic thickness evolution. Conventional process models rely on homogenised continuum assumptions that do not explicitly resolve tow-level architecture, limiting their ability to capture microstructure-dependent behaviour and restricting data-driven optimisation.

This work presents a physics-informed computational pipeline that enables systematic generation of high-fidelity datasets linking microstructural descriptors to consolidation response. A fast voxel-based preprocessor constructs three-dimensional stochastic architectures through simulated tow deposition, allowing controlled variation of tow length, width, thickness and in-plane orientation distributions. The voxelised microstructure is mapped to a finite element model, where an extended three-dimensional kinetically enriched homogenisation scheme predicts temperature-dependent compaction behaviour.

The homogenisation framework builds upon the kinetically enriched constitutive model originally developed for layered composite consolidation [1] and generalises the enrichment formulation to all voxel interfaces in three dimensions. This enables representation of inter-tow sliding and anisotropic densification within complex stochastic layouts while avoiding explicit geometric resolution of each tow, ensuring computational efficiency.

The efficiency of the framework enables automated simulation campaigns across the parametrised microstructural design space. For each generated architecture, consolidation metrics including pressure–thickness response, overall thickness reduction and spatial thickness non-uniformity associated with defect formation are extracted. The resulting datasets support training of surrogate models, including Gaussian process regression, to approximate the microstructure-to-response mapping with quantified uncertainty. By combining physics-grounded homogenisation with AI-driven surrogate modelling, the approach establishes a scalable pathway for rapid sensitivity analysis and microstructure-aware optimisation of discontinuous composite manufacturing.

References:

- [1] J. P.-H. Belnoue and S. R. Hallett, “A rapid multi-scale design tool for the prediction of wrinkle defect formation in composite components,” *Materials & Design*, vol. 187, 108388, 2020.
<https://doi.org/10.1016/j.matdes.2019.108388>.

Session Six

6 AI FOR INTELLIGENT COMPOSITES MANUFACTURING AND CONTROL

A REDUCED ORDER MODELING APPROACH TO PHYSICS-BASED SIMULATION OF AUTOMATED FIBRE PLACEMENT

Nima Bakhshi¹, Akihito Suzuki², Yukihiro Sato², Paulo Silva¹, Alireza Forghani¹, Yusei Kondo², Kento Shigekura², Kodai Shimono², Ryoji Okabe², Kana Sakon², Goran Fernlund¹, and Anoush Poursartip^{1,3}

¹ Convergent Manufacturing Technologies, Vancouver, BC, Canada

² Mitsubishi Heavy Industries, Ltd., Nagoya, Japan

³ Composites Research Network, Department of Materials Engineering,
The University of British Columbia, Vancouver, BC, Canada

Presenting Author: nima.bakhshi@convergent.ca

Automated Fiber Placement (AFP) is increasingly adopted in manufacturing of advanced aerospace structures. Utilizing industrial robotics and automation technologies, multiple narrow strips of prepreg, called prepreg tows or slit tapes, are deposited onto tooling, following a pre-designed layup path, under tightly controlled processing conditions (including temperature, compaction force and speed) to laminate composite parts. This highly automated process enables lamination of large-scale, complex structures to be achieved with higher quality, repeatability and reliability [1].

Process development for AFP is currently driven by costly and time-consuming trial and error. New material systems must undergo extensive experimental campaigns to determine their suitability for AFP lamination on a specific tool geometry, and to establish a window of process conditions for successful processing. In AFP process, various processing conditions can have complex intertwined effects often involving competing mechanisms affecting material behaviour and ultimately the final part quality. This highly manual and labour-intensive approach can be a major impediment to engaging in low risk, agile, lower-cost manufacturing [2], [3].

Physics-based process simulation has long established itself as a cornerstone in composites processing as well as other fields of science. Previous work has focused on developing a detailed high-fidelity AFP process simulation using COMPRO CCA [4] and Abaqus Explicit Solver. These models include detailed representations of key components of the AFP head, tow, substrate, and the material deposition process over a pre-defined layup path [5], [6], [7]. Further efforts were focused on developing material models [8] as well as necessary experimental methods to produce high quality data for calibrating the models [9]. This simulation framework demonstrated high ability to capture layup quality outcomes and predict key lamination defects that can develop during the process.

The current work presents a *Reduced Order Modeling (ROM)* approach for AFP process simulation. These ROM methods are developed with the objective of capturing overall trends in data in a fast, computationally efficient manner. By simplifying the underlying physics and representing only the key aspects most relevant to process outcomes, the model achieves significant gains in computation time while maintaining ability to predict trends such as number of defects per unit tow length. With incorporating a physics-based core and bringing in representations of key components of material behavior, the models can relate the simulated lamination predictions to processing conditions such as,

temperature, deposition speed, compaction force, and roller features.

In the present ROM approach to AFP, the initial configuration of the tow is represented as it is fully consolidated onto the tooling following the prescribed layup path. Residual stresses induced in the tow as a result of the deposition process are estimated during a pre-processing stage and then imposed onto the tow. Upon application of these stresses, the tow seeks a new equilibrium state through deformation, which is resisted by prepreg tack. The interplay between the stored energy available for deformation and the resisting tack interface stresses ultimately determines the occurrence and growth of defects during the process.

Comprehensive libraries of material behavior are available through COMPRO CCA [4]. Viscoelastic in-plane and bending properties are used to model prepreg tow behavior within the ROM framework, while a viscoelastic tack model represents the cohesive tacky behavior between the prepreg and the substrate. The application of this framework is demonstrated (see Figure 1) through a tow-steering problem on a flat tool with a steering radius of 1 (m). Using representative material properties, the ROM AFP simulations were compared against detailed deposition simulations under equivalent conditions. The results indicate that the ROM predictions for lamination quality are comparable to detailed simulations while achieving a 10-20x reduction in run time, suggesting a promising balance between predictive accuracy and computational efficiency.

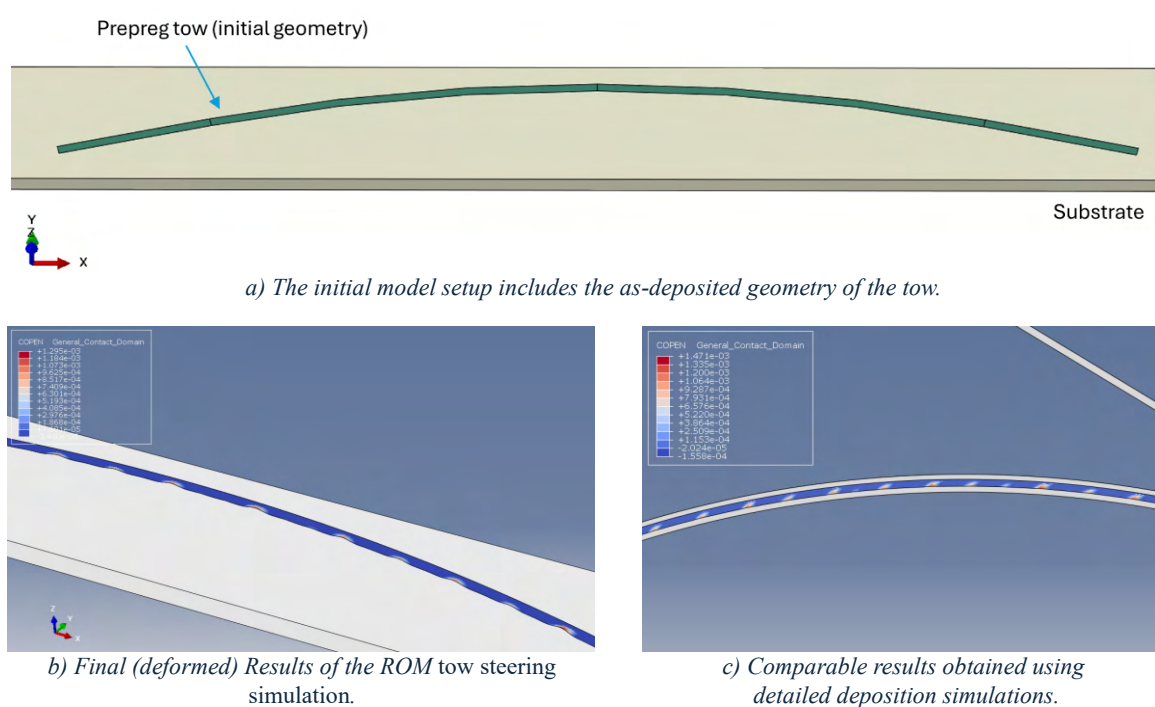


Figure 1 Reduced Order Model AFP Simulation approach applied to tow steering problem over a flat tooling. The ROM approach can produce comparable lamination quality predictions more computationally efficiently.

References:

- [1] A. Brasington, C. Sacco, J. Halbritter, R. Wehbe, and R. Harik, "Automated fiber placement: A review of history, current technologies, and future paths forward," *Compos. Part C Open Access*, vol. 6, p. 100182, Oct. 2021, doi: 10.1016/j.jcomc.2021.100182.

- [2] N. Bakhshi, “Investigation of prepreg tack through development of an AFP simulator using in-situ sensing and physics-based simulation,” University of British Columbia, 2023. Available: <https://dx.doi.org/10.14288/1.0438302>
- [3] N. Bakhshi, X. Yin, Z. Chen, J. D. W. Madden, and A. Poursartip, “Exploring Science-based Automation Using a Small AFP Demonstrator,” in *Proceedings of SAMPE 2023 Conference*, Seattle WA, Apr. 2023. doi: 10.33599/nasampe/s.23.0189.
- [4] “COMPRO Simulation Software | Convergent.” Available: <https://www.convergent.ca/products/compro-simulation-software>
- [5] V. Hutten *et al.*, “A Validation Study of a Physics-based Tack Model for an Automated Fiber Placement Process Simulation,” *SAMPE 2019 - Charlotte NC*, Apr. 2019, doi: 10.33599/nasampe/s.19.1512.
- [6] A. Forghani *et al.*, “Experimental Calibration of a Numerical Model of Prepreg Tack for Predicting AFP Process Related Defects,” presented at the Society for the Advancement of Material and Process Engineering – North America, Long Beach, CA, May 2018. Available: <https://ntrs.nasa.gov/citations/20200002539>
- [7] P. Silva *et al.*, “Simulation of Deposition Manufacturing Processes of Polymer Matrix Composites,” presented at the NAFEMS World Congress, 2019. Available: https://www.nafems.org/publications/resource_center/nwc_19_432/
- [8] A. Forghani *et al.*, “A Physics-Based Modelling Framework for Simulation of Prepreg Tack in AFP,” presented at the Society for the Advancement of Material and Process Engineering – North America, Seattle, WA, May 2017. Available: <https://www.nasampe.org/store/viewproduct.aspx?id=9296457>
- [9] M. Lane *et al.*, “Characterization Testing of Un-cured Prepreg Fabrics for Forming Process Simulation,” presented at the Proceedings of SAMPE Seattle 2023,

A Surrogate Model for Continuous Resistance Welding of Thermoplastic Composites

Marco Didone¹, Stephen Atkinson¹, Reza Vaziri¹, Anoush Poursartip¹, Steven Roy², Julieta Barroeta Robles², Marc Palardy-Sim², Marc-André Oceau², Ali Yousefpour²

¹ Composites Research Network, Departments of Civil Engineering and Materials Engineering, The University of British Columbia, Vancouver, Canada, marco.didone@ubc.ca

² National Research Council, Montréal, Canada

Continuous resistance welding (CRW), in which a localized heating zone is translated along the joint using a gantry or robotic system, offers a promising approach for joining of aerospace structural thermoplastic composite components [1]. Complexity in CRW processing increases markedly when scaling to production environments. As with other thermoplastic welding technologies, non-invasive measurement of the temperature at the weld interface (i.e. without the use of embedded thermocouples), remains infeasible, despite being critical for controlling the process in order to ensure joint strength and quality [2]. However, physics-based process simulation can mitigate this shortcoming, and thus reduce uncertainty in the weld operation.

A rigorous, systems-based computational framework for simulating the CRW process has been developed and validated for predicting thermal histories and qualitative interfacial melting [3]. To achieve this, a detailed 3D finite element (FE) model was constructed to capture the thermal response of the welded components, coupled with an electrical model that generates heat maps accounting for contact resistances and current leakage. Figure 1 presents a schematic of the CRW system, in which copper electrodes supply electrical current to the assembly, generating heat through Joule heating.

The detailed physics-based simulation was used to establish the causal relationship between process parameters and weld interface temperature, thereby guiding the selection of experimental conditions. With a validated model, useful investigations into typical processing deviations were demonstrated to be well captured with predictive control. The full model was further used to determine nominal process parameters, such as applied electric voltage and welding speed, to ensure operation within the processing window. The efficiency limitations of the full FE model, however, hinders process design optimization, real-time control, uncertainty quantification, and large-scale parametric studies that are required for industrial settings. Reduced-order or surrogate models directly address these challenges. In this study, surrogate models are developed by learning the input-output relationships of the high-fidelity FE simulations. Their efficient inverse analysis capability enables using electrical current feedback to estimate weld temperatures in real-time, forecast peak temperatures and compensate for process fluctuations through adaptive adjustment of the applied voltage and weld speed.

Figure 2 illustrates an example of a 15 electrode blocks weld geometry in which process simulation was used to guide welding speed adjustments, ensuring that the temperature remained within the desired processing window as the welding head traversed a heat-sink zone created by an aluminium insert placed between two electrode blocks within the insulation material. Comparison of Figures 2(a) and 2(b) shows that in the full FE model, a single step change in speed was necessary to maintain weld temperatures within the processing window. Figure 2(c) shows a similar plot generated using the predictive capability of a surrogate model employed to actively control the welding process using current feedback from an industrial robot which forced frequent variations of weld speed. This particular surrogate model was trained using only temporal temperature data at the centre and edge of the weld zone obtained from full FE simulations. Results from other surrogate models that structure their training process by enforcing physical constraints will also be presented.

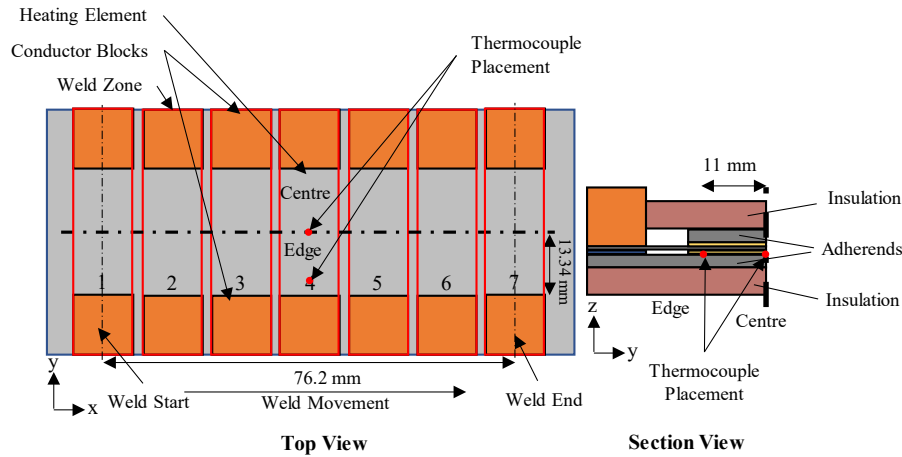


Figure 1. Schematic representation of the CRW process showing sectional views of its components

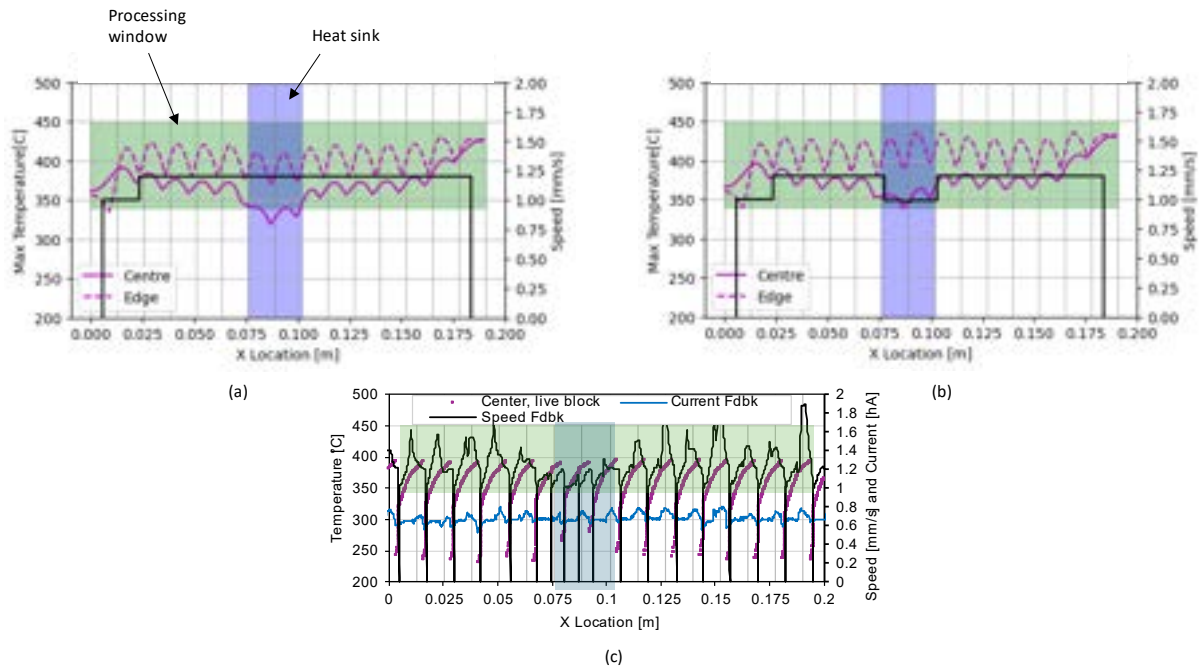


Figure 2. Predicted temperature at the interface (between the neat film and CF/PEEK adherend layers) when the welding electrode passes over an aluminium insert placed under two electrode blocks acting as a heat sink: (a) without, (b) with welding speed adjustment recommended by the full FE model, and (c) results from a surrogate model's active control of the process

References:

- [1] A. Yousefpour, M. Hojjati, and J.-P. Immarigeon, "Fusion Bonding/Welding of Thermoplastic Composites," *Journal of Thermoplastic Composite Materials*, vol. 17, no. 4, pp. 303–341, Jul. 2004.
- [2] M. Palardy-Sim *et al.*, "Towards In-line Control of Continuous Resistance Welding for Joining Structural Thermoplastic Composites," *SAMPE Journal*, vol. 59, no. 5, pp. 9–17, Sep. 2023.
- [3] S. H. Atkinson, "A process simulation framework for continuous resistance welding of thermoplastic composites," Master's Thesis, The University of British Columbia, 2024. doi: 10.14288/1.0440654.

Combining Physics-based and Data-driven Methods to Optimize Sub-Melt Consolidating Thermoplastic Tapes (OATMEAL)

Joseph G. Kirchhoff¹, Tyler B. Hudson², Wilfredo Flores², Finnian Day³, Christopher J. Stelter², Roberto J. Cano²

¹ Walker Mechanical, University of Texas at Austin, USA, kirchhoff@my.utexas.edu

² Advanced Materials and Processing Branch, NASA Langley Research Center, USA

³ Roux Institute, Northeastern University, USA

During high-rate processing of thermoplastic composites, incomplete interface healing can limit consolidation quality and final performance, particularly in semi-crystalline systems where crystallization suppresses polymer interdiffusion. To address this challenge, we developed **Out-of-Autoclave Amorphous/Crystalline Thermoplastic Materials for Energy-efficient Aerospace-grade Laminates (OATMEAL)**, a hybrid prepreg architecture consisting of fully crystallized PEEK tapes coated with amorphous PEI sheaths (see Figure 1) [1]. The PEI-rich interfacial layer is designed to promote bonding below the PEEK melting temperature, creating a sub-melt processing window for consolidation. Because excess PEI may reduce in-plane mechanical performance, the interfacial layer must be chemically effective while remaining geometrically minimal.

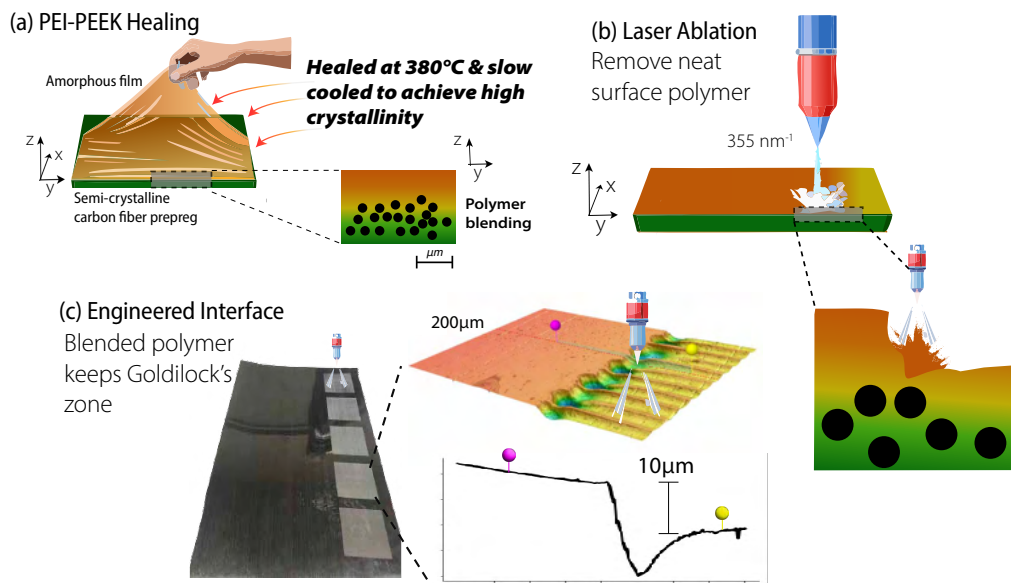


Figure 1. Overview of the OATMEAL prepreg process.

A key theme of this work is the deliberate use of different modeling strategies for different physical regimes. For the PEI-PEEK interphase, where the governing transport physics are relatively well defined, we use **AFM-IR measurements** together with **PDE-constrained diffusion optimization** to engineer interdiffusion behavior and identify processing conditions that enable healing in a “Goldilocks zone” of sufficient mobility without excessive thermal

exposure. For removal of excess PEI, however, the laser-material interaction is more complex and difficult to model mechanistically, so we instead use a **data-driven closed-loop experimental design framework** based on **Gaussian process (GP) surrogate models** for ablation depth and width.

The laser ablation workflow used **measured power, scan speed, and pulse frequency** as inputs, with each condition tested in **triplicate**. Replicate measurements were aggregated to condition-level means, and replicate scatter was propagated as **heteroscedastic observation noise** using the standard error term, with a small floor added for numerical stability. Two independent GPs, one for depth and one for width, were trained using robust multi-start marginal likelihood optimization. New experiments were selected adaptively from the physically feasible laser operating space using Bayesian design logic that balanced predicted target achievement, epistemic uncertainty, diversity, and experimental cost, while favoring faster scan speeds whenever similar ablation depths were predicted.

On an unseen **Round 4** validation set, the **planning-time GP** achieved a **depth mean absolute error (MAE) of 1.35 μm** and a **root mean square error (RMSE) of 1.77 μm** overall (see Figure 2), improving to **0.83 μm MAE** and **1.05 μm RMSE** in the practically relevant **6-12 μm** removal range. Width was more difficult to predict, with **2.06 μm MAE** and **2.78 μm RMSE** overall.

Together, these results show how a **hybrid physics/AI workflow** can be used to engineer both the chemistry and geometry of OATMEAL tapes: first-principles modeling is applied where the physics are accessible, while adaptive data-driven modeling is used where the process behavior is too complex for a tractable mechanistic description. This approach provides a practical route toward energy-efficient, high-rate thermoplastic composite manufacturing.

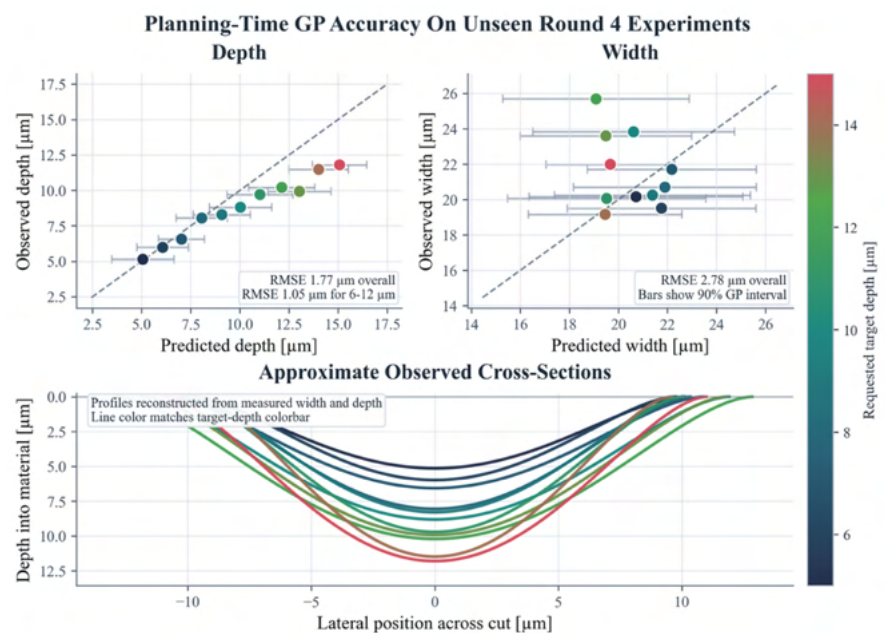


Figure 2. Gaussian Process predicts within ~1 micron accuracy.

References:

- [1] J. G.Kirchhoff, S.Khaleghi, G.Haugstad, T. B.Hudson, and M.Tehrani, "Sub-Melt Consolidation of Aerospace-Grade Thermoplastic Composites for High-Rate Processing." Adv. Mater.38, no. 9 (2026): e14390. <https://doi.org/10.1002/adma.202514390>

Real-Time Flow-Front Monitoring and Closed-Loop Injection Control in Transparent SLA-Printed Hollow Structures

Heinrich Pfander^{1#}, Dominik Platzer¹, Stefan Carosella¹ and Michael May¹

¹ Institute of Aircraft Design (IFB), University of Stuttgart, Germany,

[#]Presenting Author: pfander@ifb.uni-stuttgart.de

Short-fibre reinforcement of additively manufactured hollow structures have been shown in previous works to increase stiffness, strength and the elongation at break, yet the filling process remains insufficiently understood because in-situ monitoring of flow-front propagation and defect formation is missing. Existing simulations accurately predict the fibre distribution for the final geometry, but lack validation against real-time process data, leaving the relationship between viscosity, fibre orientation and void formation poorly understood and with it, the potential for targeted process improvement [1]. In prior work, the authors address this by developing a camera-based, robust, real-time flow monitoring system capable of detecting flow-front progression, filling dynamics and void formation. Hollow structures are produced via stereolithography (SLA), exploiting the optical transparency of the resin to provide direct visual access to the filling process without modification of the part geometry. An AI-based segmentation model is applied to each camera frame to extract binary flow-front maps in real time, from which flow-front velocity is continuously derived throughout the injection. The gathered experimental data are compared with process simulation predictions to validate the simulation model under realistic processing conditions, with deviations attributed to viscosity and fibre effects during the injection process. This serves as a basis for data-driven model calibration and a step towards scalable automated quality assurance in fibre-reinforced additive manufacturing.

The present work realises the closed-loop control step foreshadowed by this prior work. Flow-front velocity, derived in real time from successive AI segmentation outputs, is the primary control variable. Deviations between the measured velocity and the simulation-predicted reference are used directly as the control signal: a drop in velocity below the predicted profile indicates a risk of void formation or incomplete filling, triggering a corrective increase in injection pressure. This physically motivated, deviation-based approach keeps the control logic simple and interpretable while being grounded in the validated simulation model.

The primary outcome is a closed-loop injection system in which the AI-based flow-front segmentation, the validated simulation, and the pressure control are integrated into a single automated pipeline. The quantitative validation of the velocity signal against simulation predictions provides the deviation metric that drives the control response, with the simulation serving as a continuously updated reference throughout the injection. The system is currently under development, and experimental validation results are expected to be presented at the conference.

Keywords: closed-loop control, additive manufacturing, short-fiber injection, flow monitoring, process simulation

References:

- [1] D. Platzer, S. Carosella and P. Middendorf, "Nachträgliche Kohlenstoffkurzfaserverstärkung stereolithografisch gefertigter Strukturen," 29. Stuttgarter Kunststoffkolloquium, C. Bonten and M. Kreutzbruck, Eds., Schriftenreihe / Institut für Kunststofftechnik, Stuttgart: IKT, Universität Stuttgart, Feb. 2025.

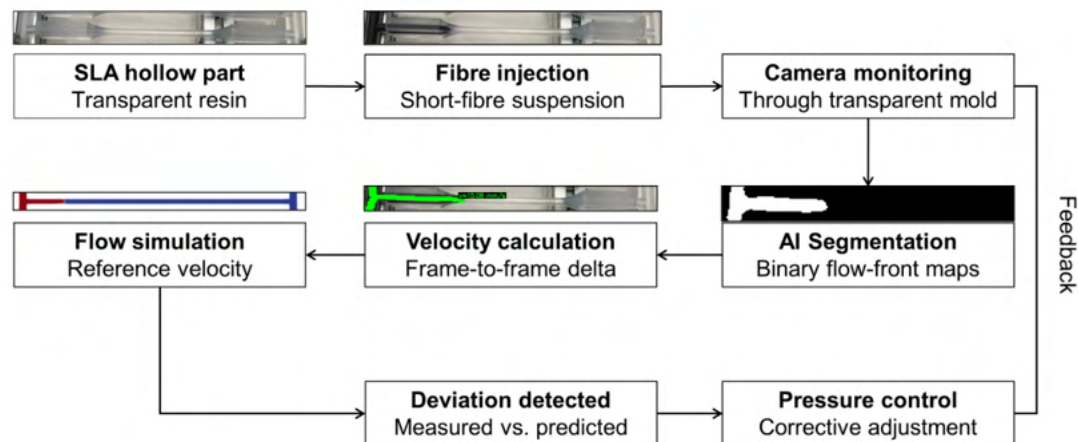


Figure 1: Workflow for AI-driven closed-loop control of short-fiber injection in SLA-printed hollow structures.

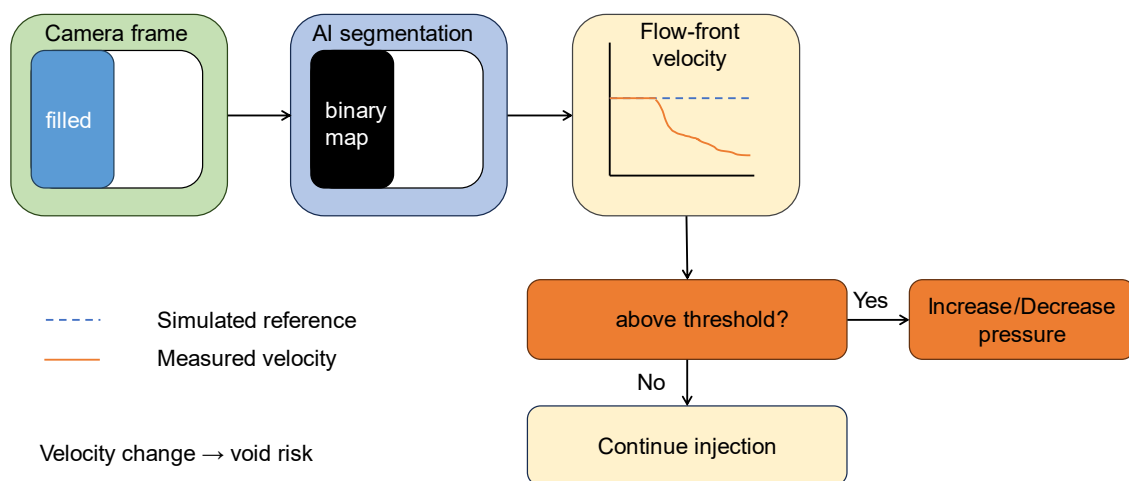


Figure 2: Flow-front velocity deviation as control signal: measured velocity versus simulation reference triggering corrective pressure adjustment