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DATA-DRIVEN PREDICTION OF STRESS RESPONSE FOR INELASTIC DISCRETE RVE

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Abstract: *Multiscale homogenization enables the calculation of the macroscopic stress response of a discrete periodic representative volume element (RVE) of a (quasi) brittle materials subjected to a macroscopic strain, accurately capturing their nonlinear inelastic behaviour. Wider application of the RVE as a microstructural constitutive model is hindered by its high computational cost. This paper investigates two data-driven approaches to approximate the effective response of the RVE. 3D RVE is loaded by uniaxial macroscopic strain and the response is approximated using polynomial chaos expansion (PCE) and neural networks. Both approaches incorporate a predefined history variable to incorporate the path dependency, while the second also tries to leverage recurrent neural networks (RNNs) to learn the load path dependency autonomously. The results show that the RNN can reach the same accuracy as a feed-forward network with a history variable given enough training data. The PCE provides good results but does not reach the precision of the other methods.*

Keywords: Homogenization, Softening, Recurrent neural network, Polynomial chaos expansion

1. Introduction

Discrete particle-based lattice models are highly effective for capturing the fracture behavior of quasi-brittle heterogeneous materials such as concrete (Schlangen and Garboczi, 1997). They accurately model the hardening, softening, and unloading-reloading regimes while depending on simple vector-based constitutive relations. However, their high computational cost makes them impractical for large-scale simulations of real-size structures. Their advantages can be exploited for practical applications by incorporating them as a micro or meso scale model in a multi-scale homogenization scheme (Rezakhani et al., 2017).

In this approach, meso-scale discrete model is used as a periodic Representative Volume Element (RVE) loaded by the macroscopic strain path, and the macroscopic history-dependent stress path is computed. While this method significantly reduces computational overhead compared to a full-scale discrete model, RVE computations remain demanding, driving the search for computationally efficient approximations of its macroscopic response.

Polynomial Chaos Expansion (PCE) and Neural Networks (NNs) are two data-driven approaches widely used in mechanics for their ability to approximate highly nonlinear functions while keeping computational costs manageable. NNs have proven to be able to predict path-dependent and time-dependent responses of nonlinear materials (Wang et al., 2024). This study aims to compare the effectiveness of these methods in predicting the effective stress of the RVE under uniaxial loading, capturing softening, hardening, and unloading-reloading behaviors.

PCE represents a spectral expansion of the original stochastic problem in a polynomial basis orthogonal with respect to input random variables (Wiener, 1938; Ghanem and Spanos, 1991; Blatman and Sudret, 2011). Recently, physics-informed PCE has been proposed by Novák et al. (2024). This extension of the standard PCE is designed to incorporate both stochastic and deterministic input variables. In this pilot study, we used the same framework, though no stochastic variables are present in the investigated example.

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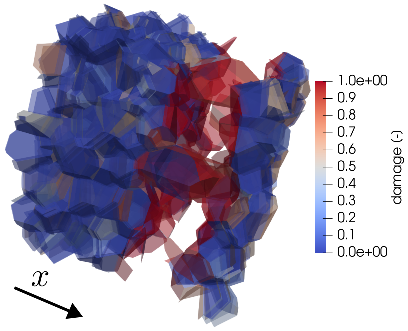

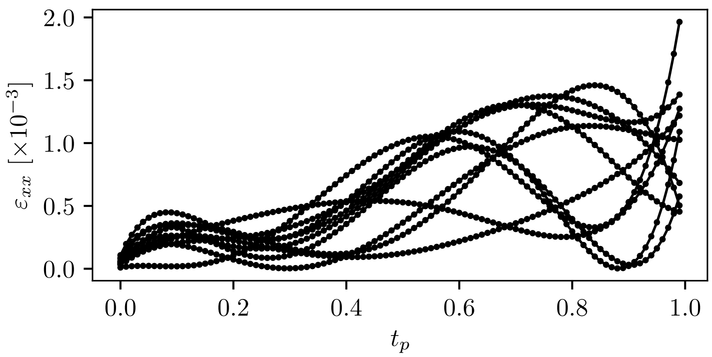

Fig. 1: Left-hand side: facets of RVE with crack perpendicular to the loading direction x; right-hand side: several random load paths $\varepsilon_{xx}(t_p)$

2. Homogenization of a discrete RVE

To obtain effective macroscopic behavior of a microstructure model the asymptotic expansion homogenization method can be employed. Here the material microstructure is explicitly modeled in a periodic RVE (Kouznetsova et al., 2002). In this work, the Lattice Discrete Particle Model (LDPM) (Cusatis et al., 2011) is used to represent a concrete material at meso-scale. The model consists of discrete particles connected with the constitutive relations prescribed on the contact facet of the particles. The constitutive relations allow damage initiation and accumulation at each facet, leading to inelastic hardening and post-peak softening behavior in the macroscopic response.

A lattice geometry is constructed inside a cube with a side length of 50 mm and periodic boundary conditions. The model is shown in Fig. 1. Given a macroscopic strain tensor $\varepsilon = \{\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{zz}, \varepsilon_{yz}, \varepsilon_{xz}, \varepsilon_{xy}\}$ a strain vector ϵ is applied to all RVE facets. After solving a set of non-linear balance equations the micro-scale displacements and rotations of the RVEs particles and tractions of the facets are obtained. Then the averaged effective macroscopic stress tensor $\sigma = \{\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{xz}, \sigma_{xy}\}$ can be calculated. The procedure is described in detail in (Eliáš and Cusatis, 2022).

3. Data-driven surrogates for inelastic material modeling

The data-driven prediction of the discrete RVE's macroscopic stress tensor is a similar problem to approximating history- and time-dependent material models, like elastoplasticity and elastoviscosity. In both cases, the information about the current load state—here the strain tensor ε—is insufficient to predict the current stress state accurately. The history dependence must be considered, namely in the unloading reloading states in the case of the fracture softening RVE. Various approaches exist to address the history or time dependence in constitutive modeling (Maia et al., 2023; Mendizabal et al., 2020; Wang et al., 2024). In this work, two methods are explored: manually defining a history variable that is supplied as additional input to the surrogate and autonomous discovery of the history dependence by recurrent neural networks (RNNs).

In the presented work, the RVEs are loaded by macroscopic uniaxial strain tensor $\varepsilon_u = \{\varepsilon_{xx}, 0, 0, 0, 0, 0\}$ with the ε_{xx} varying along a defined strain path. Only the σ_{xx} component of the macroscopic stress tensor is monitored reducing the problem to a prediction of input-output pairs $\varepsilon_{xx} : \sigma_{xx}$.

The loading paths of $\varepsilon_{xx}(t_p)$ varying with a pseudo-time t_p were generated as Lagrange interpolation polynomials interpolated through 6 points with $t_p = (0, 0.2, 0.4, 0.6, 0.8, 1.0)$ and $\varepsilon_{xx}(t_p) = i \cdot t_p \cdot 0.002$, where i is randomly picked from uniform distribution $U \sim (0, 1)$. Additionally, the condition that $\varepsilon_{xx}(t_p)$ is always non-negative was imposed by rejecting those random paths that violate it. In this manner, 1000 strain paths were generated, each sampled at uniformly spaced 100 t_p values between 0 and 1, resulting in 1000 sequences of 100 ε_{xx} values. Due to the imposed constraints, the ε_{xx} maximum value is about 0.002 and the RVE is always loaded in tension. However, the strain decreases and increases at various t_p values, resulting in unloading-reloading regimes. Several paths can be seen in Fig. 1. The RVE with lattice geometry generated in a cube of edge size 50 mm was loaded by the strain paths, resulting in 1000 corresponding σ_{xx} sequences.

3.1. Predefined history variable

Once the onset of the damage occurs, a decrease of ε_{xx} leads to states in which one ε_{xx} value corresponds to two σ_{xx} different values, depending whether the current state is in the loading or unloading-reloading phase. The influence of t_p history needs to be taken into account for correct σ_{xx} value prediction. For this a history variable can be manually defined. In this work, the maximum reached strain $\varepsilon_{xx}^{\max}(t_p)$ is used. This way, the input-output data pairs used for the training and inference phases read $(\varepsilon_{xx}(t_p), \varepsilon_{xx}^{\max}(t_p)) : \sigma_{xx}(t_p)$. These can be predicted by a standard feed-forward neural network (FFNN) or PCE. A simple network with one hidden layer with 512 neurons and ReLu activation was used.

3.2. Self-discovery of history dependence by RNN

For higher-dimensional generalization, defining the history variable is problematic. Recurrent neural networks can bypass this by self-discovering time dependencies in data sequences. In this work, the Gated recurrent unit (GRU) based neural network is used for its advantages over other RNN implementations, such as its low computational cost and effective handling of long-term dependencies (Tsantekidis et al., 2022). The network architecture comprises a GRU unit with 2 layers each with 100 hidden neurons followed by two linear layers with 128 neurons and ReLu activation. The sequence-to-sequence approach was used for GRU-NN training and inference. In practical applications, inference can be modified to export hidden-state tensors at each step alongside stress prediction, feeding them back with strain values in the next step. The method is described in detail in (Mendizabal et al., 2020).

4. Results

The 1000 sequences were divided into 800 training and 200 testing samples. The PCE and FFNN with the history variable as well as the GRU RNN were trained using varying sample sizes, ranging from 10 to all 800 available samples. The architecture and hyperparameters of all methods remained the same. Fig. 2 (left-hand side) shows the mean and maximum relative square error of the σ_{xx} predictions. For a low number of samples, the FFNN provides the best result. With an increasing number of samples, the accuracy of all models increases, with the GRU surpassing the FFNN's accuracy, which is to be expected as the GRU's architecture used has bigger representational power. Since the training subset is randomly selected, the error does not always decrease with more samples, highlighting the importance of careful data selection.

The results show that with enough training data, the RNN can autonomously discover the history dependence. The PCE model with an adaptive least-angle regression algorithm reaches a lower level of prediction

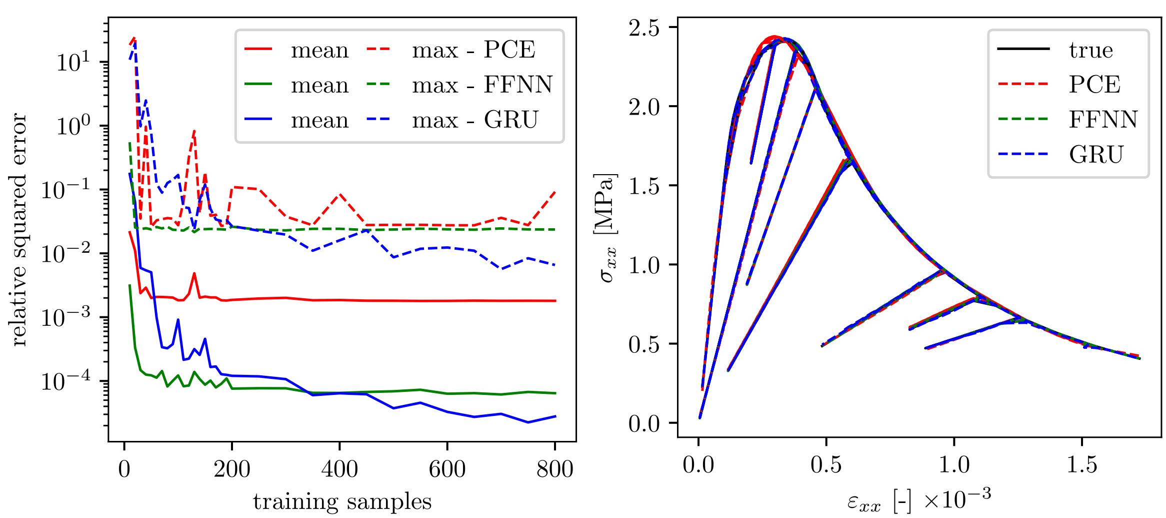

Fig. 2: Left-hand side: the mean and maximum squared error of prediction of PCE, FFNN, and GRU models trained on different numbers of samples; right-hand side: is a comparison of predicted macroscopic stress tensor σ_{xx} component for several strain paths from the testing set

accuracy, only surpassing the GRU at very low sample numbers. Overall, all of the methods succeed in capturing the behaviour in the unloading-reloading regimes. This can be seen in Fig. 2 (right-hand side). It shows the response prediction to several loading paths from the testing samples. The constant t_p sampling step results in nonconstant $\varepsilon_{xx}(t_p)$ step, which might be a complication for RNNs (Wang et al., 2024). In the presented case, the GRU network handles this well.

5. Conclusions

By manually specifying a history variable and using it as additional input information for (i) a feed-forward neural network or (ii) a polynomial chaos expansion model, a data-driven approximation of the macroscopic response of an inelastic discrete RVE to a non-monotonic uniaxial macroscopic strain loading was constructed. The predictions of such surrogate models can closely match the correct results computed by the LDPM simulation. However, the manual identification of the history variable presents a challenge for higher-dimensional problems and also represents a subjective choice rather than an underlying physical principle. In contrast, (iii) the recurrent neural networks discover the history dependencies in sequence data automatically and show similar accuracy to the FFNN providing the training dataset is large enough. While this work includes predictions only for one component of the macroscopic stress tensor, they show a path for predicting the full stress tensor. Furthermore, while the presented models are purely data-driven, physical constraints can be incorporated potentially leading to robust metamodels of discrete RVEs macroscopic response.

Acknowledgments

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