Supplementary Information

Deep Generative Spatiotemporal Learning for Integrating Fracture Mechanics in Composite Materials: Inverse Design, Discovery, and Optimization

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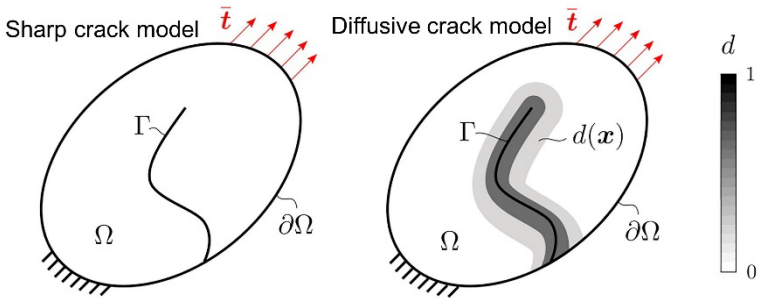
Supplementary Note 1. Phase fields model to simulate crack propagation in composite material

In this study, we adopt a phase field approach utilizing a hybrid formulation,[1] inspired by Griffith's thermodynamics. This method, tailored to characterize the intricate failure behaviors of CMs, provides foundational data for training our deep learning model. As depicted in **Supplementary Fig**. **1**, the topology of the sharp crack is represented by the phase field scalar parameter, $d(\boldsymbol{x})$. This parameter indicates the extent of the material's damage or fracture: a value of 1 signifies total failure, while 0 indicates no damage. The phase-field methodology offers a comprehensive framework, capably simulating various failure mechanisms in CMs, such as reinforcement breakage due to external load transfer, and matrix cracking. Additionally, the hybrid approach enables the prediction of failure scenarios under combined loading. Our primary objective is to create an advanced deep learning model that serves as an effective surrogate, substantially reducing the inference time of crack phase field simulations. Also, generating a simulated dataset that approximates real-world material behavior is the most fundamental to developing a robust deep learning model with high practicality. In that regard, the 'hybrid' energy degradation formulation integrates the key principles of earlier developed isotropic and anisotropic formulations, providing realistic simulation framework. In this hybrid paradigm, crack evolution is predominantly driven by the tensile portion of the strain energy, a characteristic derived directly from the anisotropic formulation. This feature is advantageous as it inhibits crack evolution under compressive loading, aligning with real-world observations where uncontrolled crack propagation due to compressive loads is seldom seen. Unlike the anisotropic formulation, the degradation of the material's elastic modulus occurs uniformly in all directions, mirroring the isotropic formulation. This uniform degradation ensures that elements sustaining significant damage progressively lose their load-bearing capability, irrespective of the external load's direction. By harmoniously merging distinctive features from both isotropic and anisotropic methodologies, the hybrid formulation is crafted. Consequently,

it furnishes a more precise and realistic simulation framework for modeling the complex processes of deformation and eventual failure in CMs. Our objective is to validate the STGNet's predictability for extrapolation problems, particularly for unseen configurations that demonstrates exceptional mechanical properties beyond those included in the training set, essential for optimizing CM design. Therefore, we generate dataset with various crack propagation scenarios from a wide variety of combinations of constituents by leveraging the strengths of crack phase field model. To generate the dataset of the entire failure process of CMs, we execute the crack phase field model through the Abaqus CAE's User Element (UEL) subroutine with a staggered solution scheme. For this simulation, we consider two-dimensional CM configurations under plane stress conditions, simulated in displacement-controlled analysis with constant time step size. This setup includes perfectly bonded 70 stiff blocks and 51 soft material blocks, arranged in an 11×11 square array. 132×132 structured quadrilateral meshes are utilized for the finite element simulation. A single edge pre-crack with a length of 2.5mm was introduced centrally to initiate crack propagation, bypassing both the upper and lower boundaries. The selected material properties for the constituents (stiff and soft phases) are listed in **Supplementary Table 1**, where E designates Young's modulus, ν is Poisson's ratio, and g_c is critical energy release rate. Note that although quasi-static crack phase field modeling is employed, the methods utilized in this study can equivalently be applied to mechanically dynamic problems (e.g., dynamic crack propagation), provided that equispaced or, at least, equivalent variable time steps are used for datasets.



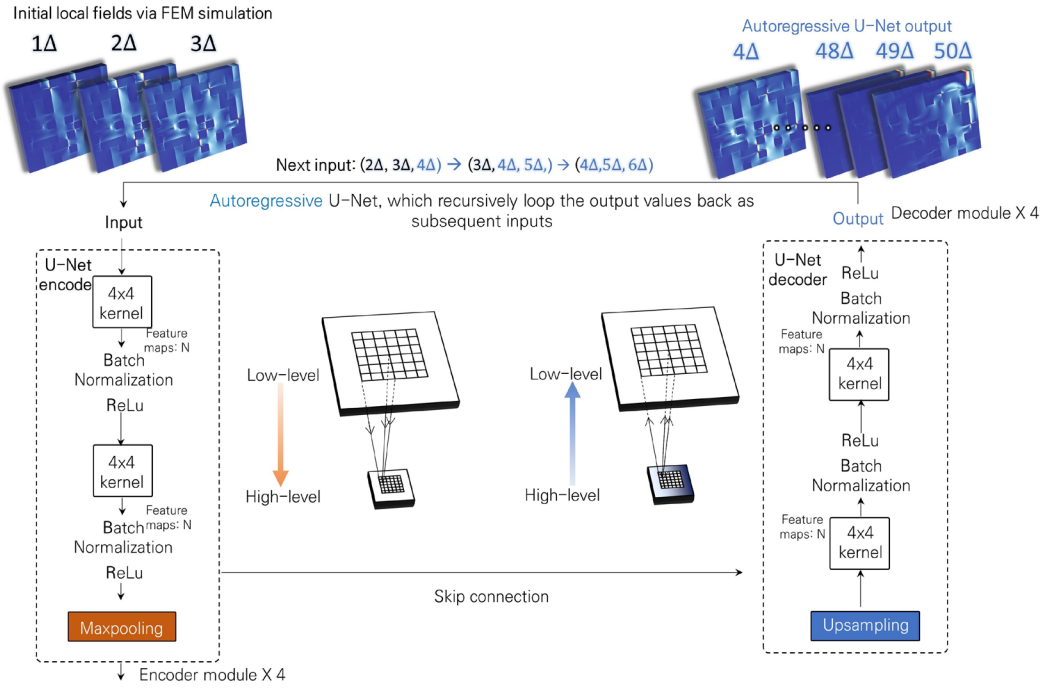
Supplementary Fig. 1. Two-dimensional crack topology: sharp crack model (left), diffusive crack model described by phase field function ***d(x)*** (right).

Parameters	E_{stiff} (MPa)	$g_{c,\text{stiff}}$ (J/ m^2)	ν_{stiff}	E_{soft}	$g_{c,\text{soft}}$ (J/ m^2)	ν_{soft}	Mesh size (mm)	Number of mesh	Applied strain
Values	2,100	50	0.3	21	50	0.3	0.08	17,000	0.015

Supplementary Table 1. Material properties of composite constituents.

Supplementary Note 2. Baseline (autoregressive U-Net) algorithm

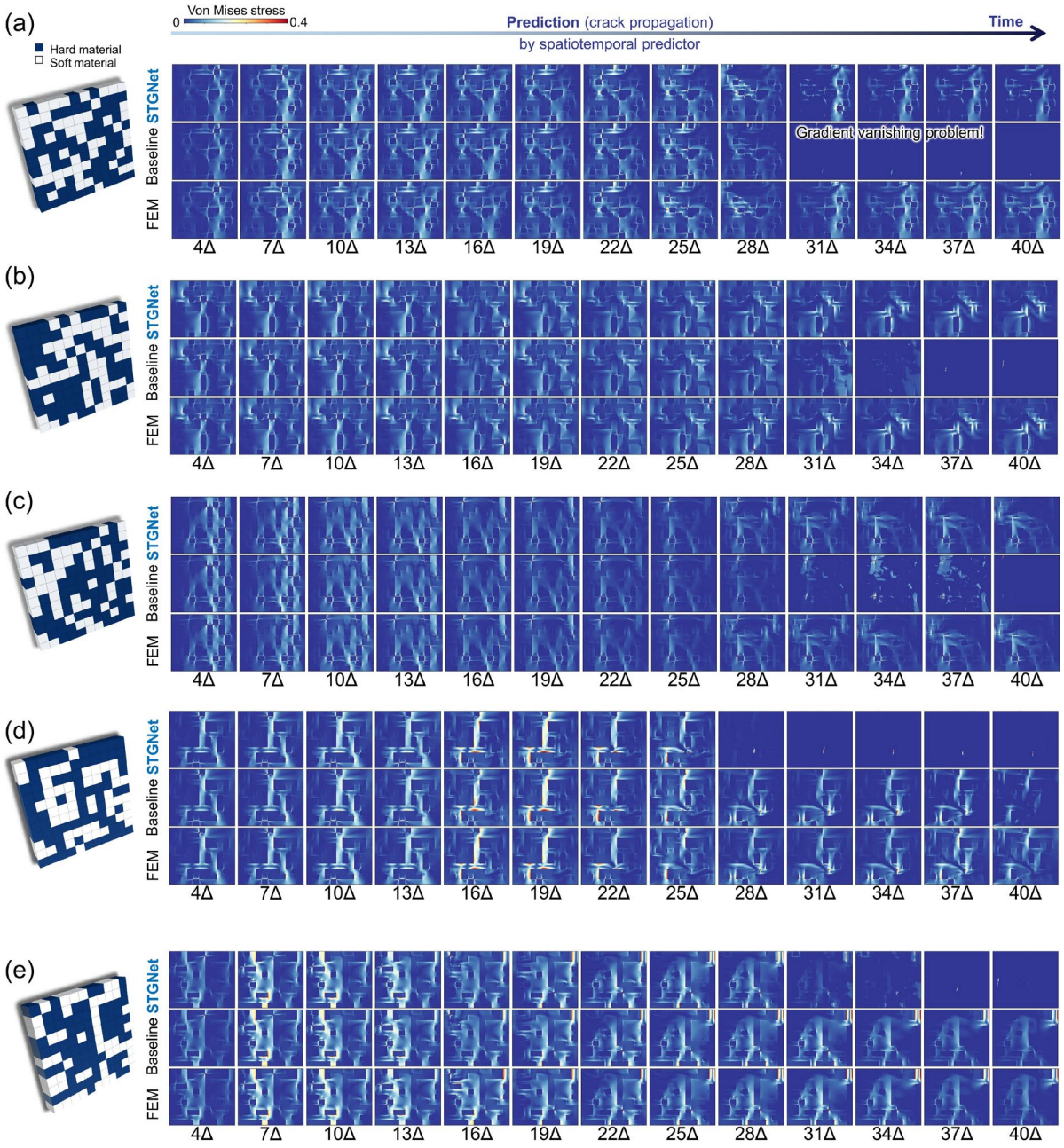
To evaluate STGNet's powerful predictive capability for spatiotemporal dynamics, we conduct a comparative analysis with a baseline model. This baseline employs an autoregressive U-Net, a cutting-edge algorithm widely used in predicting the spatiotemporal dynamics in various research fields such as heat, fluids, and materials sciences.[2-4] As illustrated in **Supplementary Fig. 2**, local fields derived from the initial steps via FEM are fed into the baseline model to forecast subsequent local fields. These predicted fields are then channel-stacked and recursively inputted for extended length predictions. However, this method of recycling outputs as inputs may engender long-term dependency challenges, potentially impairing the model's proficiency in predicting novel configurations. To ensure a fair comparison between STGNet and the baseline model, we maintained a consistent number of convolutional feature maps, 64, across both models, thus standardizing the learning parameters irrespective of layer depth variations.



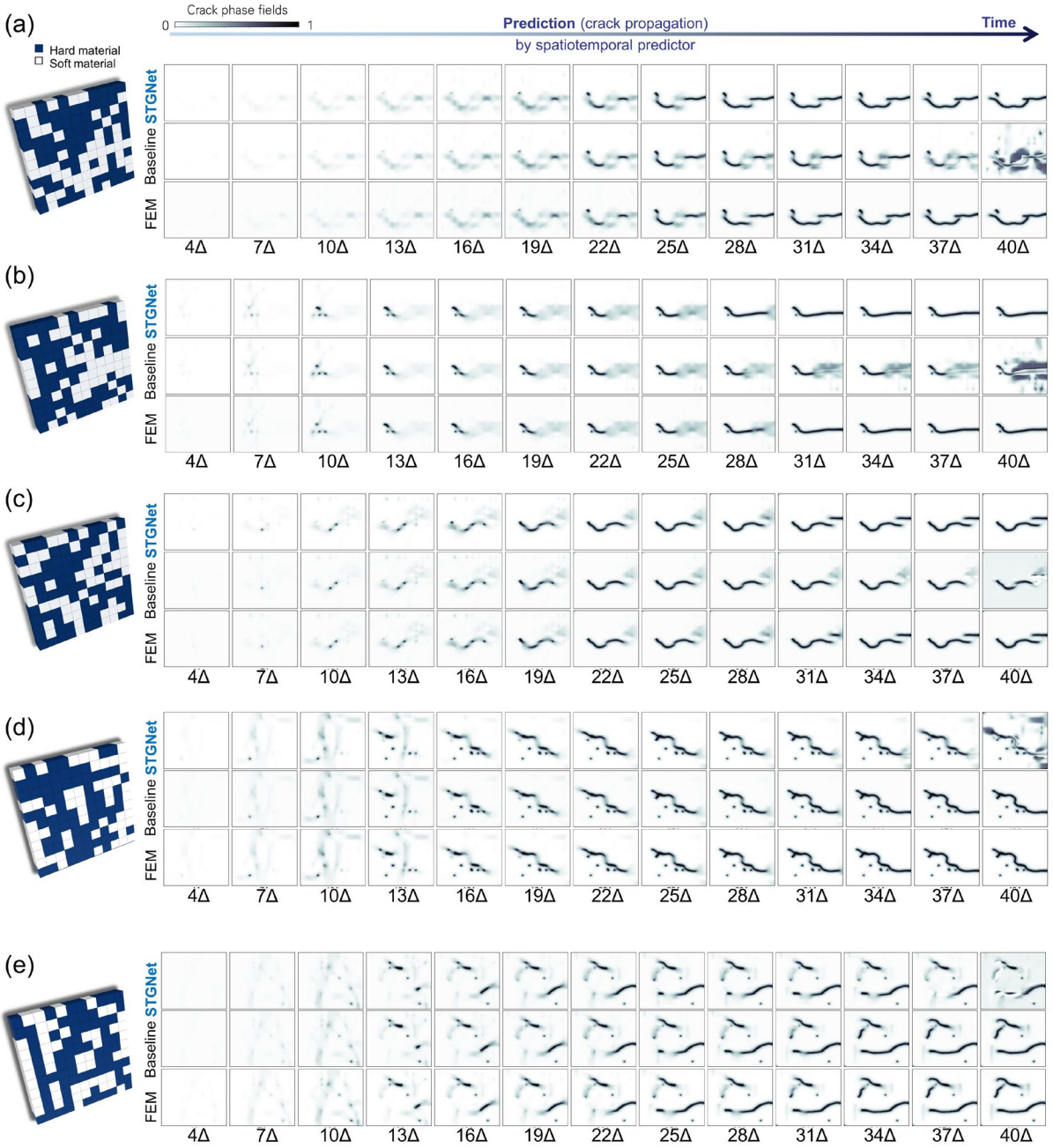
Supplementary Fig. 2. Baseline algorithm: autoregressive U-Net to predict spatiotemporal dynamics such as stress evolution and crack propagation in composite material.

Supplementary Note 3.

In the main manuscript, we verified the superiority of STGNet in predicting stress evolution and crack propagation in CMs, and to further verify the prediction ability of STGNet for more diverse CM morphologies, we compared the prediction ability on a random array of unseen CMs with more diverse crack scenarios as shown in **Supplementary Fig. 3 and 4**.



Supplementary Fig. 3. Stress evolution prediction results within the CM and comparison with FEM and baseline. We test the three unseen CM configuration (**a-d**).

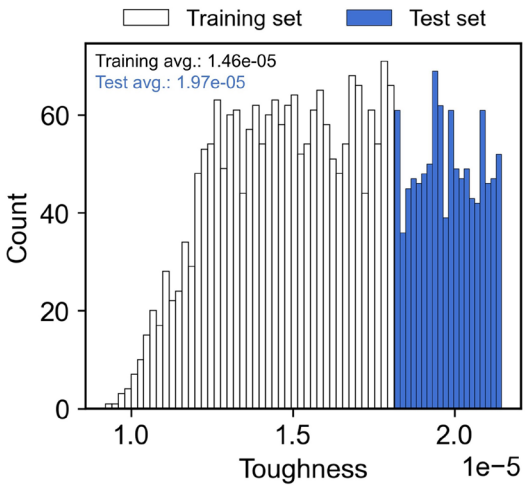


Supplementary Fig. 4. Crack propagation prediction results within the CM and comparison with FEM and baseline. We test the three unseen CM configuration (**a-d**).

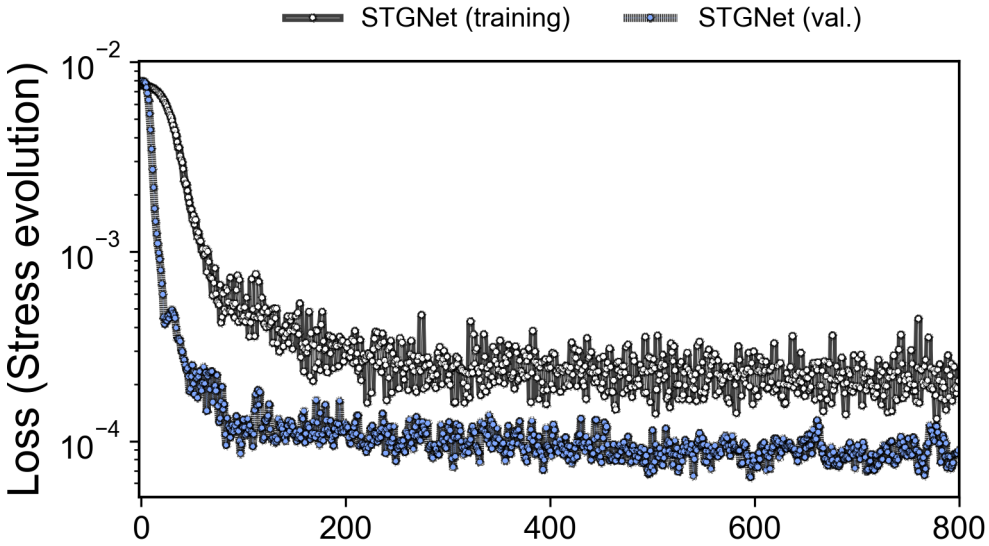
Supplementary Note 4. Detailed training process of STGNet

The ultimate goal of this study is to predict the stress evolution and crack propagation of materials with superior mechanical properties that the trained deep learning model has not seen before. Therefore, in this study, we generate 4,000 composites with random shapes and create corresponding stress evolution and crack propagation data through phase fields simulation. The materials are then sorted based on the mechanical characteristic of toughness (area under stress-strain curve), which indicates their capacity to withstand fracture. The top 25% of these materials (1,000 samples) are selected to test the model's generalization ability, including its capacity to extrapolate toughness beyond the training data. The remaining 75% (3,000 samples) are used to train the STGNet (**Supplementary Fig. 5**).

Moreover, it is crucial to assess the balance between the training set and the unused validation set to indicate whether the STGNet has been sufficiently trained. **Supplementary Fig**. **6** demonstrates that the STGNet has successfully achieved learning convergence. Particularly, the learning rate is reduced by a factor of ten every 200 epochs to further optimize the search, and as shown in **Supplementary Fig**. **6,** it is evident that STGNet has successfully demonstrates its generalizability in predicting the stress evolution. In this study, the use of the ABAQUS MACRO FUNCTION to generate training and testing datasets minimized the tediousness of repetitive tasks due to configuration changes. Additionally, utilizing three desktop CPUs, it took approximately 29 days to generate total 4,000 dataset (both training and test). The training time for STGNet used in this study is about 5 hours.



Supplementary Fig. 5. Training/test set for developing and validating STGNet



Supplementary Fig. 6. History of training/validation set of STGNet in predicting stress evolution.

Supplementary Reference

1. H. Jeong, S. Signetti, T.S. Han, S. Ryu, *Comput. Mater. Sci.* **2018**, 155.

2. Z. Niu, V.J. Pinfield, B. Wu, H. Wang, K. Jiao, D.Y.C. Leung, J. Xuan, *Energy Environ. Sci.* **2021**, 14.

3. S. Mo, N. Zabaras, X. Shi, J. Wu, *Water Resour. Res.* **2019**, 55.