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A recurrent machine learning structure for few-shot constitutive model optimization: Application to Geomechanics

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Abstract: In practice, a purely data-driven approach for building a generic 2D or 3D stress-strain relationship without introducing physical constraints (assumptions) is rather difficult to be embedded in boundary value problems' (BVP) calculations, as the strain paths may be highly variable. With machine learning (ML)-based constitutive models, it is not the 'best' predictions that lead to the success of the computation, but, conversely, rather the worst predictions that often lead to the failure of the computation. To address the problem of insufficient generalization, the material 'cell' is proposed with the assumptions of the so-called Critical-State-Unified-Hardening (CSUH) [1] model working as the physics constrains in the PyTorch framework. Based on strain-stress sequence data from explicit FEM-DEM (exFEM-DEM) simulations, the parameters of a material 'cell' were optimized with the Adam algorithm and error backpropagation. Eight sets of ($\epsilon_{ij} - \sigma_{ij}$) sequences in one exFEM-DEM BVP simulation are used for model training, and two different BVP simulations are utilised to assess the optimized model.

Keywords: Machine Learning, Constitutive Modeling, Granular Materials, FEM-DEM, Optimization

1 Introduction

With the advent of ML, especially neural networks ($\mathcal{NN}$), recent research focuses on rebuilding constitutive models (i.e. mapping $\epsilon_{ij} \rightarrow \sigma_{ij}$) via ML methods. However, it is impossible to cover the entire $(\epsilon_{ij}, \mathcal{I})$-space without simplifying assumptions. Such models are known to generalize poorly, and high prediction errors can cause BVP calculations to become nonsensical and/or crash. Most studies focus on improving the best prediction accuracy. But, unfortunately, there is rarely a proper method to guarantee the ML model's poorest performance is above some acceptable threshold. Here we introduce the CSUH model as the physical constraint for the ML model to improve the generalization.

2 Methodology

All constitutive models can generally be represented as

$$\mathcal{I} = \mathcal{M}\left(\dot{\epsilon}_{ij}, \mathcal{I}_0\right) \ , \tag{1}$$

where $\mathcal{I}$ is the set of state variables, including but not limited to the stress tensor σ_{ij}, $\mathcal{I}_0$ is the initial state before the strain increment $\dot{\epsilon}_{ij}$, and $\mathcal{M}$ is the material 'cell' employed in the recurrent structure, as is shown in Fig. 1(a). This equation is very similar to the recurrent neural network format $h = \mathrm{RNNCell}(x, h_0)$, where $\mathrm{RNNCell}$ is a network cell, x is the input, h is the hidden state (Fig. 1(b)). This implies that the training process of $\mathcal{M}$ is very similar to the training process of a recurrent neural network given the CSUH-assumptions, i.e. $\mathcal{M} \triangleq$ RNNCell | CSUH formulas.

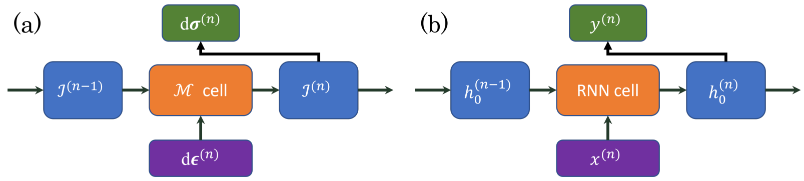

Figure 1: The comparison of the architecture of the material cell and a RNN cell-based ML method

3 Conclusions

The comparison of biaxial compression simulations is displayed in Fig. 2. The curves of maximum a mean the largest value among all of the accelerations of the nodes.

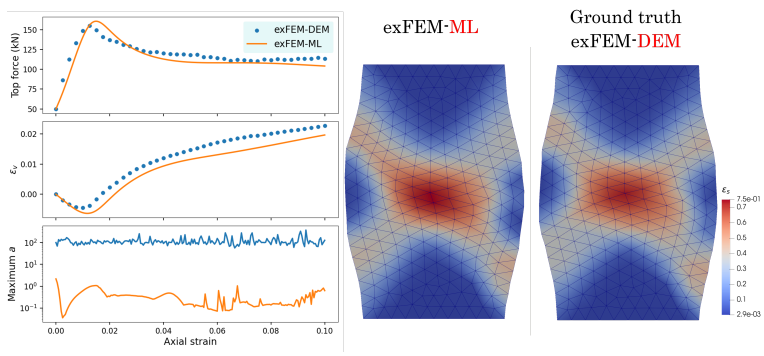

Figure 2: Comparison of the biaxial compression in exFEM-DEM and exFEM-ML

The physics-constrained $\mathcal{M}$-cell trained on the datasets collected from the exFEM-DEM simulations can be used to properly reproduce the exFEM-DEM simulation under various circumstances. The physics constraints are effectively implemented by recognizing the state equations with the training process of a recurrent structure and improving the model's generalization [2]. Recurrent neural networks are known to induce a corresponding Gaussian process [3], posing a possible route for incorporating further prior knowledge on the underlying PDE [4].

References

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