Data-driven Discrete-continuum Method for Partially Saturated Micro-polar Porous Media

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ABSTRACT

We present hybrid data-driven approach to model multi-physical process in fluid-infiltrating porous media across length scales. Unlike single-physical problems where data-driven model is often used as a replacement of the solid constitutive law, a hydro-mechanical problem often leads to more complex hierarchical relations among physical quantities which in return complicate the design of the data-driven solver. When artificial neural network is used, additional issues may arise when constraints and rules, such as material frame indifference, cannot be explicitly enforced without artificially expanding the training dataset. In this work, we introduce a component-based strategy in which a multiphysical problem is viewed as a directed graph, a network consisting of inter-connected vertices representing physical quantities. This strategy enables modelers to couple data-driven model with conventional mathematical expression methods by considering different hierarchical relations among data. Depending on the availability of data, hybridization of data-driven and mathematical models may take different forms. To enforce material frame indifference efficiently, we employ spectral decomposition to handle the invariant and spin terms via Lie algebra.

1 Introduction

The emergence and growing importance of machine learning and data science have altered the way prediction, forecasting and analysis are done across engineering disciplines. In solid mechanics, previous work on data-driven modeling applied in computational mechanics has placed a significant emphasis on the single-physics solid mechanics problems, where the information flow or the hierarchy of the computational model is simply a sequence as illustrated in Figure 1. In this small subset of engineering problems, the relationship between strain and displacement, and between the balance of linear momentum and stress are considered ”definition”, while the relationship between the stress and strain (material constitutive law) is considered the most ad-hoc portion of the model. These material laws are therefore replaced by data-driven constitutive laws, obtained either through supervised machine learning (cf. Ghaboussi et al. [1], Lefik et al. [6]) or, recently, through constrained variational principles (cf. Kirchdoerfer and Ortiz [3]).

Figure 1. Hierarchy of single-physics solid mechanics problem. Black arrow represents a definition or a "universal principle"; red arrow represents either a phenomenological relation or an operator that is defined not based on first principles.

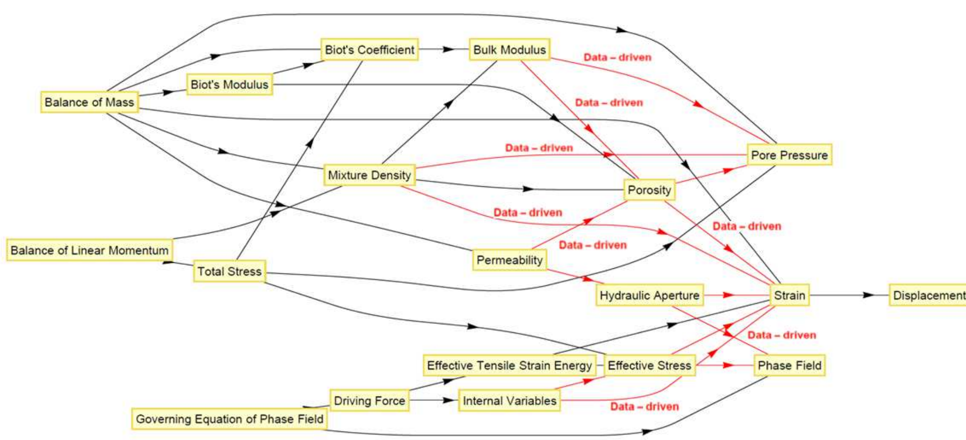


Figure 2. Hierarchy of a phase field or eigen-fracture hydraulic fracture model of fully saturated porous media. Black arrow represents a definition or a "universal principle"; red arrow represents either a phenomenological relation or an operator that is defined not based on first principles (cf. Wang and Sun [16]).

The underlying philosophy of this treatment is due to the assumptions that (1) phenomenological law is always the most ad-hoc part of the numerical boundary value problem mired in empiricism and arbitrariness and (2) there exists a clean and binary cut between definitive governing equations and ad-hoc constitutive laws. These assumptions, nevertheless, are invalid for multi-physical problems in which the complex multi-physical coupling mechanisms are interrelated and therefore hard to be replaced by a single data-driven model. The lack of clear cut between phenomenological models and robust principles are further complicated by many subtle and hard-to-detect coupling mechanisms that may affect the macroscopic outcomes in a variety of significance across spatial and temporal scales, as shown in the example illustrated in Figure 2. The objective of this work is to create an adaptive graph-based framework to introduce data-driven models for multi-physical poromechanics problems, with special emphasis on the prediction of path-dependent behaviors. Our specific contributions are:

- **Graph-based hybrid meta-modeling:** We introduce a meta-modeling approach that instills different forms of knowledge as building blocks for complex multi-physical systems in a directed graph. This directed graph represents the hierarchy of information processed in a computational model that utilizes a combination of classical and data-driven models. The relations among physical quantities are considered as edges that link those building blocks together to form a computational model.

- **Adaptability:** Through a series of forward and backward propagation, the configuration of the directed graph may evolve until it yields the optimal prediction ability measured by the objective function that compares the forward predictions with the available data. In this work, the machine learning process is not only used to generate the data-driven constitutive laws, but is also used to generate the optimal directed graph and select proper edges (data-driven laws obtained, phenomenological laws, hierarchical RVE models) across different length scales.

- **Extended Database:** We employ data-fusion process to combine experimental data of different scales (e.g. stress-strain curve, micro-CT images, digital image correlation) and micro-mechanical simulations calibrated from experimental data to enhance forward prediction capacity [7, 8, 14, 15, 17]. In the case where macroscopic experimental data are either limited or do not provide sufficient constraints for training neural networks (e.g. using tensile test results for torsion predictions), micro-mechanical models are first calibrated and then extend the training set via virtual experiments.

2 Supervised Learning with Constraints

For multi-physical poromechanics problems, the computer models can be generated from a mixture of first-principle constraints supplemented by constitutive laws in a complex hierarchical coupling relations [11, 12, 13]. While some of the rules or constraints such as balance of linear momentum can be enforced explicitly in the computational framework, other important rules such as thermodynamic laws and material indifference are often not obeyed by a data-driven model as pointed out in Lefik and Schrefler [5]. For instance, the previous data-driven models may not obey the principle of objectivity due to the fact that components of the second-order tensors written in terms of a particular basis (e.g. stress, strain, permeability) are mistakenly treated as individual inputs by the artificial neural network. As an example of the model selection process, we consider two different configurations of the directed graph and use the machine learning to evolve the directed graph until the principle of objectivity is fulfilled. In the original case, we use the classical artificial neural network model in Ghaboussi et al. [1], Lefik and Schrefler [5] where strain components are used as input and stress components as output. In the second case, we modify the direct graph such that we use the invariants and parameterized rotations as vertices to form the directed graph. For instance, the spectral decomposition is applied on strain and stress tensors, and the the principal values and principal directions are used to preserve the tensor properties.

$$\boldsymbol{\sigma} = \sum_{A=1}^{3} \sigma_A \boldsymbol{n}_{\sigma}^{(A)} \otimes \boldsymbol{n}_{\sigma}^{(A)}, \quad \boldsymbol{\epsilon} = \sum_{A=1}^{3} \epsilon_A \boldsymbol{n}_{\epsilon}^{(A)} \otimes \boldsymbol{n}_{\epsilon}^{(A)} \tag{1}$$

where σ_A and $\boldsymbol{n}_{\sigma}^{(A)}$ are eigenvalues and eigenvectors of the stress tensor $\boldsymbol{\sigma}$, respectively. ϵ_A and $\boldsymbol{n}_{\epsilon}^{(A)}$ are eigenvalues and eigenvectors of the strain tensor $\boldsymbol{\epsilon}$, respectively. The data-driven model computes the stress and strain using an incremental update. Given the change in principal strains and the change of Euler angles, the neural network, after the proper supervised machine learning procedure, predicts the incremental changes of principal stresses and the infinitesimal rotation of principal stress direction at the tangent space of the special orthogonal group SO(3) where the rotation tensor $\boldsymbol{R}$ belongs. Thus the rotation tensors are parameterized using the following expansion [4, 9]. In the incremental form, the rotation matrix at time t_n is updated by

$$\boldsymbol{R} = \exp[\tilde{\boldsymbol{\Psi}}] = \sum_{k=0}^{\infty} \frac{\tilde{\boldsymbol{\Psi}}^k}{k!} \; ; \; \boldsymbol{R}_n = \boldsymbol{R}_{n-1} \exp[\Delta \tilde{\boldsymbol{\Psi}}_n] \tag{2}$$

where $\tilde{\boldsymbol{\Psi}}$ is a skew-symmetric matrix that is defined by three components $\tilde{\Psi}_{23}$, $\tilde{\Psi}_{13}$, $\tilde{\Psi}_{12}$. As the data of the input and output of the neural network are both stored in coordinate-free form, the data-driven model is inherently objective. In the following sections, we showcase a number of numerical examples where this model selection is used to create hybrid models to predict path-dependent behaviors (e.g. elasto-plastic responses, fracture) of fluid-infiltrating porous media.

2.1 Data-driven Eigen-fracture Model

In this study, a material element is allowed to be simultaneously in crack set C and compaction band CB in the proposed model, i.e., $C \cap CB \neq \emptyset$. A compaction band zone could become crack, as observed in borehole breakout experiments that anti-dilatant failure zone occurs at the tip of fracture-like breakout in sandstone with high porosity. The regularized energy-dissipation functional in the context of fluid-saturated brittle porous media reads (cf. Wang and Sun [16]),

$$\begin{aligned} F_{(\epsilon_C,\epsilon_{CB})}(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^*,p^f,t) = & \int_\Omega \frac{1}{2}(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^*) : \boldsymbol{C}^e : (\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}^*) dV - \int_{\Gamma_t} \bar{\boldsymbol{T}} \cdot \boldsymbol{u} dS \\ & + \int_\Omega \frac{M}{2}[(1-b)\varepsilon_v - \frac{p^f}{M}]^2 dV + \int_0^t [\int_\Omega \bar{s} p^f dV - \int_{\Gamma_q} \bar{\boldsymbol{q}} \cdot p^f \boldsymbol{dS}] d\tau \\ & + G_C \frac{|C_{\epsilon_C}|}{2\epsilon_C} + G_{CB} \frac{|C_{\epsilon_{CB}}|}{2\epsilon_{CB}} + \mathcal{D}_f(\boldsymbol{\varepsilon},\boldsymbol{\varepsilon}^*,p^f). \end{aligned} \tag{3}$$

where Γ_t is the boundary on which the traction $\bar{\boldsymbol{T}}$ is applied, Γ_q is the boundary on which the flux $\bar{\boldsymbol{q}}$ is prescribed, and $\bar{s}$ is the source flux. Here, we introduce the data-driven algorithm for the last three energy functionals that represent the energy required to create crack surface, compaction band surface and the fluid dissipation energy. Instead of providing explicit mathematical expressions for these three energy functional, they are determined from the experimental data provided to us.

3 Numerical Example 1: Data-driven FEM model for shear band behaviors

We employ a hybrid FEM-ANN (Artificial Neural Network) coupled framework to model strong discontinuity interface as illustrated in 3. The data-driven constitutive law is used in the assumed strain elements to embed strong discontinuity in finite elements. In this idealized system, the overall macroscopic responses are often dominated by the frictional responses of the interfaces. Yet, proposing a constitutive law that adequately incorporates the complex mechanisms, such as wearing, particle re-arrangements, fragmentation and fracturing of grains, and the effect of moisture and pore pressure remains a difficult task. Here our goal is to test the capability of the data-driven model by using experimental data as the training set to predict the results of a biaxial compression test of an unsaturated specimen. While a subset of stress-strain, fluid pressure and water retention curve of data is used as the training set, the forward prediction is compared against experimental data that is not included in the calibration process such that an assessment on the accuracy of the predictions can be made. Micro-scale information of unsaturated porous media are also available from micro-CT technology [2, 17]. Here, we will consider a data-fusion strategy in which experimental data is used to construct a small-scale discrete element model. This model is in return used as a surrogate to extend database so that the original data can be used to predict deformation modes that are not directly observed from the original database.

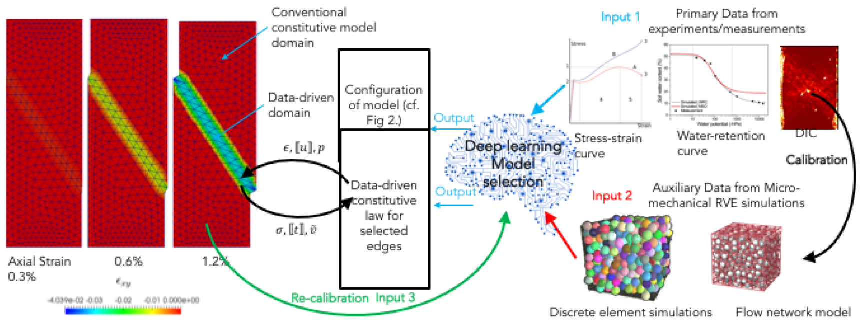
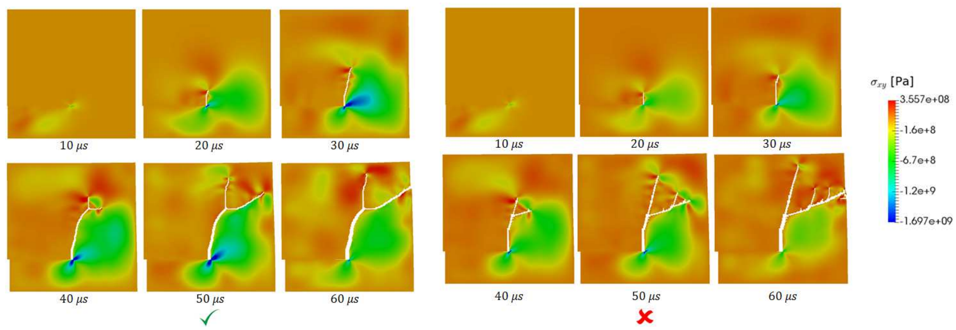


Figure 3. Machine learning in meta-modeling. The experimental data consists of macroscopic data and micro-scale information [2]. Micro-mechanical models are calibrated and additional simulations are performed to extend the data set. The ensemble of data is divided into training data and verification data. The configuration of directed graph of model is determined by supervised machine learning. Predictions are made by the current model and they are compared against the verification data.

4 Numerical Example 2: Data-driven nonlocal eigen-fracture model for hydraulic fracture problems

This example aims at illustrating the application of machine learning in developing robust data-driven model for modeling fractures. The starting point is a non-local eigen-erosion model [10, 16]. While there exist multiple possibilities of introducing artificial neural networks in replacing the phenomenological relations. Among the alternatives, a data-driven model based on strain energy and its gradient, and another crack-tracking model based on principal stresses are compared. The training data of the neural networks in each models consist of simulation results from eigen-erosion model and may be extended by experimental data. According to the simulation results on dynamic fracture compared in Fig. 4, the nonlocal strain energy based data-driven model is more accurate and robust, and thus is superior than the principal stress model. Machine learning techniques can be introduced to provide help in deciding the best data-driven model design among all possibilities, if sufficient data can be used as training set for model selection. Note that the metrics of the model selected is not limited to quantitative measurements of error, but also constraints. For instance, in the case of the Kalthoff-Winkler tests, one may simply filter out all configurations that lead to non-physical branching as shown in Figure 4(b).



(a) nonlocal energy based fracture model **(b)** stress-invariant based fracture model

Figure 4. Comparison of strain energy and principal stress based data-driven fracture models. The results consist of crack-path evolution in Kalthoff-Winkler test with impact velocity of 50 m/s.

5 Conclusion

We employ a data-fusion process to combine experimental data and micro-mechanical simulations as training set. By providing a new methodology that systematically compares, analyzes and produces data-driven computational models, the research will provide a thought-provoking way not just to deepen understanding of multi-physics processes, but an effective way to compare forward prediction power of data-driven and classical models.

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