Integrated Machine Learning and Numerical Modeling for Multiscale Analyses of Coupled Processes in Geosystems

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Abstract. Understanding the formation and evolution of geosystems as a result of coupled processes from microscale structure to core-scale samples is critically important for predicting meso- to macro-scale multi-physical behavior, thus providing effective control of subsurface energy recovery and storage activities. In this paper, we present integrated machine learning and numerical modeling approaches that we have developed to understand fundamental geosystem behavior, to predict their mesoscale behavior, and to analyze large-scale performance of such geosystems subject to multi-physical couplings. First of all, we will present a high-level summary of our developed modelling capabilities based on the numerical manifold method [1]. Then we will present theoretical comparison between machine learning and numerical modeling [2]. Using current machine learning techniques on image recognition, we make flexible use of these techniques to integrate experimental data with numerical modeling. By using a convolutional neural network, U-net, we show results of fractures recognized from rock images [3]. By using a machine learning approach referred to as neural style transfer, we will show automatic and efficient mesh generation and optimization from rock images [2]. With a microscale model for capturing dynamic contacts between geomaterials with arbitrary shapes of grains and interfaces [4], we extend this model by accounting for hydro-mechanical couplings and realistic geometry using digital representations of rocks [1]. Using different examples, we show the unique capabilities to simulate coupled processes in fractures at different scales and microscale granular systems, while applying differing physical laws, coupling priorities, and solutions for evolving geometry at multiple scales [5]. We will conclude with perspectives on solutions to bridge the gaps between fundamental and applied geosciences by integrating machine learning and numerical modeling.

1. Introduction
Geosystems are unique because they are stressed, fluid-filled, and heated. Materials within the Earth system consist of a variety of minerals and structures that respond differently to coupled processes, and these minerals form porous, fractured, granular systems at distinct scales. Understanding the formation and evolution of these structures as a result of coupled processes from microscale structure to core-scale samples is critically important for predicting meso- to macro-scale multi-physical geosystem behavior, thus providing effective control of subsurface energy recovery and storage activities such as hydrocarbon recovery, geothermal energy, and nuclear waste disposal.

In this paper, we present integrated machine learning and numerical modelling for analyzing multiscale coupled processes in geosystems, including porous, fractured and granular systems. In Section 2, we first briefly show a high-level summary of our developed modelling capabilities. Then
we compare and discuss the similarities and opportunities between machine learning and numerical modelling. In Section 3, we show a number of examples including machine learning applications in image recognition and mesh optimization, multiscale coupled processes modelling of fractures at different scales, and microscale modelling of granular systems for providing understanding of phenomena at larger scales. In Section 4, we reach the conclusions.

2. Numerical Modeling and Machine Learning for Analyzing Multiscale Coupled Processes

2.1. Multiscale Modeling of Coupled Processes in Geosystems

Previously, we have developed comprehensive model capabilities to simulate coupled processes in porous, fractured and granular systems at different scales. The modeling capabilities involve different governing equations, constitutive relationships, HM couplings, and approaches for addressing intersections and shearing of interfaces at different scales [1,5].

![Figure 1. Overview of the multi-scale coupled processes models based on the NMM [1].](image)

A high-level summary of the modeling capabilities is shown in Figure 1. From the left to the right, we show the developing steps from the continuous to discontinuous media [1,2,4-8]. Radiating from the direct coupling of conservation of solid momentum and conservation of fluid mass, discontinuum mechanics with calculation of dynamic contacts is applied for the two discontinuous scales, i.e., the discrete fracture networks and microscale asperities and grains. In addition, different and indirect couplings apply with different constitutive behavior and physical laws.

2.2. Machine Learning and Its Relationship with Numerical Modeling

Machine learning (ML) has been an increasingly popular research approach that has been applied in disciplines ranging from social to natural sciences, geosciences and engineering in recent years. Based on a theoretical comparison, a number of similarities were found between ML and numerical modeling if similar interpolation structure are used [2]. The compared items are listed in Table 1.

The major difference is that in ML the weighting factors \( \theta \) need to be derived while \( x \) are given. In numerical modeling, \( x \) needs to be solved and weight factors are typically constructed by shape functions of numerical grids. If the physical meanings of \( x \) and \( \theta \) are swapped, ML can be identical to numerical modeling in terms of constructing the hypothesis, cost function and minimizing the cost function to derive the \( \theta \). Because of these similarities, computer software that was designed for ML and numerical modeling may be shared.

Whether ML or deep learning can be applied widely for physical analysis of geosciences depends on two important questions:

1. If there is a lack of data, can machine learning perform like a numerical model?
2. What can machine learning do to bridge the fields of experiments and numerical modeling?
The similarity between machine learning and numerical modeling derived in this section provides the theoretical demonstration that machine learning can function like a numerical model. However, building on 60 years of experience in the development of numerical models for analyzing physics across temporal and spatial scales, numerical model supervised machine learning could be a promising pathway to integrate the advantages of both.

**Table 1.** Theoretical comparison between numerical modeling and machine learning [2].

| Numerical modeling | Machine learning |
|--------------------|------------------|
| Linear interpolation: \( \varphi = \mathbf{w}^T \mathbf{\phi} \) | Linear hypothesis: \( h = \mathbf{\theta}^T \mathbf{x} \) |
| Higher-order interpolation: \( \mathbf{f} = \mathbf{A}(\mathbf{w}^T) \mathbf{L}(\varphi) \) | Neural network: \( \mathbf{h} = g(\mathbf{\theta}^T \mathbf{a}) \), … \( \mathbf{a} = \mathbf{\theta}^T \mathbf{x} \) |
| Total potential energy: \( \Pi = \beta [\mathbf{D}(\mathbf{\phi})] \) | Cost function: \( j = \gamma [f(h - y)] \) |
| Penalty method for boundary constraints: \( \Pi_{bc} = \frac{1}{2} \eta (\varphi - \bar{\varphi})^T (\varphi - \bar{\varphi}) \) | Regularization: \( j_{reg} = \lambda \mathbf{\theta}^T \mathbf{\theta} \) |
| Iteration (e.g., Newton-Raphson iteration): \( \varphi_j^{k+1} = \varphi_j^k - \frac{1}{k} R^k \mathbf{\phi_j}^k \frac{\partial R^k}{\partial \varphi_j^k} \) | Gradient descent: \( \mathbf{\theta}_j^{k+1} = \mathbf{\theta}_j^k - \alpha \frac{\partial j}{\partial \mathbf{\theta}_j^k} \) |

Between experiments and numerical modeling, there are at least two challenging steps: (1) image processing may require considerable effort when attempted using traditional approaches, and (2) determination of physical properties can be difficult. These challenges can be overcome with the help of machine learning. In addition, machine learning can be easily applied to predict statistical trends and to classify patterns. With the development of convolutional neural networks (CNN), ML has been increasingly used in the fields of image processing, but prediction of the dynamic evolution of geometry can be challenging. Thus, ML supervised by experiments and numerical modeling may be a promising approach if there are sufficient datasets.

3. Applications

3.1. Image Recognition and Mesh Optimization by Using Machine Learning

3.1.1. Image Recognition with a Convolutional Neural Network In the first example, we applied a CNN model to recognize fractures from the image at the core scale [3]. We trained the CNN model using 60 images containing different crack patterns and validated the model using other 15 images. All the images were resized to 600 × 600 pixels and fed to the neural network in batches with each batch of three images. The model was trained on RGB and Grayscale images with the estimation of average loss for every 50 epochs. As we validated the trained CNN model on the validation set, the best inference obtained for an RGB input image based on prediction on the grayscale model with provided ground truth is shown in Figure 2, where ground truth refers to the accuracy of the training set’s classification for CNN.

To evaluate our model, we used the dice score or mean Intersection over Union (IoU) as a performance metric. The dice score obtained for the prediction result is 72.54% based on the model's inference and the predicted mask.
3.1.2. Mesh Generation and Optimization with Neural Style Transfer

Then we applied a ML approach named neural style transfer (NST) to generate and optimize mesh for an image of rock containing several dominant and rough fractures [2]. We tried two different densities of triangles as the style. Figure 3 shows one of the results. As can be noted, the NST learned the boundaries of rock and fractures from the rock image and applied the triangular styles to the images that were recognized. The sizes of triangles in the generated mesh are the same as in the style image. With the size and shape of the triangles kept in the generated image, the machine rearranged the orientations of the triangles to accommodate the fractures and rock matrix.

![Figure 3. NST generated mesh for rough fractures with denser meshes and thicker mesh lines.](image)

From this example we show that because the generation is automatic despite the complexity of the geometric features, this new NST technique can potentially save a great deal of effort for mesh generation and optimization while achieving a good balance between the density of the mesh and the presentation of the geometric features.

3.2. Modeling Fractures at Multiple Scales

3.2.1. Closure of Fractures Impacted by Geometry and Distribution of Asperities

In this example, we calculated mechanical compression of rough fractures with explicit representation of the asperities with later confinement [4]. Here we show two cases with different profiles of asperity geometry and distribution: (1) evenly distributed smaller asperities, and (2) non-evenly distributed asperities with two major asperities. The sizes of the domains are the same: 10 mm × 5 mm. The Young’s modulus is 4GPa and the Poisson ratio is 0.3. The Young’s modulus of the two columns on the left and right sides is 40GPa.

Figure 4 shows vertical (left) and shear (right) stresses. When reaching equilibrium, the average value of closure for case (1) is 0.8mm and for case (2) is 0.5mm. We observed that both the vertical stress and the shear stress concentrate at the contacting areas evenly through the fracture for case (1), whereas for case (2) the dominant contacting asperities govern the closure as well as stress concentration.
Figure 4. Calculated normal (left) and shear (right) stresses (Pa) of a compressed fracture when reaching equilibrium.

3.2.2. Modeling Discrete Rough Fractures with Continuous and Discontinuous Models In this example, we used an image of a network of rough fractures and applied two different models to simulate its mechanical behavior induced by compaction [1]. These two models are: (1) a continuous model where the fractures are represented as porous and deformable zones with a softer material than the rock matrix, and (2) a discontinuous model where the fractures are represented as discontinuous rough surfaces. In both models, the asperities are explicitly represented. The model domain for this example is 10m × 8m. For each model, a vertical loading of 0.42 MPa is applied on the top. The other three boundaries are fixed. For both models, the Young’s modulus is set to 4GPa and the Poisson’s ratio is 0.3. In the continuous model, the solid material within the fractures surfaces is assumed to have a Young’s modulus of 4 MPa, which is three orders of magnitude lower than the surrounding rock matrix. The Poisson’s ratio is the same as the rock matrix. In the discontinuous model, the loading and confinement columns have a Young’s modulus of 4GPa. The fractures have a friction angle of 30°.

![Image of stress distribution](image)

Figure 5. Calculated vertical stress (Unit: Pa) with the continuous model (left) and with the discontinuous rough interface model (right).

The vertical stress calculated by the two different models is shown in Figure 5. From this example we concluded that because the discontinuous model captures the dynamical changes of contacts with large displacements on the right and the stress re-distribution as a result of the dynamic changes of contacts, the results appear to be quite different than those obtained by the continuous model. We show that when rough fractures are not filled with minerals and when a number of rough fractures form a blocky system, dynamic contacts play an important role for the geometric, multi-physical evolution of the system.

3.2.3. Consolidation Impacted by a Discrete Fracture Network We calculated consolidation of a 100×100 m porous domain containing 25 arbitrary fractures with a 10KPa traction applied on the top surface which is free to drain [5]. The other three boundaries are impermeable. The initial hydraulic head is 100 m over the entire domain. For the rock matrix, the Young’s modulus is 4MPa, Poisson’s ratio is 0, and the permeability coefficient is 2.5×10⁻⁸ m/s; For the discrete fractures, the initial mechanical aperture is 0, the shear stiffness and normal stiffness are both 1×10⁶ Pa/m, the ratio of
hydraulic aperture to mechanical aperture is 0.5, and the residual aperture is 10µm. This vertical compaction occurred gradually while water is gradually drained from the fully saturated porous fractured media through the top surface. Figure 6 shows the results of vertical displacement (left) and the pore pressure (right). We observe discontinuities associated with some of the fractures in the displacement and/or pore pressure field(s), which may be associated with opening and shearing of these fractures. We also observe heterogeneous distribution of displacement and pressure in Figure 6, indicating complex changing hydraulic properties as well as the strong hydromechanical pore-volume coupling occurred.

Figure 6. Simulated vertical displacement (m) and pore pressure (Pa).

3.3. Microscale Modeling of Geomaterials in Sedimentary Rocks

3.3.1. Modeling a Grain Pack with a Cataclastic Deformation Zone In this example, we investigated the compaction of a sandstone with a cataclastic deformation zone with our microscale model [1]. In our model, the 5mm × 8 mm domain is represented with three different materials: grains with a Young’s modulus of 4GPa and a Poisson’s ratio of 0.2, fragmented grains with a Young’s modulus of 0.2 GPa and a Poisson’s ratio of 0.2, and a cataclastic deformation zone with a Young’s modulus of 0.2 GPa and a Poisson’s ratio of 0.2. On the left, right and bottom boundaries, the sample is confined. On the top, a vertical loading of 7.5MPa is applied. We assume the friction angle is zero because of the fluid. The system is drained so that there is no sufficient fluid pressure built up rapidly to impact the compaction process.

The horizontal, vertical and shear stresses when reaching equilibrium are shown in Figure 7. We can see high compressive horizontal and vertical stress bands are formed in both directions. At the bending area in the center, all stress components reach very high values, indicating a high possibility of failure in this region.

Figure 7. Calculated horizontal, vertical and shear stresses (Unit: Pa) when reaching equilibrium.

This example confirms a conclusion in the earlier paper by the authors [4]: the sequential evolution of geomaterials as responses to stress is motion, deformation and accumulation of high stress at local contacting areas (especially at sharp corners). In addition, through this example, we find the fact that the damage zone with softer material can accommodate larger deformations, and therefore dominate
contact evolution and redistribution of stress of a granular system toward a system with minimized porosity.

3.3.2. Microscale Modeling of Granular Salt: Insights for Salt Creep In this example, we conducted microscale modeling of salt compaction for understanding the creep of salt [9]. In our simulation, we extracted the geometry of halite aggregate from an image and explicitly represented the geometry and the structure of the aggregates. We simulated the initial compaction due to reorganization of the halite aggregate, and the second-stage compaction as results of pressure solution and microfracture growth. With consideration of microfractures and pressure solution, we are also able to study their impacts on porosity loss and redistribution of stress within the granular system. Figure 8 shows the geometric evolution of the halite grains before compaction, and after initial and secondary compaction. Figure 9 shows the redistribution of the high-stress band from the initial and secondary compaction.

![Figure 8. Geometric evolution of the halite grains before compaction, and after initial and secondary compaction.](image)

![Figure 9. Vertical stress after initial and secondary compaction (Pa).](image)

Based on our simulations, we found that (1) the dynamic changes of salt granular systems involving reorganization of grain aggregates, creation of microfractures and pressure solution can repeatedly occur, therefore potentially contributing to long-term creep behavior of salt at larger scales; and (2) sharp corners of mineral grains can dominate the structural changes and loss of porosity of the system, which can be further altered by creation of new microfractures and/or pressure solution.

4. Conclusions
In order to address the challenges associated with computational geometry and complex multiphysics in geosystems, we presented integrated machine learning and numerical modelling in this study. First, we applied a convolutional neural network (CNN) for recognizing a rough fracture from an image and achieved acceptable accurate result. Then we made use of neural style transfer (NST) to generate and optimize meshes from rock images. By optimizing the cost function to achieve approximation to represent both the content and the style, numerical meshes were generated and optimized. Because the mesh generation routine is automatic, the NST technique can be very promising for applications of simple mesh patterns (e.g., evenly sized or adaptively refined triangles, rectangles, spheres) to generate and optimize meshes for complex geometric features in various geosystems.
We applied previously developed models based on NMM to analyze processes in different systems involving single rough fractures, discrete rough fractures and a granular system under different multi-physical conditions. We used different geometric representations of fractures and granular systems and developed numerical models with different governing equations and constitutive relationships to study coupled processes at different scales. We achieved the following key findings from our simulations:

- Accurate representation of geometric features of fractures at different scales is essential;
- Interfacial or microscale evolution of fractures depends on the abnormal features (sharp corners of minerals, major asperities) and THMC coupling;
- The sequential evolution of geomaterials responding to stress is motion, deformation and high stress;
- Mechanical behavior differs between loosely packed and tightly packed blocky/granular systems;
- Interfacial or microscale evolution of fractures as a result of THMC coupling leads to structural or physical changes at upper scales.

Because of the challenges of image processing and determination of physical properties from numerical modelling and experiments, machine learning provides an excellent opportunity to address these challenges. On the other hand, by using realistic geometric representation from rock images, by applying reasonable physical laws and coupling priorities, and by successfully tackling the challenges associated with calculation of dynamic contacts in deformable discontinuous materials, our multiscale modeling capabilities presented here have shown to be promising for analyses of a number of geosciences activities. In the future, more integrated study of experiments, machine learning and numerical modelling will be conducted for advancing fundamental understanding and optimizing energy recovery and storage in the subsurface geosystems.

Acknowledgments
This research was supported by US Department of Energy (DOE), including the Office of Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division, and the Office of Nuclear Energy, Spent Fuel and Waste Disposition Campaign, both under Contract No. DE-AC02-05CH11231 with Berkeley Lab.

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