Machine Learning aided Phase-Field Method in Constitutive Modeling of Concrete Structures

Adalberto Horácio de Oliveira Mendes[1], Hugo Mouro Leão[1], Saulo Silvestre de Castro[1] , Roque Luiz da Silva Pitangueira[1]

[1]*Dept. of Structural Engineering, Federal University of Minas Gerais*
Av. Antonio Carlos, 6627, Pampulha, Belo Horizonte, 31270-901, Minas Gerais, Brazil
adalbertohom@gmail.com, hugomleao@yahoo.com.br, saullo9@yahoo.com, roque@dees.ufmg.br

Abstract. Phase-field modeling has emerged as a promising approach for modelling crack propagation. Different from Griffith's theory, which deals with discrete cracks, phase-field modeling transforms cracks into diffusive entities that propagate within a defined region, regulated by a length scale parameter. This methodology introduces a phase-field variable as a novel nodal degree of freedom, governed by an additional equation integrated into the model. This variable quantifies the damage of the material at each point, with zero representing intact material and unity indicating complete damage. However, the practical implementation of phase-field modeling presents significant computational challenges. Its requirement of very refined meshes makes the process computationally expensive. In this context, machine learning techniques can be used to simulate the constitutive model and ensure that the process enhance efficiency. The article aims to use the machine learning technique to train a neural network capable of simulating the constitutive behavior of a phase-field model. The validation of this approach will be carried out by comparing its results with those obtained through finite element numerical analysis. All simulations will be conducted using the INSANE software.

Keywords: Machine Learning, Neural Networks, Multilayer Perceptron, Phase-Field.

1 Introduction

The theoretical development of fracture mechanics took its first steps with Griffith's theory that considers an initial crack in the body evolves when the energy of that body reaches to the critical energy release rate [1]. Although very promising, this theory had limitations such as dependence on an initial crack and the inability to describe the crack path. After a long journey taken by the scientific community, phase-field models have emerged as a robust alternative that can overcome these limitations. These models can detect crack nucleation and describe its path with no explicit representation, by using a continuous field variable (ϕ) that represents the damage of a material point and creates a smooth transition between between the undamaged ($\phi = 0$) and the fully damaged material ($\phi = 1$). For that, a length scale parameter is employed in order to define the size of that transition region. Despite their advantages, phase-field modelling faces significant computational challenges. Since the need for very refined meshes for accurate analysis makes the process computationally expensive. In this context, artificial intelligence (AI) offers a promising solution to mitigate these challenges. Through machine learning (ML) techniques, that interpret external data, learn from it, and use this learning to achieve specific goals. A very widely applied ML technique is neural networks (NN), which consists of computational models inspired by the biological structure of neurons. Artificial neural networks (ANN) can significantly reduce the computational cost in finite element simulations [2]. Neural Network-Based Constitutive Models (NNCM) can effectively model the mechanical behavior of materials using stress-strain data, material theory, and additional information [3]. The purpose of this work is to present the using of a Multilayer Feedforward Neural Network, also known as a Multilayer Perceptron (MLP), to predict phase-field values based on associated stresses and strains values. Through this approach, it is aimed to obtain a computational more efficient way to obtain the values for the field variable.

2 Phase-field models

The phase field models are based on two essential functions: the crack surface density function ($\gamma(\phi, \nabla\phi)$), responsible for smear the Grifith's sharp crack over a smoothed region, and the energetic degradation function ($g(\phi)$). Wu [4] has proposed a generalization for ($\gamma(\phi, \nabla\phi)$):

$$\gamma(\phi, \nabla\phi) = \frac{1}{C_0}\left[\frac{1}{l_0}\alpha(\phi) + l_0 \mid \nabla\phi \mid^2\right] \tag{1}$$

where $\alpha(\phi)$, known as the geometrical crack function, is a monotonically increasing function that determines how the shape of the smoothed region and must satisfy $\alpha(0) = 0$ and $\alpha(1) = 1$, C_0 is a constant calculated by $C_0 = 4\int_0^1 \alpha^{1/2}\, d\phi$. In order to prevent crack in compressed regions, phase-field models also incorporates an additive decomposition into the strain energy density $\psi(\epsilon)$, in such way that.

$$\psi(\epsilon) = g(\phi)\psi_0^+(\epsilon) + \psi_0^-(\epsilon) \tag{2}$$

The counterpart ψ_0^+ represents the strain energy density that comes from traction and ψ_0^- from compression. It is important to emphasize that split is applied only to anisotropic models. In isotropic models, the function g multiplies the entire strain energy density function. In phase-field models, those isotropic and anisotropic are related to that split between compressed and tractioned regions, not to the material properties. Therefore, the total energy functional that describes the fracture problem, considering phase-field models, is given by:

$$E_t = \int_\Omega \psi(\overline{\epsilon}(\overline{u}), \phi)\, dV + \int_B G_c\gamma(\phi, \nabla\phi)\, dV - \int_\Omega \overline{b}\cdot\overline{u}\, dV - \int_{\partial\Omega} \overline{t}\cdot\overline{u}\, dA \tag{3}$$

where Ω is the body domain, B is the degraded domain, G_c is the critical energy release rate, u is the displacement vector, and b and t are the body and surface forces, respectively. Thus, according to Wu [5], the weak form for the phase-field model equations is expressed as:

$$\begin{cases} \int_\Omega \sigma : \delta\epsilon\, dV = \delta P_{\text{ext}} \\ \int_B \left[g'(\phi)\overline{\psi}\delta\phi + G_c\delta\gamma\right] dV \geq 0 \end{cases}, \quad \text{com } \delta\gamma = \frac{1}{C_0}\left[\frac{1}{l_0}\alpha'(\phi)\delta\phi + 2l_0\nabla\phi\cdot\nabla\delta\phi\right] \tag{4}$$

The data used to train the artificial intelligence model in this work were based on the anisotropic constitutive model of Miehe et al. [6]. Due to the spectral decomposition of the strain tensor (See eq. 5, 6 and 7), this model can completely supress cracks in compressed regions. More details about this constitutive model can be found in the work of Miehe [7] and Leão [8].

$$\underline{\epsilon} = \sum_{n=1}^{3} \epsilon_n \overline{p}_n \otimes \overline{p}_n = \underline{\epsilon}^+ + \underline{\epsilon}^- \tag{5}$$

$$\underline{\epsilon}^+ = \sum_{n=1}^{3} \langle\epsilon_n\rangle_+ \overline{p}_n \otimes \overline{p}_n \tag{6}$$

$$\underline{\epsilon}^- = \sum_{n=1}^{3} \langle\epsilon_n\rangle_- \overline{p}_n \otimes \overline{p}_n \tag{7}$$

3 Machine Learning models

Machine Learning, as defined by Samuel in the late 1950s, involves the development of algorithms that enable computers to learn from data without explicit programming. Today, ML is recognized as a subset of artificial intelligence that designs algorithms capable of identifying patterns in data to generalize and predict future events with high accuracy. This capability makes ML suitable for solving complex problems that traditional methods cannot effectively address [9–12].

In this study, the focus was on Supervised Learning Algorithms, which require labeled training data to learn tasks. These algorithms analyse input features (attributes) to predict target values (labels) by estimating the probability of the label given the features. The research explored the feasibility of predicting the Phase Field in a numerical simulation using Artificial Neural Network, which is briefly explained.

Artificial Neural Networks (ANNs) are computational models inspired by the central nervous system of living beings. They consist of numerous simple processing units called neurons, which work in parallel to store and utilize knowledge. ANNs are effective in pattern recognition tasks, making them suitable for both classification and regression problems. The structure of an artificial neuron is conceptually similar to that of a biological neuron.

An artificial neuron receives input signals, each of which is weighted by a synaptic weight. The neuron's activity is calculated as the weighted sum of these inputs, with an added bias. The neuron's output is determined by an activation function applied to this activity. Synaptic weights are usually initialized randomly but are adjusted during training to minimize the error, which is measured by a cost function. This process is crucial for optimizing the model's predictive accuracy. The Perceptron, the simplest form of an artificial neuron, was initially proposed by Rosenblatt in 1958 and remains foundational in modern neural network design.

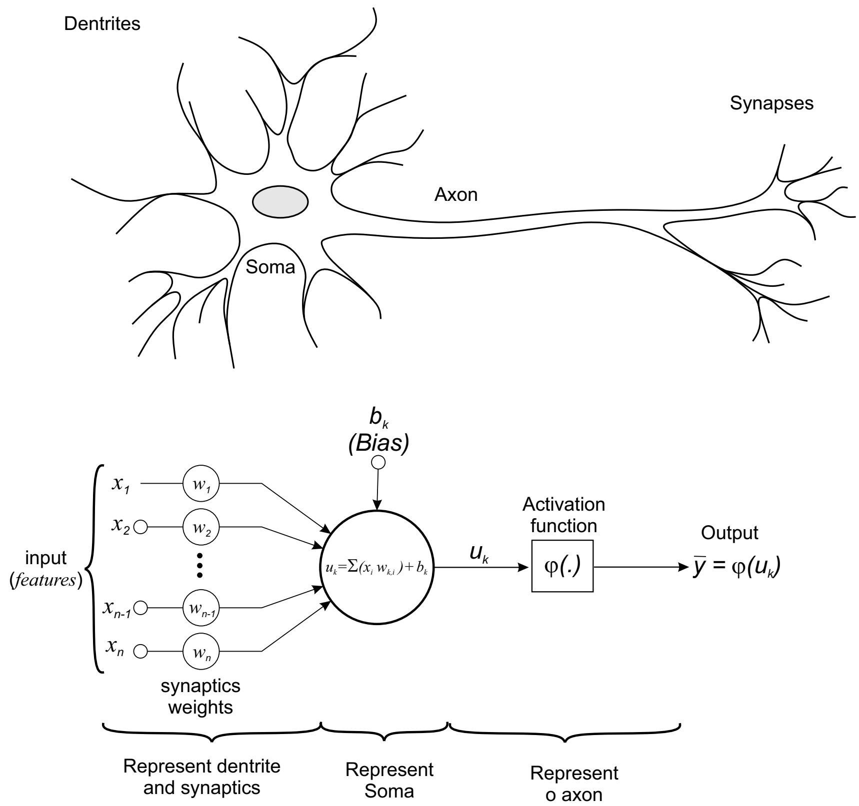


Figure 1. Idealization of the first artificial neuron proposed by

A neural network typically consists of multiple layers of artificial neurons, including an input layer, one or more hidden layers, and an output layer. The input layer receives the features representing the problem, while the output layer produces the network's predictions. Hidden layers, which vary in number and neuron density, process the information between these layers. In densely connected layers, every neuron in one layer is connected to all neurons in the next.

The Backpropagation algorithm, introduced by Rumelhart and colleagues in 1986, is a key training method for Multilayer Perceptrons (MLPs), a common type of ANN. While not the only training algorithm, Backpropagation is foundational and has influenced many subsequent algorithms used in training ANNs [9–12].

4 Methodology

As discussed in Sections 1 and 2, phase field models have a high capacity to represent quasi-brittle media, incurring substantial computational costs. To overcome this limitation, the authors are developing a methodology to create a constitutive model based on phase field theory, assisted by ML models. This methodology involves numerical simulations to generate a database correlating deformation states with corresponding phase fields (material damage). With this database, the goal is to train an ML model capable of predicting the phase field from a given state of deformation. The primary objective is to incorporate this model into a constitutive model based on phase field theory, aiming for a significant reduction in computational cost. As demonstrated in Section 2, the determination of the phase field requires a computationally expensive iterative process. To make this proposal feasible, the numerical models used for generating the training dataset must be realistic and duly validated in the literature.

This study presents the results of the first ML model trained to predict the phase field associated with a deformation state. For this purpose, training data from a numerical simulation that replicated the tensile test of a plate with asymmetric notches, as presented by Molnar and Gravouil (2017), were used. The experiment was simulated within the INSANE system, employing the Miehe constitutive model. The model setup, encompassing geometry, loading, and boundary conditions, is depicted in Figure. The material properties utilized in the simulation are as follows: Young's modulus $E = 21876.0\,\text{kN/mm}^2$, Poisson's ratio $\nu = 0.18$, critical energy release rate $G_c = 1.8 \times 10^{-2}\,\text{kN/mm}$, and length scale parameter $l_0 = 2.234\,\text{mm}$.

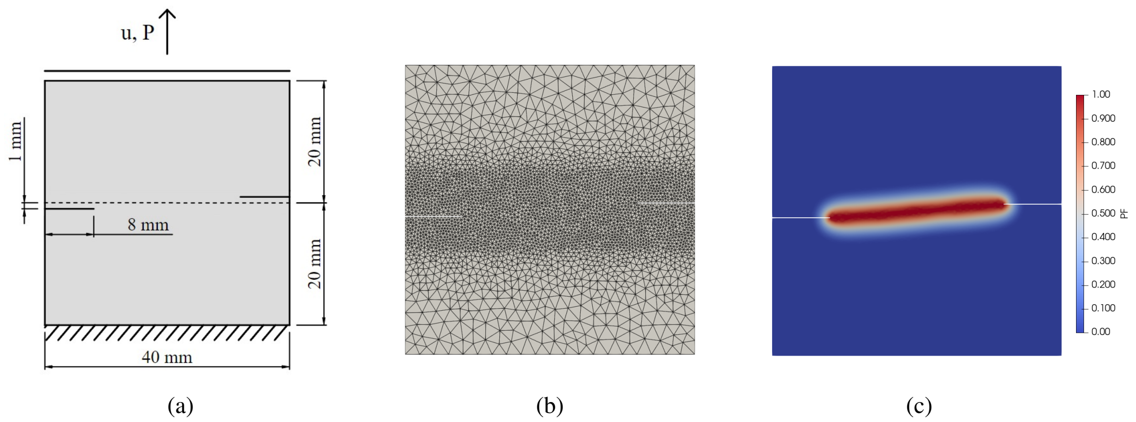
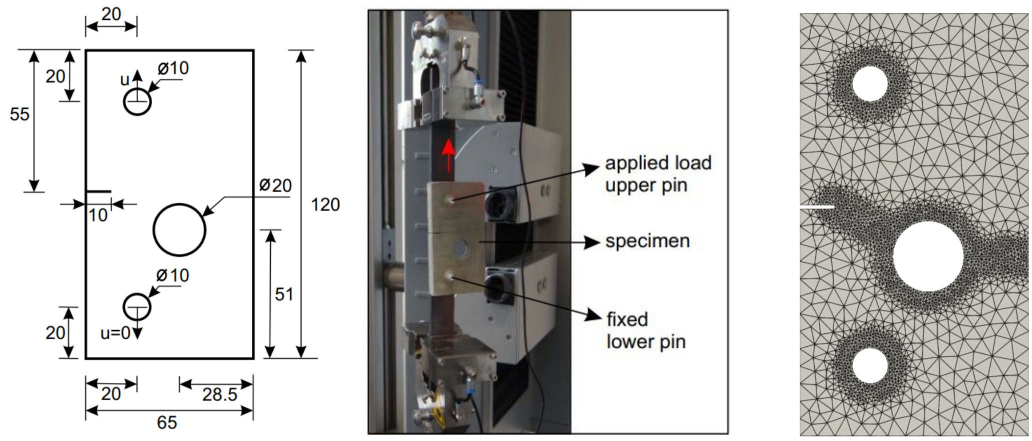


Figure 2. (a) asymmetric double notched tensile test; (b) mesh asymmetric double notched tensile test; (c) Phase field result the last step.

A multi-layer perceptron (MLP) model with three hidden layers, comprising 50, 150, and 50 neurons, respectively, was developed. The ReLU activation function was employed in the hidden layers, and the identity function was used in the output layer. The model was trained over 50 epochs using the Adam optimization algorithm with a learning rate of 0.05. Implementation was carried out using the Scikit-learn library. The adopted features include the strain state (the three components), the fracture driving force, and the historical driving force.

To validate the ML model, we attempted to simulate the damage observed in the tests studied by [13]. The geometry, boundary conditions, and experimental setup are depicted in Fig.3a and 3b. The specimen is a notched plate subjected to loading via a top pin and a fixed lower pin, featuring a hole offset from the center to induce mixed-mode fracture.



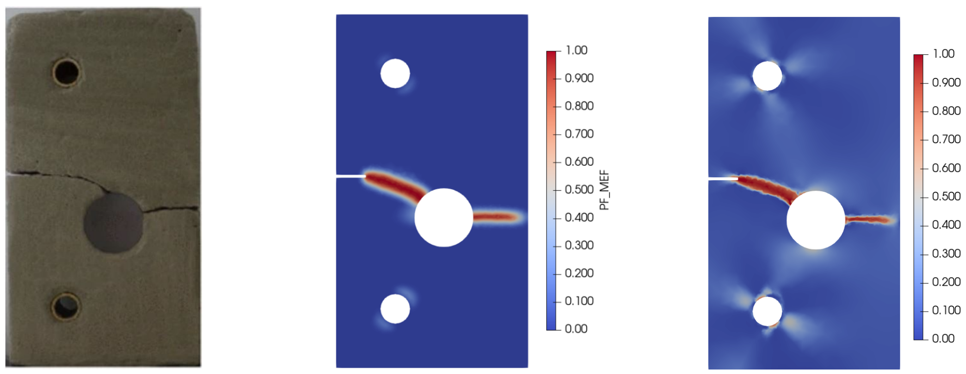
(a) (b) (c)

Figure 3. (a) Test dimensions notched plate with hole; (b) Test notched plate with hole; (c) Mesh Plate notched with hole.

For a comparison between the expected values from a numerical simulation by Finite Element Method (FEM), simulations were performed using fixed displacement increments of $\Delta u = 1 \times 10^{-4}$ mm throughout. The mesh consists of 4550 triangular elements with refinement in areas where cracking is anticipated. It is important to note that the same material properties used in the numerical simulation were employed to generate the training dataset.

5 Results

The computational results of validation test are presented in Figure 4.



(a) (b) (c)

Figure 4. (a) Experimental observation of fractured specimen; (b) Predicted crack path by MEF method; (c) The crack path by the ML method.

A photo of one of the fractured specimens is shown in Fig. 4a. A curved crack develops from the notch to the large hole, followed by a secondary straight crack extending from the hole to the sample edge.

The results displayed in Figure 4c. indicate that the ML model demonstrated good agreement with the values obtained both in numerical simulation and as indicated in the experimental results. Although some predictions of the ML model exhibited deviations compared to the values obtained via the Finite Element Method (FEM), these deviations are minor and expected, given that the model was trained with a limited database, encompassing a small diversity of deformation states. These preliminary results demonstrate the potential of the method, as even with reduced training data, the results adhere to expectations. It is noteworthy that these results are derived from the initial studies of the research group, and as the investigation progresses, more robust results are anticipated, which will be presented in future publications.

The experiment highlights that using ML models to predict phase field values from deformations is a highly promising approach. An adequately trained ML model can significantly reduce the computational cost of simulations utilizing constitutive models based on Phase Fields, as the ML model can eliminate the need to solve a system of equations in the problem-solving process.

6 Conclusion

The results obtained demonstrate that the ML model holds significant potential for predicting phase field values from deformations, despite some deviations observed relative to traditional methods such as FEM. These deviations, being of small magnitude and expected due to training with a limited database, do not compromise the validity of the method; rather, they underscore the need to expand the training data to enhance the model's accuracy. In conclusion, the use of ML models emerges as a promising alternative for reducing computational costs in complex simulations, such as those based on Phase Fields. As research progresses and models are refined with a more robust database, it is anticipated that these models will complement traditional methods, resulting in more efficient and accurate simulation processes.

References

[1] D. Broek. *Elementary engineering fracture mechanics*. Springer Science & Business Media, 2012.
[2] M. Stoffel, F. Bamer, and B. Markert. Artificial neural networks and intelligent finite elements in non-linear structural mechanics. *Thin-Walled Structures*, vol. 131, pp. 102–106, 2018.
[3] J. Ghaboussi, J. Garrett Jr, and X. Wu. Knowledge-based modeling of material behavior with neural networks. *Journal of engineering mechanics*, vol. 117, n. 1, pp. 132–153, 1991.
[4] J.-Y. Wu. A unified phase-field theory for the mechanics of damage and quasi-brittle failure. *Journal of the Mechanics and Physics of Solids*, vol. 103, pp. 72–99, 2017.
[5] J.-Y. Wu, V. P. Nguyen, C. T. Nguyen, D. Sutula, S. Sinaie, and S. P. Bordas. Phase-field modeling of fracture. *Advances in applied mechanics*, vol. 53, pp. 1–183, 2020.
[6] C. Miehe, F. Welschinger, and M. Hofacker. Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field fe implementations. *International journal for numerical methods in engineering*, vol. 83, n. 10, pp. 1273–1311, 2010a.
[7] C. Miehe, M. Hofacker, and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, vol. 199, n. 45-48, pp. 2765–2778, 2010b.
[8] H. M. Leão and others. A critical study on phase-field modelling of fracture, 2021.
[9] S. Haykin. *Neural networks: a comprehensive foundation*. Prentice Hall PTR, 1994.
[10] T. M. Mitchell and others. Machine learning, 1997.
[11] M. Awad and R. Khanna. *Machine Learning*, pp. 1–18. Apress, Berkeley, CA, 2015.
[12] I. Goodfellow, Y. Bengio, and A. Courville. *Deep learning*. MIT press, 2016.
[13] M. Ambati, T. Gerasimov, and L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Computational Mechanics*, vol. 55, pp. 383–405, 2015.