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REDUCED-ORDER MODELING OF THE DEFORMATION RESPONSE OF POLYCRYSTALLINE AGGREGATES

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Modeling the crystal-scale deformation of polycrystalline aggregates is computationally costly. Cheaper models are necessary to crystal-scale behavior in simulations of large-scale engineering components in aerospace assets. Here, a computational framework to develop reduced order crystal plasticity models to describe the deformation response of polycrystalline aggregates has been developed. This was achieved through training a convex neural network via large datasets generated from crystal plasticity finite element simulations. This framework has been demonstrated by creating a computationally inexpensive model which relates the state of the material to its macroscopic yield behavior. Data from the reduced order model was qualitatively compared against simulated data, with robust correlation. The framework was developed to be extendable to consider increasingly complex material descriptions to further the generality, accuracy, and precision in its predictions.

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1. Summary

The behavior of metallic alloys is influenced by the microscopic state of the material [1, 2]. Modeling the macroscopic mechanical deformation response of metallic alloys via full-field crystal plasticity simulations to lend insight into their mechanical behavior is often computationally expensive. Owing to the high computational cost, simulations are often limited to only small, representative volumes of material [3, 4]. Consequently, simulations of relatively large-scale engineering components in machines do not directly consider the material state and rely instead on centuries-old theories to predict how and when a component will fail [5, 6]. It is thus necessary to develop computationally cheap models to integrate crystal-scale behavior in component-scale simulations to better predict material failure.

In this study, the applicability of machine learning techniques to develop reduced-order crystal plasticity models was investigated via the creation of a computational framework to train reduced-order models [7]. In particular, convex neural networks (CNN) were utilized to develop a computationally inexpensive model which directly relates the microscopic state of a material to its macroscopic yield behavior. This computational framework was trained considering the crystallographic texture of the material, and results indicated that the reduced-order model was qualitatively adept at reproducing the correct macroscopic yield behavior for a material with a given crystallographic texture. Various textures were utilized to train the material, and both extrapolative and interpolative predictions proved successful.

The framework was designed to be fully extendable. In this way, future iterations of the model may consider increasingly complex material descriptions, as well as evolution of material state (i.e., behavior beyond initial macroscopic yield). It is recommended that the model be trained to be more generalized, as well as to consider material state evolution. Further, it is recommended that the reduced-order model be implemented in a finite element framework to facilitate component-scale simulations.

2. Introduction

Design engineers tasked with designing components for machines rely on an understanding of macroscopic material properties to predict how and when a component will fail, either due to static fracture or fatigue. The macroscopic behavior (i.e., mechanical material properties) of polycrystalline metallic alloys is well-known to be influenced by the microscopic material state: namely the anisotropic single-crystal mechanical response and the crystallographic texture of the material [1, 2, 3, 4]. However, the majority of models available to design engineers fail to include these effects, and machines are over-designed, with conservative estimates of how and when components will fail. Better predictions of material properties is necessary to increase performance, efficiency, and sustainability of modern machines.

Historically, macroscopic material properties were exclusively gathered experimentally [8, 9]. However, experimental determination of yield surfaces is often relatively costly, and is limited to only a single material state (i.e., results from one material state do not necessarily indicate the behavior of another). Thus, experimental databases are often limited, and new determination of material behavior is likewise focused on only singular material states as necessary.

Consequently, design engineers often employ centuries-old theories regarding the yield behavior of materials. Namely, the Tresca yield criterion and the von Mises yield criterion are still the most-often used models to predict macroscopic yield behavior, owing to their computationally cheap, closed-form solutions [5, 6, 10]. However, neither model considers the state of the material, and instead make the broad assumption that material behavior is isotropic, which is only true for a very small subset of structural materials [11]. Using these theories, the calculation of yield is often either over- or under-predicted. The result is that designers tend to implement generous factors of safety to offset any potential under-prediction, leading to significant weight gains in machines.

In the past century, various methods have been developed in an attempt to relate the state of the material to its macroscopic behavior. Early model development focused on homogenization techniques to find upper- and lower-bounds to material properties (i.e., Taylor and Sachs models [12, 13]). More recently, computational efforts have focused on quasi-homogenization schemes (e.g., viscoplastic self consistent models [14]), and state-of-the-art full-field crystal plasticity finite element modeling (CPFEM) [15, 16, 17].

CPFEM considers accurate representations of the microscopic state of the material, as well as sophisticated crystal-scale deformation models. While the predictions of CPFEM simulations are often the most accurate and precise of any existing modeling framework bridging these length scales, they come at a relatively high computational cost [2]. Low-fidelity simulations often require high-end computational workstations, while high-fidelity simulations may require high performance computing clusters. Consequently, CPFEM simulations are often limited in scope to only small volumes of material. Their implementation into simulations at larger length scales is thus prohibited given current computational capabilities, as the computational cost of a component-scale simulation directly considering CPFEM simulations to predict local behavior would be astronomically high.

To better predict the mechanical response of machine components – and thus better predict how and when they will fail – it is thus necessary to develop models that have limited computational cost, yet capture the essence of full-field CPFEM models. These so-called reduced-order models

are able to be directly implemented in component-scale simulations, owing to their reduction in computation time to render mechanical predictions.

Recently, machine learning methods have emerged as a way to develop understanding of trends in large datasets that may not be readily apparent to the human eye or via traditional analysis methods. In particular to understanding material behavior, machine learning methods have been applied to predict the intra-grain stress state based on descriptors of the grain state [18, 19]. Further, machine learning models are often composed of relatively simple mathematical operations, allow for fast computation (relative to CPFEM simulations). It is thus envisioned that given large datasets regarding the yield behavior of materials with a fixed material state, machine learning can be utilized to render a model relating the material state to the material properties at relatively low computational cost – i.e., a reduced-order model.

By using these reduced order models, design engineers can have increased confidence in their failure predictions compared to historical models. This will both allow for a better prediction of component lifecycles thus increasing safety of machines, as well as the reduction of often excessive factors of safety, increasing performance, efficiency, and sustainability of machines.

3. Methods, Assumptions, and Procedures

In this study, we employ a workflow to develop a reduced-order crystal plasticity model relating the microscopic state of the material to the macroscopic material properties (i.e., material behavior) [7]. Broadly speaking, this is achieved by generating large datasets of yield points via CPFEM simulations for a given material state under specific loading to characterize the macroscopic yield surface. These datapoints are then fed as training points to a convex neural network (CNN), which learns the relationship between the material state and the resulting macroscopic yield surface. The broad overview of the workflow is summarized in Figure 1, and specific details follow.

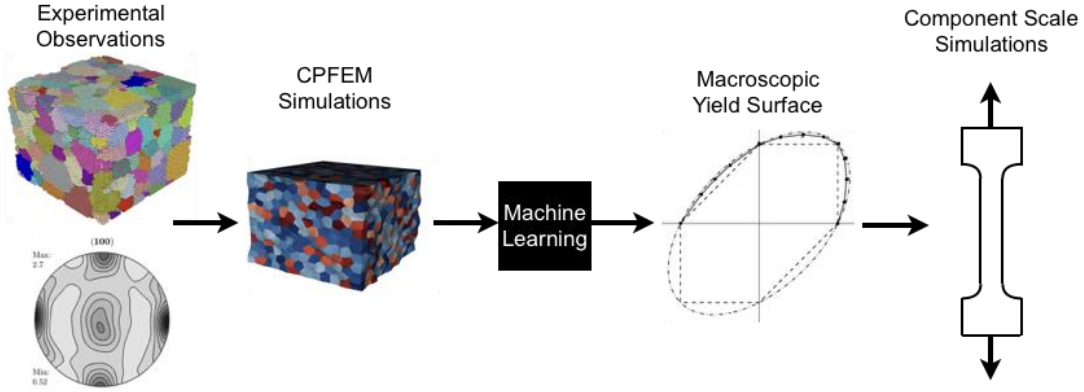

Figure 1. Workflow used to train the reduced-order crystal plasticity model. Experimental observations inform the creation and evaluation of representative simulations, which can be performed with a variety of loading conditions to elucidate the yield surface. This data is fed to a machine learning algorithm (CNN) which formulates a model which can predict the macroscopic yield surface, which may then be implemented in component scale simulations.

3.1 Yield Surface Generation

Ultimately, the CNN requires a description of the material state and a description of the resulting macroscopic yield surface as input. In terms of the CNN framework, it is agnostic as to whether this data is derived from experimental observations or from synthetic predictions. In order to train the model, many different material states and their resulting yield surfaces are necessary. Access to such experimental data is lacking, owing in large part to the difficulty in producing said datasets. However, studies have shown that CPFEM is adept at predicting bulk properties such as yield. Therefore, this study focused on generating large synthetic datasets via CPFEM. Generation of the datasets for this study consisted of the generation of 9 cube-component textures (Figure 2) with varying degrees of intensity. For each texture (i.e., material state), 72 different biaxial loading conditions were applied to the point of macroscopic yield (Figure 2). In this way, for each texture, a finely resolved biaxial yield surface could be constructed. Note that the method is not limited to biaxial loading, and indeed can consider generalized load states – for ease of visualization and demonstration of the framework, the 2D loading case was first considered.

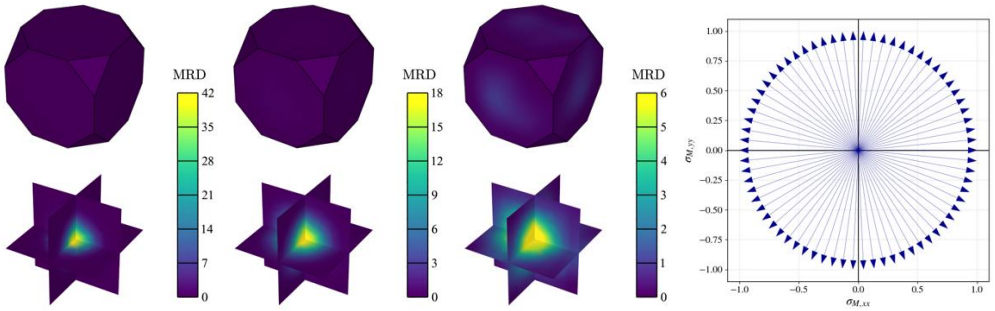

Figure 2. Three example textures (left), with angular spread equal to 5°, 15°, and 25° (left to right), and prescribed loading vectors in biaxial plane (right) used to generate yield surface data via CPFEM simulations.

3.2 Convex Neural Network Training

For each material state, a corresponding yield surface is generated via CPFEM modeling (Section 3.1). This data serves as the direct input to the CNN machine learning framework as so-called training data. While other machine learning frameworks were considered for this application (e.g., Gaussian process regression, or GPR), the advantage of the CNN framework is in its natural enforcement of convexity in the solution that it produces. For metallic alloys, Drucker's postulate implies that the macroscopic yield surface must be of a convex shape to be physically proper. In this way, the use of a CNN framework provides physical constraints to the solution, and further does not require the input data to itself be convex, allowing for the input points from CPFEM to be non-convex (expected, due to minor numerical error in the simulations). Note that other machine learning frameworks, such as GPR, proved to be extremely sensitive to the convexity of the input, leading to non-physical predictions.

The data is ultimately supplied to the CNN simultaneously, such that it can recognize and learn as much about the relationship between the material state and the resulting yield surface as possible. Likewise, the model that is returned upon training of the CNN will be as generalized as the dataset supplied.

4. Results and Discussion

4.1 Results

The CNN was trained with 9 variations of a cube-component texture (examples show in Figure 2), each with a yield surface calculated via CPFEM performed with 72 different biaxial loading conditions (Figure 2). The resulting reduced-order model thus relates the material state to the macroscopic yield surface. In an effort to test the predictive capabilities of the CNN, two separate techniques were used for assessment.

First, in-sample (or interpolative) predictions were made. Interpolative predictions are made between training points. In the case of this study, this equates to the prediction of a yield surface for a crystallographic texture within the range of the crystallographic textures used for training. Figure 3 contains results from two interpolative predictions. Further, Figure 4 depicts the training and test loss for the two cases seen in Figure 3.

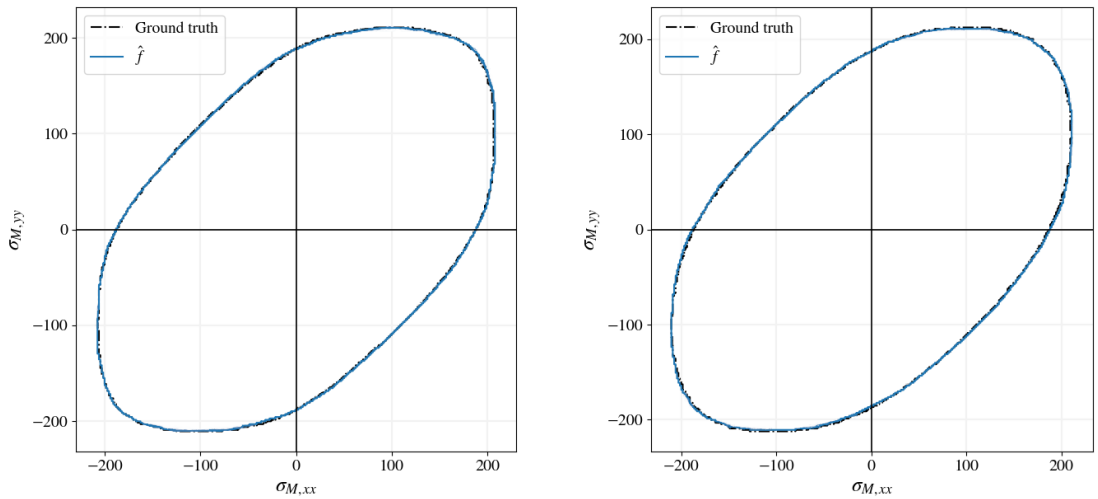

Figure 3. Interpolative predictions for a cube-component texture of spread 12.5 degrees (left) and 17.5 degrees (right). Plots depict both the predicted yield surface and that from ground truth (from CPFEM simulations).

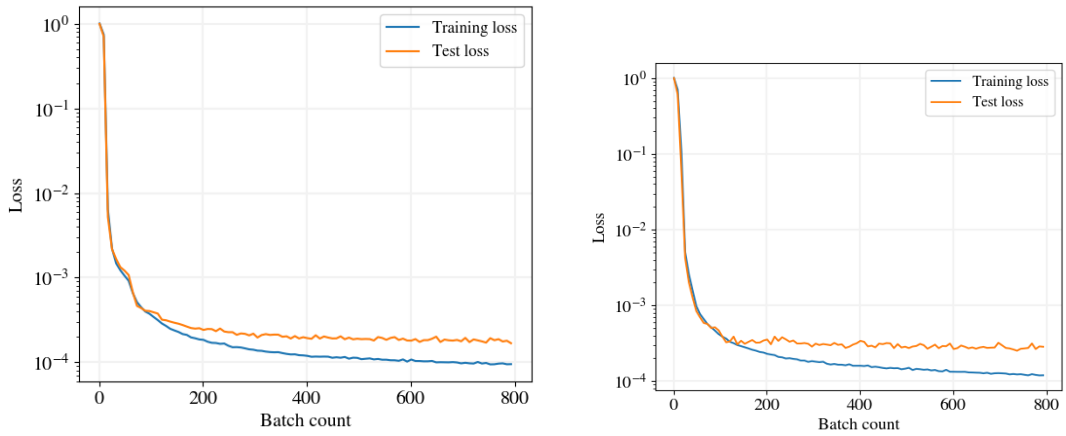

Figure 4. Training and test loss for a cube-component texture of spread 12.5 degrees (left) and 17.5 degrees (right).

Next, the model was tested via out-of-sample (or extrapolative) predictions. Extrapolative predictions are made outside of training points. In the case of this study, this equates to the prediction of a yield surface for a crystallographic texture outside of the range of the crystallographic textures used for training. Figure 5 contains results from two extrapolative predictions. Further, Figure 6 depicts the training and test loss for the two cases seen in Figure 5. Loss is broadly defined as the badness or error of a prediction compared to the ground truth data, with lower loss indicating less error (0 loss indicating a perfect fit). Different categories of loss indicate the sets of data being compared: training loss compares the truth vs. predicted values on data sets used for training, test loss compares the same on data sets used for testing.

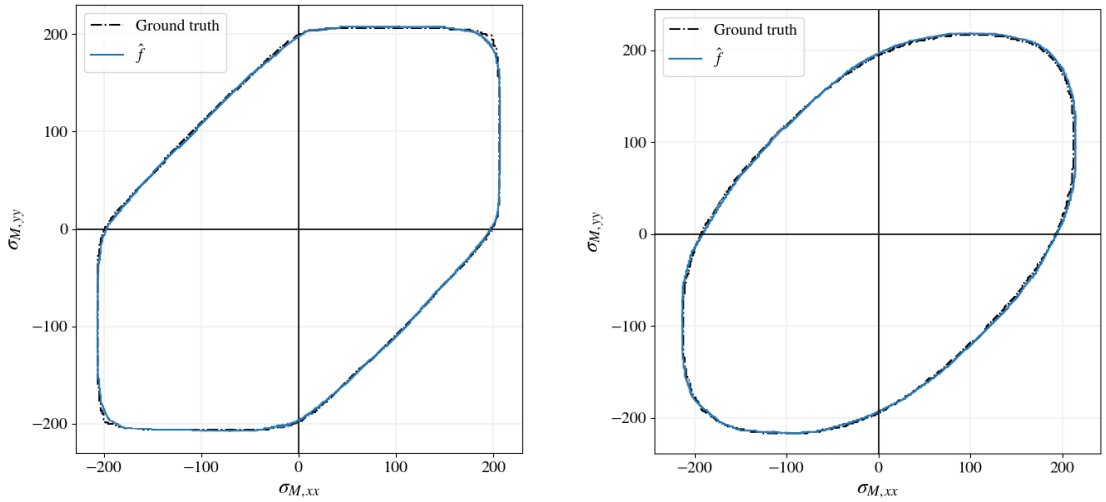

Figure 5. Extrapolative predictions for a cube-component texture of spread 5 degrees (left) and 25 degrees (right). Plots depict both the predicted yield surface and that from ground truth (from CPFEM simulations).

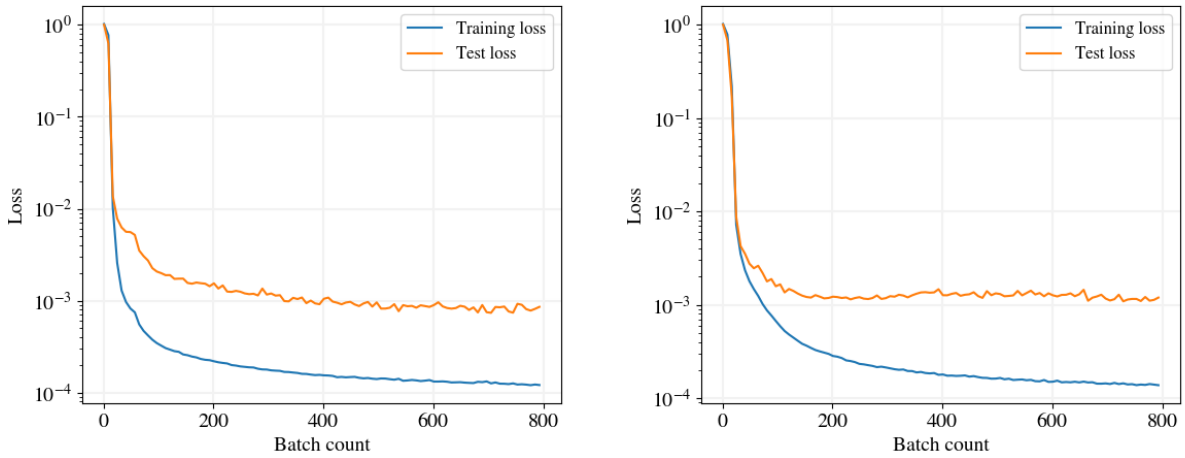

Figure 6. Training and test loss for a cube-component texture of spread 5 degrees (left) and 25 degrees (right).

4.2 Discussion

Broadly, both the interpolative and extrapolative studies render qualitatively and quantitatively good predictions between the ground truth (results from CPFEM simulations) and the machine learning predictions. This lends credibility to the CNN's ability to generate a reduced-order model capable of predicting the macroscopic material properties of a material of a given state (here: macroscopic yield and crystallographic texture, respectively).
Focusing first on the interpolative predictions, the comparison between the yield surfaces derived from CPFEM simulations and those predicted via the trained model are qualitatively good (Figure 3). There is almost indistinguishable overlap between the prediction and the ground truth, thus demonstrating that the reduced-order model is able to capture the complex behavior relating a material state to the macroscopic yield surface, for textures within the range of those used for training.

This sentiment is further bolstered by the training and test loss (Figure 4). The training loss indicates that the comparison between the ground truth and predictions decreases as a function of batch count (or model iterations), indeed converging to a low value of 10^{-4}. Interestingly, the test loss, or the comparison between the ground truth and the interpolative prediction, likewise decreases and converges to a similar loss value as the data points used for training. This quantitatively demonstrates the ability of the CNN to make interpolative predictions.

Likewise, focusing on the extrapolative predictions, similar trends are evident. First, the qualitative comparison between the predicted yield surfaces and the ground truth is strong (Figure 5), again exhibiting almost indistinguishable overlap, albeit with some deviation at the vertices of the yield surface for the yield surface corresponding to the more acute texture (5 degrees, left on Figure 5).

Likewise, the training loss is quantitatively similar to the training loss for the interpolative study – indicating that the machine learning algorithm is adept again at predicting directly at the training points (Figure 6). While the overall test loss, however, is greater than that used for the interpolative study, it is still a very small value and orders of magnitude below the starting loss. This indicates that extrapolative predictions are potentially more fraught for the CNN framework, and care should be taken to use training datasets which encompass expected ranges of a given material state, thus mitigating the necessity to make extrapolative predictions (though it is worth stressing that these predictions are still qualitatively and quantitatively robust, however slightly lower in confidence than the interpolative predictions).

5. Conclusion

Overall, the study presents the construction of a convex neural network (CNN) framework to be used to learn the relationship between material state and macroscopic material properties. As proof of concept, this framework was demonstrated on a material state described in terms of a sample's crystallographic texture, and yield surfaces determined via biaxial planar loading. The reduced-order model as trained by the CNN framework proved adept (both qualitatively and quantitatively) at both interpolative and extrapolative predictions, lending a high degree of confidence in its abilities. The framework thus stands poised to train more generalized models describing the relationship between a material's state and the macroscopic behavior.

Further, outlook of continued work is strong. The CNN framework developed in this study was purposefully made to be easily extensible to consider increasingly more complex phenomena. It is the recommendation of the author that the framework be extended to consider more complex material descriptions (beyond simply crystallographic texture) and material behaviors (e.g., behavior evolution beyond the initial yield of the material). Further, more generalized loading conditions and textures should be explored to create a fuller view of the macroscopic yield surface of the material. Finally, the models produced by the framework are (once trained) available to be implemented in finite element frameworks in the place of historic yield criteria (i.e., Tresca or von Mises). This would allow for a computationally inexpensive way to bridge crystal-scale behavior with component-scale behavior. Such a finite element framework could be updated with future iterations of reduced-order models produced via CNN frameworks or similar.

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LIST OF SYMBOLS, ABBREVIATIONS, AND ACRONYMS

AFRL	Air Force Research Laboratory
CNN	Convex neural network
CPFEM	Crystal plasticity finite element modeling/method
GPR	Gaussian process regression
RXCM	Metals Branch, Structural Materials Division, Materials and Manufacturing Directorate
WPAFB	Wright-Patterson Air Force Base