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

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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.

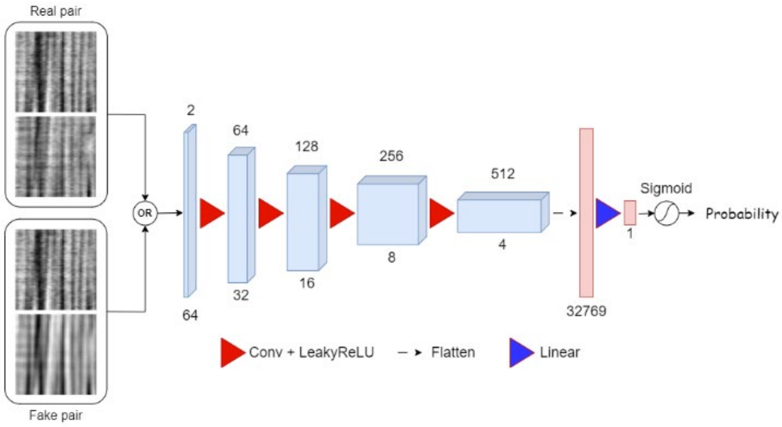

Figure 1. Discriminator architecture. The input is an image pair concatenated along the channel axis.

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.

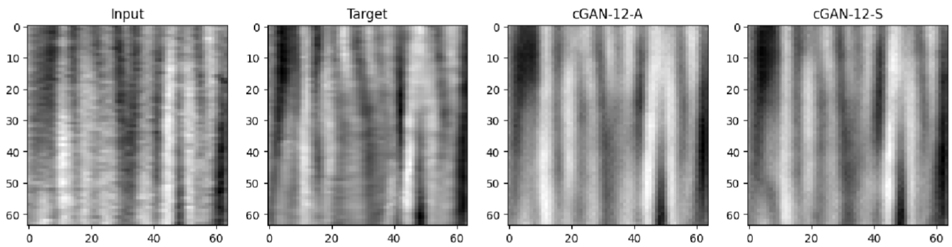

Figure 2. A generation example of cGAN-12-A and cGAN-12-S on 00-to-12 validation set.

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.