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Interpretable and Flexible Generalization of Evolving Computational Materials' Framework for Heterogeneous Composite Structures

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Abstract

Recently, computational material models accelerated innovations by harnessing machine learning (ML) methods, but they face challenges. It is difficult to incorporate internal heterogeneity and diverse boundary conditions (BC's) into existing ML methods, and weak interpretability of ML poses challenges. This paper generalizes a recently developed self-evolving computational material models framework built upon physics-ingrained ML-friendly new features via information convolution and the Bayesian evolutionary algorithm. This paper proposes a new material-specific information index (II), which is capable of autonomously quantifying the internal heterogeneity and diverse BC's. Also, this paper introduces highly flexible cubic regression spline (CRS)-based link functions which can offer mathematical expressions of salient material coefficients of the existing computational material models in terms of convolved II. Thereby, this paper suggests a novel means by which ML can directly leverage internal heterogeneity and diverse BC's to autonomously evolve computational material models while keeping interpretability. Validations using a wide spectrum of large-scale reinforced composite structures confirm the favorable performance of the generalization. Example expansions of nonlinear shear of quasi-brittle materials and progressive compressive buckling of reinforcing steel underpin efficiency and accuracy of the generalization. This paper adds a meaningful avenue for accelerating the fusion of computational material models and ML.

Keywords: Evolutionary algorithm, cubic regression spline, computational material model, machine learning for heterogeneity, machine learning for varying boundary conditions, nonlinear analysis of reinforced concrete structures

1 Introduction

Traditionally, computational material models ($\mathcal{M}$'s) are derived from the statistical fitting of data sets obtained from well-designed small-scale laboratory experiments under specific boundary conditions (BC's) to represent the analyses of real-world structures (Figure 1B). However, machine learning (ML) methods have approved their power in learning complex data over the past decades. Therefore, researchers in computational mechanics and structures sometimes apply different ML methods such as decision tree or deep learning to predict different targets in the structural system (Mangalthu et al. [1]; Lee and Lee [2]; Luo and Paal [3]) (Figure 1C).

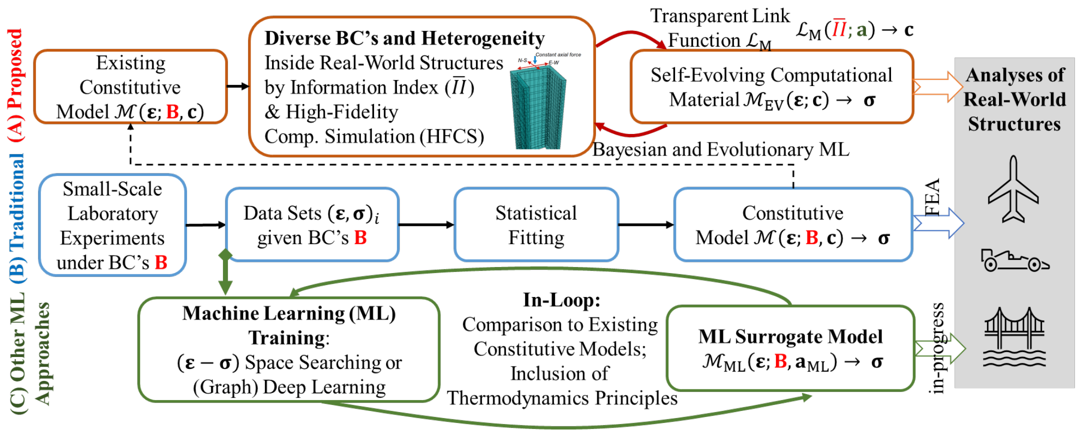


Figure 1: A comparison of (A) the proposed glass-box framework, (B) the traditional $\mathcal{M}$'s, (C) the current ML-based approaches.

Despite their meaningful contributions to our understanding of materials and structures, there are two critical challenges, the lack of interpretability and the limited description of the internal complexity of heterogeneous materials and diverse BC's. In terms of the first challenge of interpretability, most existing ML methods rarely present detailed explanations behind the input-output relations, rendering them a "black-box" approach. Regarding the second challenge of incomplete data, ML approaches essentially depend on training the data sets obtained from the laboratory tests to develop an alternate model representing or replacing the constitutive model. However, these training data sets can hardly contain the entire space of all possible physical conditions. Therefore, to overcome the two critical challenges, this work adopts and generalizes a "glass-box" computational material model framework developed by Cho [4] (Figure 1A). The major novelty of the glass-box framework is twofold. First, it can combine fundamental physics principles and spatial convolution to generate convolved information index (II) so that ML autonomously identifies internal heterogeneity and complex BC's within real-world structures. Second, the glass-box framework offers room for transparent link functions (LF's) that can solve the hidden rules behind the material coefficients of adopted computational material mechanisms. However, in the initial work, the glass-box framework contains only two material models with a simple two-parameter form LF, requiring significant generality, flexibility, and expandability for broader applicability. This paper generalizes the glass-box framework by proposing a set of new convolved II's necessary for the extension to additional material mechanisms such as the nonlinear shear of cracked quasi-brittle materials and reinforcing steel's progressive buckling mechanisms. Also, this paper generalizes the glass-box framework by including the cubic regression spline (CRS) (Wood [5]; Hastie and Tibshirani [6]).

2 Methods

There are significant similarities between the adopted glass-box framework and the convolutional neural network (CNN), in which both can provide a spatially weighted averaging to collect information from adjacent regions and come up with new information measures. However, the steps of the glass-box framework are straightforward and briefly summarized herein. More details can be found in Bazroun et al. [7].

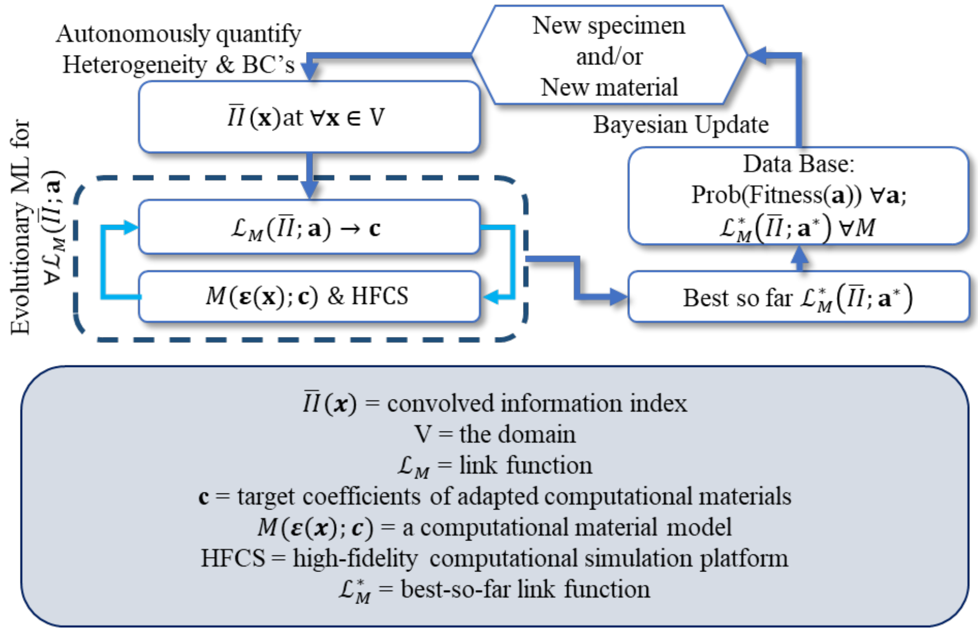
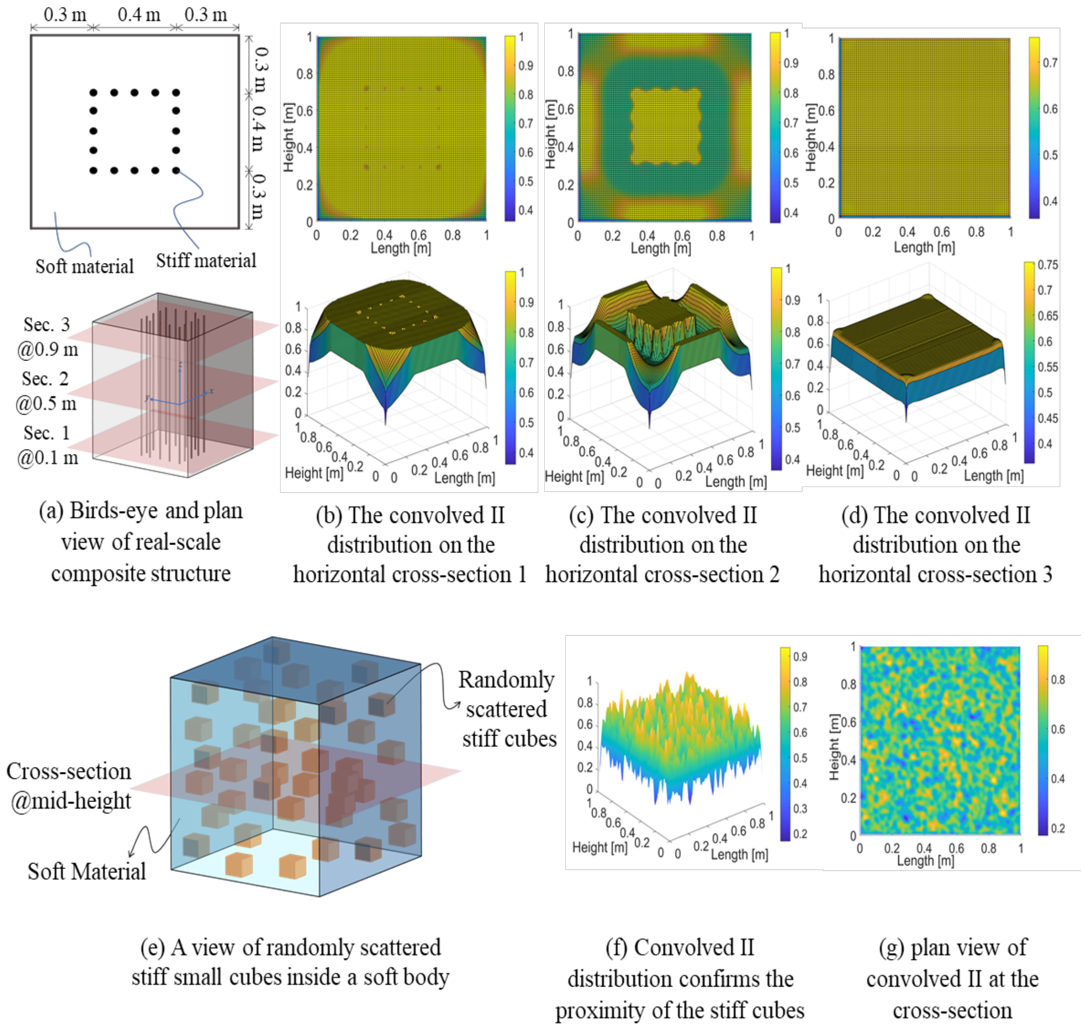


Figure 2: Flowchart of the proposed glass-box framework.

As shown in Figure 2, convolved II first determines the laboratory-reality similarity and leads the ML method to internal heterogeneity and BC's at the material point level inside the physical system (Figure 3). There is no limit to derive domain-specific II, and there is always sufficient room to include engineering principles or basic mechanics for the desired physical information. Hence, Bazroun et al. [7] proposed a new convolved II to help evolutionary ML improve significant material coefficients of a complex progressive reinforcing steel bar buckling model, which is highly challenging to capture by experimental efforts (Dhakal and Maekawa [8]). However, this new convolved II can quantify the impact of surrounding brittle materials on the reinforcing steel. Then, multiple LF's of multiple M's interact within the loops of generations and organisms in genetic algorithms (GA) and high-fidelity computational simulation platform (HFCS) for standard selection, spawning, and evolution of GA. Herein, LF seeks to offer a mathematical expression between convolved II and M. Hence, this work suggests a highly flexible CRS-based LF which can be represented as Eq. (1). II-based perception of randomly embedded stiff materials (adapted from Bazroun et al. [7]).

$$\mathcal{L}_M(\bar{\mathit{II}};\mathbf{a}) = a_1 b_1(\bar{\mathit{II}}) + a_2 b_2(\bar{\mathit{II}}) + \sum_i a_{i+2} b_{i+2}(\bar{\mathit{II}}) \tag{1}$$

where a_i is the unknown free parameter of the basis function, and $b_i(x)$ is the ith basis function. Also, in terms of M, this study selects different microphysical mechanisms (Figure 4). First, the multi-directional, fixed-type smeared crack model is adopted since it can maintain the actual crack direction and accepts at most three orthogonal cracks (Thorenfeldt [9]; Taucer et al. [10]; Reinhardt [11]; Cho [12]). Next, this study adopts the nonlinear reinforcing steel bar mechanism based on the generalized Menegotto-Pinto hysteresis that can utilize the topological information of surrounding concrete's damage of the center bar capable of describing progressive compressive buckling of the bar (Cho [13]). Finally, new experimental data of different test systems are used by Bayesian updates with the prior best of the LF to strengthen the best-so-far LF.



(a) Birds-eye and plan view of real-scale composite structure

(b) The convolved II distribution on the horizontal cross-section 1

(c) The convolved II distribution on the horizontal cross-section 2

(d) The convolved II distribution on the horizontal cross-section 3

(e) A view of randomly scattered stiff small cubes inside a soft body

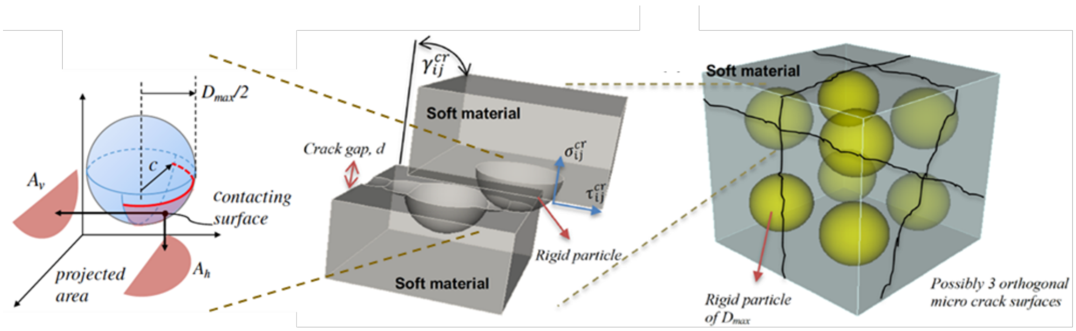
(f) Convolved II distribution confirms the proximity of the stiff cubes

(g) plan view of convolved II at the cross-section

Figure 3: Examples of (a-d) II-based perception of stiff objects, BC's, and (e-g) heterogeneity.

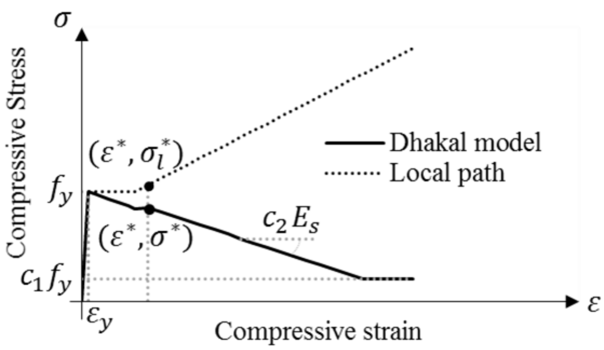
3 Results

One of the notable strengths of the proposed glass-box framework lies in its expandability. Generally, its evolutionary algorithm is long gene-based storage that can be easily extended by adding more gene expressions for more material models (Fig. 5). Therefore, to investigate the proposed framework's performance, a rectangular wall (named WSH 5) and a U-shaped wall (named TUB) have been used to train the glass-box framework. The geometric, material properties, and reinforcement information of the two walls, experimented by Dazio et al. [14] and Beyer et al. [15], respectively, are summarized in Bazroun et al. [7].



(a) 3D nonlinear shear mechanism-based soft matrix-rigid hemisphere interlocking (adapted from Cho [12], Cho [13])

(b) Multi-directional smeared crack mechanism allowing three orthogonal cracks over random-sized aggregates (adapted from Cho [4])



(c) buckling model proposed by (Dhakal and Maekawa [8]) where σ_l^* is point wise stress corresponding to ε^* (strain at the onset of buckling)

Figure 4: Adopted microphysical mechanisms.

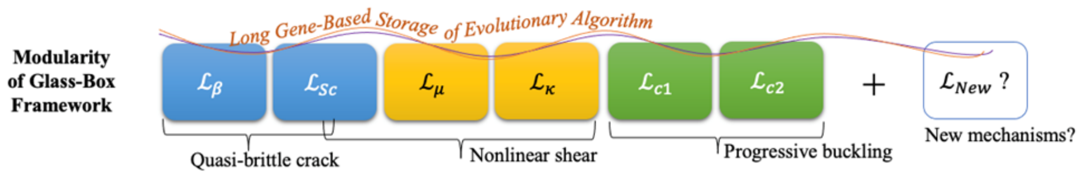


Figure 5: The modularity of the glass-box framework.

As shown in Figure 6, the best-so-far result for each wall compares the prediction in terms of force and displacements using the glass-box framework of 6- and 2-coefficients (denoted as Model I and Model II, respectively) and a parallel multi-scale finite element analysis platform named VEEL (Cho [13]; Cho and Porter [16]). The results clearly show that the minimum error of the best-so-far generation of WSH5 using Model I, which is 0.6%, is less than the default VEEL (4.3%) and Model II (0.7%). Also, using the prior best of WSH5 for testing TUB shows better accuracy in Model I than using Model II and default VEEL, in which the minimum error using Model I is 3.1% while it is 6.5% and 3.9% with using default VEEL and Model II, respectively. However, as shown in Figure 7, increasing generations increases the accuracy, but it costs more computational time and computing memory.

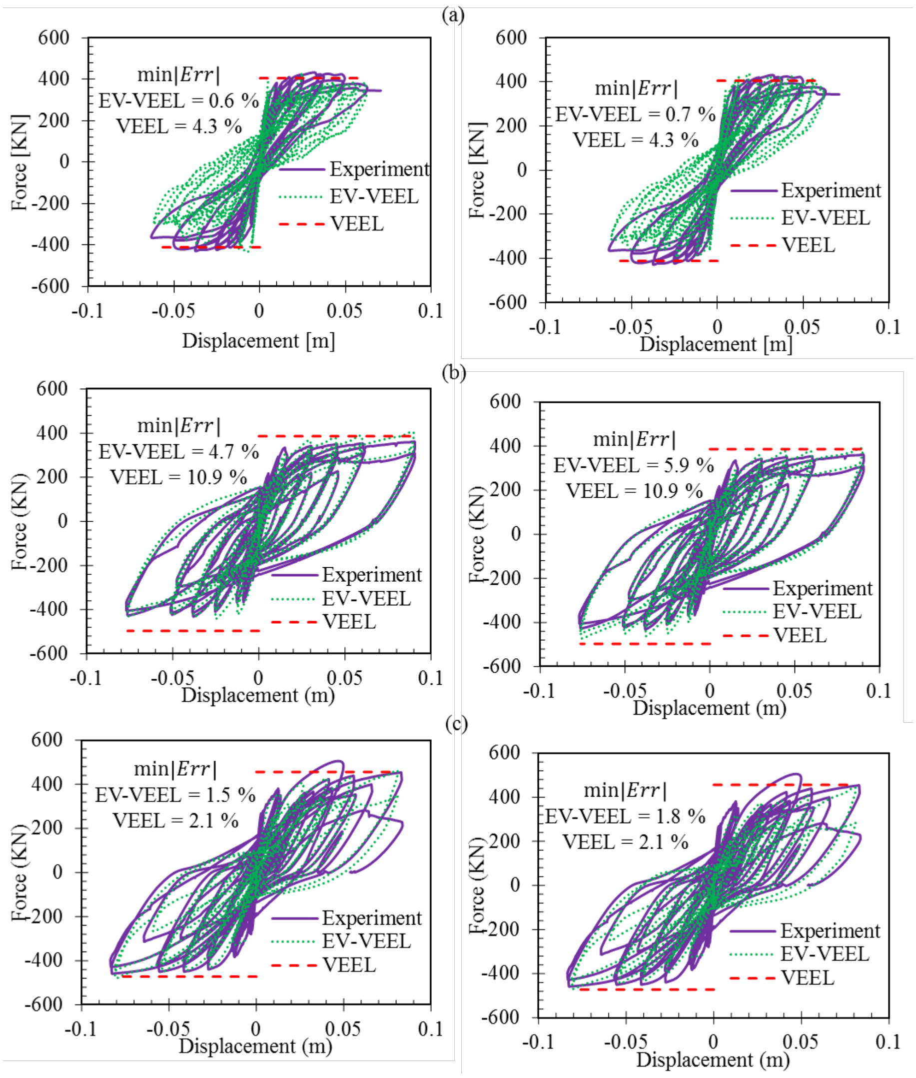


Figure 6: Comparison between the accuracy of Model I (left column), Model II (right column), and VEEL for the walls WSH5 and TUB: (a) results for WSH 5; (b) results of north-south direction loading for TUB; (c) results of east-west direction loading for TUB.

Furthermore, Figure 8 shows that the framework can provide a mathematical expression since the GA can learn the hidden relationship between the convolved II and material coefficients through LF using a single target LF. Hence, an example of identified physical rule about β and the II in a clear CRS form at the i_{th} material point $\boldsymbol{x}_{(i)}$ can be given by

$$\begin{aligned}\beta(\boldsymbol{x}_{(i)}) &= a_1 + a_2 \times \overline{II}(\boldsymbol{x}_{(i)}) + \sum\nolimits_{j=1}^{3} a_{j+2} \times b_{j+2}\, \overline{II}(\boldsymbol{x}_{(i)}) \\ &= a_1 + a_2 \times \mathbb{E}_{\mathcal{N}(\boldsymbol{x}_{(i)},L^2)}(II) + \sum\nolimits_{j=1}^{3} a_{j+2} \times b_{j+2}\, \mathbb{E}_{\mathcal{N}(\boldsymbol{x}_{(i)},L^2)}(II)\end{aligned} \tag{2}$$

As proof of generality and versatility, extensions of the glass-box approach of this paper to nano-scale and millimeter-scale structures' phenomena can be found in Cho et al. [17, 18].

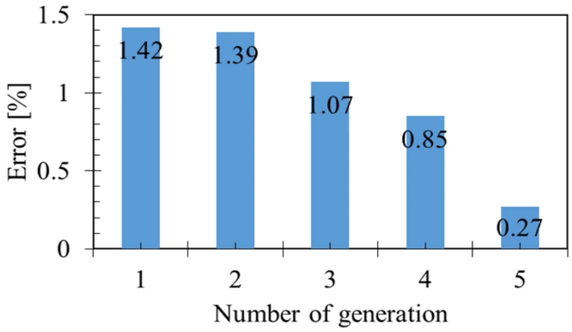


Figure 7: Results of the gradual evolution.

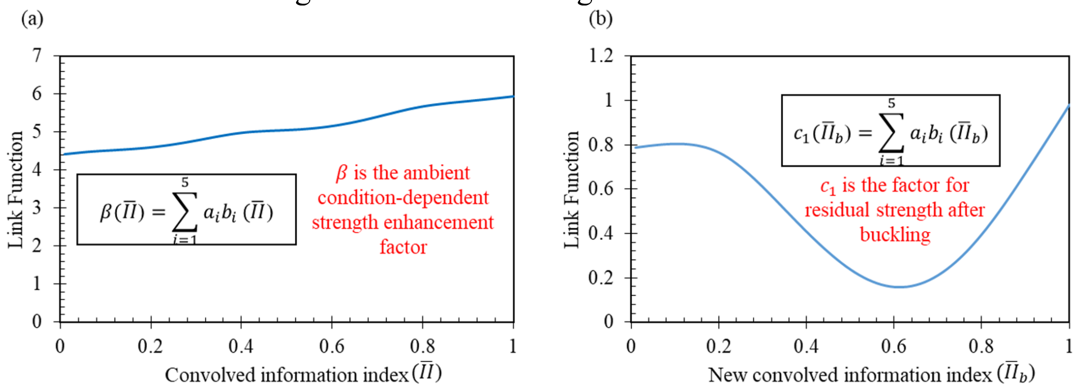


Figure 8: Material coefficients through an LF: (a) an example of material coefficient that affects the strength of the brittle material; (b) an example of material coefficient that affects the buckling of the reinforcement steel.

4 Conclusions and Contributions

This paper describes how to generalize the glass-box computational material framework by proposing (1) a new material-oriented convolved information index (denoted as $\overline{II}_b$) and (2) highly flexible cubic regression spline (CRS)-based link function (LF), and the conclusion can be summarized as follow: (1) Convolved information index (II) can serve as physics-ingrained ML-friendly new features; (2) The new convolved II helps the glass-box framework leverages complex internal material heterogeneity and diverse BC's inside large-scale structures; (3) The glass-box framework can honor and leverage the existing material models while selectively replacing the decisive material coefficients; (4) Testing the large-scale reinforced composite structures confirmed that CRS-based LF's could improve accuracy compared to the manually calibrated high-fidelity simulations; (5) CRS-based LF plays an important role in identifying hidden rules between the convolved II and additional physical mechanisms; (6) The new convolved II demonstrates the expandability of the glass-box framework to incorporate a new material mechanism.

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