Multiscale Thermodynamics-Informed Neural Networks (MuTINN) for Nonlinear Prediction of Recycled Composite Behavior

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Abstract

The growing demand for sustainable materials has driven significant interest in the development and recycling of continuous fiber-reinforced thermoplastic composites, which are valued for their lightweight properties and high mechanical performance. However, mechanical recycling of these materials introduces microstructural changes such as porosity, fiber misalignment, and voids, which degrade mechanical properties and limit their reuse. In a previous study, the authors developed a multiscale model capable of capturing the mechanical responses of recycled composites, focusing on the microstructural complexity and degradation caused by the recycling process [1]. Building on this foundation, the present work adopts a novel Multiscale Thermodynamics-Informed Neural Networks (MuTINN) model [2], which couples the multiscale framework with data-driven modeling to enable efficient and accurate multiscale simulation of the mechanical behavior of recycled thermoplastic composite structures. Figure 1 provides a graphical abstract of the MuTINN approach, illustrating the integration of thermodynamic principles, neural networks, and Finite Element Analysis (FEA) to bridge microstructural behavior with macroscale structural predictions.
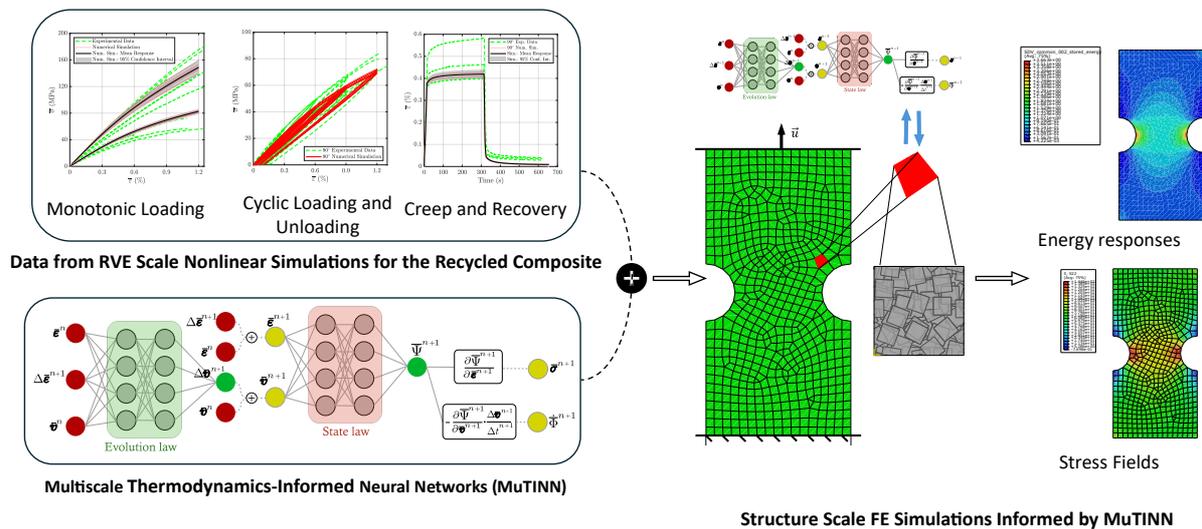

Figure 1: Graphical abstract of the MuTINN approach, illustrating the integration of thermodynamic principles, neural networks, and finite element analysis to link microstructural behavior with macroscale structural predictions.

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The MuTINN model integrates thermodynamic principles with Artificial Neural Networks (ANNs) to capture the complex behavior of recycled composites. It employs two interconnected ANNs: one for the evolution law, predicting the increment of quantities of interest (e.g., accumulated plastic strain), and another for the state law, predicting the Helmholtz free energy. This approach eliminates the need for memory-based networks, such as Recurrent Neural Networks (RNNs), by introducing Internal State Variables (ISVs) derived from microscale averages. The model is trained on a dataset generated from finite element simulations of a Representative Volume Element (RVE) under various loading conditions, ensuring robust predictions for both seen and unseen scenarios. Key innovations of the MuTINN model include its ability to account for the anisotropic nature of recycled composites by defining quantities of interest based on local material orientation. This allows the model to capture the heterogeneous behavior of the material at the macroscale.

The MuTINN model has been successfully integrated into commercial FEA software via a Meta-UMAT framework, enabling efficient multiscale simulations (FE-MuTINN) with a reduced computation time compared to standard FE^2. Validation of the MuTINN model against experimental data and finite element-based periodic homogenization demonstrates its accuracy in predicting mechanical responses, including stresses, and energy quantities. The model performs particularly well for uniaxial and biaxial loading conditions, with slight discrepancies observed in dissipation energy at higher deformations due to the omission of viscoelastic effects. Despite this, the model's predictions align closely with experimental results, confirming its reliability for practical applications. A key advantage of the MuTINN approach is its computational efficiency. While traditional FE-based periodic homogenization requires several minutes per time step, MuTINN completes the same computations in seconds. This efficiency is demonstrated in structural-level simulations, where the models accurately predict macroscopic strain fields and quantities of interest across different material domains, highlighting the material's anisotropic response.

In conclusion, the MuTINN model represents a significant advancement in the modeling of recycled thermoplastic composites. By combining thermodynamic principles with machine learning, it offers a computationally efficient and accurate tool for predicting the mechanical behavior of these materials, facilitating their development and optimization in a circular economy. The integration of MuTINN into commercial FEA software bridges the gap between microstructural complexity and macroscale structural analysis, supporting the broader adoption of recycled composites in industries such as automotive, aerospace, and construction.

References

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