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Predictive modeling of dynamic fracture growth in brittle materials with machine learning

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ABSTRACT

We use simulation data from a high fidelity Finite-Discrete Element Model to build an efficient Machine Learning (ML) approach to predict fracture growth and coalescence. Our goal is for the ML approach to be used as an emulator in place of the computationally intensive high fidelity models in an uncertainty quantification framework where thousands of forward runs are required. The failure of materials with various fracture configurations (size, orientation and the number of initial cracks) are explored and used as data to train our ML model. This novel approach has shown promise in predicting spatial (path to failure) and temporal (time to failure) aspects of brittle material failure. Predictions of where dominant fracture paths formed within a material were ~85% accurate and the time of material failure deviated from the actual failure time by an average of ~16%. Additionally, the ML model achieves a reduction in computational cost by multiple orders of magnitude.

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1. Introduction

Failure in brittle materials occurs through the propagation of fractures and has been investigated for over a century due to its many applications in industry (aviation systems [1], subsurface fracturing [2], etc.) and inherent scientific curiosity [3–5]. Brittle materials are materials in which cracks of atomic sharpness essentially propagate by bond ruptures [6]. Unlike ductile failure behavior, brittle solids fail with little warning along grain boundaries [3] or in the case of geomaterials, fractures propagate along interstitials [7]. Once fracturing has begun, the fractures will have a strong tendency to propagate since they are driven by internally stored elastic energy. Accurately predicting failure at the macroscale requires knowledge of the dynamically evolving microstructure, including features such as grain boundaries and interstitials, and also accounting for fracture interactions with the microstructure and other fractures present in the system. Many approaches have been taken to address the failure of a material at different length scales including analytical and numerical methods [8–13,4]. Modeling micro- and meso-scale fracture mechanics is computationally expensive and hence, cannot be directly applied to large components or systems crucial for many applications. Rather, the physics on these scales must be averaged or scaled-up and incorporated into continuum models used at the macroscale. Again, on the continuum scale, it becomes a computational burden to account for the complexities of fracture networks, including all possible fracture orientations and lengths, so significant sub-scale information is often lost when moving upwards in length scales.

In this manuscript we take advantage of recent advances in machine learning to develop a computationally efficient, reduced order model of a high fidelity model that accounts for the evolution of discrete fractures. The high fidelity model includes the majority of the physics necessary to predict failure, but is computationally prohibitive and too data intensive to be effective at the macroscale (e.g. several meters and greater). We demonstrate that our reduced order model mimics the high fidelity model for a given set of initial and boundary conditions at 2–4 orders of magnitude speed up. The eventual goal is to use the workflow demonstrated in this manuscript to incorporate sub-scale information using our efficient machine learning emulators into macroscale continuum constitutive models for more accurate failure predictions.

2. Background

A common approach for macroscale continuum failure models is to utilize average mesoscale quantities informed from higher fidelity modeling approaches where discrete fracture evolution can be captured, including mechanisms such as, velocities of tip growth, process zone stress states, and/or coalescence. The lower length scale models are used to derive upscaled relationships and

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determine quantities such as effective moduli to be used in the continuum scale model [14–17].

Analytical models for fracture propagation have also been valuable for modeling and understanding fracture growth since they are computationally inexpensive and are connected to physical insight. In general, analytical approaches, including that of Griffith [9,10] and Paris [11], must make broad assumptions in order to remain tractable. Hence, they neglect complexities such as fractures coalescence, variable orientation, and fracture nucleation and focus on understanding how pre-existing fractures grow due to the stress state present, and contain no interaction terms with other fractures. These assumptions can have a large impact on results since many materials, without a dominant fracture in the macroscale, have been shown experimentally and numerically to interact extensively before failure is reached. High fidelity numerical models provide an alternative to these analytical models allowing for the majority of physics to be considered but these models are often computationally prohibitive at the macroscale. Currently a popular approach for modeling fracture dynamics is with the use of Finite Element Methods (FEM) [18] or Finite Discrete Element Methods (FDEM) [19]. Advantageously, both methods can account for individual fractures, and interactions between many fractures within a network. The key differences between FEM and FDEM methodologies is in how the cracks propagate, along edges with voids representing cracks (FDEM) or moving the crack boundaries through the mesh using cohesive elements, mesh refinement, or other numerical methods (FEM). The obstacle to properly modeling failure aspects at the macroscale such as time to failure or damage evolution lies in finding the connection between how lower scale phenomena affect the material strength and damage. The geometry, orientation, and size of individual fractures are a few of the many mesoscale features that influence macro-scale behavior.

The high fidelity model we have chosen to model fracture propagation to inform the ML approach is the Hybrid Optimization Software Suite (HOSS), a FDEM analysis tool that can account for the complexity of a fracture network's growth over periods of time [20]. This approach can result in billions of unknowns for a relatively small system (10^6 fractures) resulting in a computationally intractable problem at larger scales of interest to many applications. For example, running a 3D simulation of geomaterial on the scale of 1 m $\times$ 1 m $\times$ 1 m with a fine enough mesh to resolve individual fractures would require about 500,000 CPU hours. Thus, bridging the gap between these two scales is a major obstacle.

In order to circumvent the cost of running high-fidelity models like HOSS directly at the macroscale to model a large spatial and temporal region, we have developed a machine learning (ML) approach to learn and abstract the information that HOSS can provide, but at a much lower computational cost. Our long-term goal is to use ML as the bridge that spans the gap between meso- and macroscales for failure prediction. ML is a field that deals with the design, development and implementation of techniques that permit computers to learn based on data [21,22]. There have been successful applications of ML across many fields like natural language processing [23], object recognition [24], and bioinformatics [25]. ML is classified into three categories based on the objective of the technique; supervised ML, unsupervised ML and reinforcement learning. Of these techniques, supervised ML has been employed because of its focus on finding a mathematical function that maps inputs to outputs. Examples of supervised ML techniques include random forests (RF) [26], support vector machines (SVM) [27] and artificial neural networks (ANNs) [28].

In the context of materials, ML has recently been used [29] to tune mesh-based parameters in an FEM model such as element stiffness, number of elements, etc. to match experimental data of fracturing in a small steel frame. Using neural networks, they achieved a 10% increase in accuracy in simulation output compared to experimental results, but at the cost of substantial growth in computational burden. Additionally for this approach to be successful, a large amount of experimental data is required to ensure over fit of the neural network doesn't occur. Over fit is when the ML model begins predicting noise or errors in the data, usually due to the high number of trainable parameters compared to observations available. In contrast to the above approach, we have generated an ML method that is trained to learn the physics of fracture propagation and interaction leading to coalescence and eventually, failure based on hundreds of HOSS simulation outputs. We extract vital patterns and trends from the high-fidelity data to build a predictive model that can emulate the HOSS simulations in a fraction of the time.

The remainder of this article is organized as follows. We present a brief description of the FDEM software HOSS in Section 3, and outline our ML methodologies in Section 4. Section 5 contains the Results and Discussions of the different ML methods compared against HOSS and discuss our conclusions in Section 6.

3. FDEM model: HOSS

HOSS (Hybrid Optimization Software Suite) is a multi-physics numerical tool based on the combined finite-discrete element method (FDEM). The FDEM was proposed in the early 1990s as an alternative to describe the transition from continuum to discrete material behavior that occurs upon failure, i.e., fracture and fragmentation processes of brittle geologic materials. One of the key aspects of FDEM formulation is the minimization of the assumptions made regarding the behavior of the material; fracture and fragmentation processes are described explicitly based on conservation laws. In an FDEM framework the solid domains (called discrete elements) are discretized into finite elements. Cracks must be finely resolved spatially, with dozens to hundreds of finite elements along the length of each crack. The governing equation of the FDEM systems are based on Newton's laws [30] and are solved by using an explicit (time marching) central difference method, which makes it necessary to use very small timesteps to update the system state dynamically. As a result, even simulations involving laboratory size samples with thousands of microcracks can result in petabytes of data. Additionally, since the initial state of defects and microcracks in the samples can never be known exactly, predictive capability in an uncertainty quantification framework requiring thousands of simulations is computationally intractable. A full description of the method is outside the scope of this paper; however, the interested reader can refer to the following comprehensive references for more details: [30–32].

4. Methods

In this section, we describe the ML approach to extracting, learning and predicting material behavior. The data is extracted from a set of 200, 2 dimensional HOSS simulations of a geomaterial that is 2 meters by 3 meters. These geomaterials contain 20 randomly distributed fractures that have a uniform length of 30 cm. The lengths of initial fractures were constricted to uniform lengths since larger lengths of initial fractures tend to dominate fracture propagation and failure. Our interest was in fracture coalescence, thus eliminating the dominance of longer fractures with uniform lengths gave us a clearer view of this phenomena. These initial fractures varied between three orientations, 0, 60 and 120 degrees to the applied load on the material. The material is pulled from the top at a constant velocity of 0.3 meters per second, the bottom boundary is fixed. The simulation ended when a continuous frac-