Predicting Mechanically Driven Full-field Quantities of Interest with Deep Learning-based Metamodel

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Motivation and Summary

Full-fidelity simulation techniques such as Finite Element Analysis, while effective, can be prohibitively computationally expensive for exploring the massive input parameter space of heterogeneous materials. Machine learning-based metamodels, on the other hand, can predict mechanical behavior at a fraction of the computational cost compared to full fidelity simulations. Notably, there has been a recent increase in interest in the challenging problem of predicting full-field QoI (e.g., displacement/strain fields) for mechanics driven problems. Designing ML models for these problems is challenging because even outside the Mechanics research community, deep learning approaches to image-to-image mapping and full-field image analysis are far from fully understood.

Our Contribution

1) We made a significant extension to the Mechanical MNIST [1] dataset by adding Finite Element simulation results of quasi-static brittle fracture in a heterogeneous material captured with the phase-field method.
2) We investigated multiple Deep Neural Network architectures and subsequently established a strong baseline performance for predicting full-field QoI.

Mechanical MNIST Crack path (Fig. 1)

For our new dataset, "Mechanical MNIST Crack Path," we modeled quasi-static brittle fracture-using the phase field method- in a two dimensional heterogeneous material domain with inclusions whose positions are dictated by the Fashion MNIST bitmap. We published our dataset under open-source licenses, hoping it will allow other researchers to readily evaluate alternative metamodeling strategies against the baseline performance that we report here. We have published two versions of our datset. The most accessible version contains:

1) A 64 × 64 array corresponding to the rigidity ratio to capture heterogeneous material distribution,
2) The binary damage field at the final level of applied displacement reported over a uniform 256 × 256 grid,
3) The force-displacement curves for each simulation (which are not addressed in this manuscript).

And a larger more detailed version is available as well [2].

Metamodel: MultiRes-WNet (Fig. 2)

We proposed a modified version of the U-Net architecture, the "MultiRes-WNet", for predicting full-field mechanics based QoI.

Key modifications to the UNet architecture include:

1) Stacking two UNets in series,
2) Using depthwise separable convolutions,
3) Replacing double convolutions at each layer with a block of serial convolutions with internal residual paths,
4) Adding several convolutional filters to the residual path connecting encoder output to the decoder input.

Results (Fig. 3)

Full-field Displacement Prediction

For the metamodels trained with all 60000 training points (including data augmentation for the Mechanical MNIST Fashion datasets), we observed a Mean Absolute Percentage Error of 0.27% and 0.34% for Uniaxial Extension and 0.50% and 0.80% for Equibiaxial Extension in the Mechanical MNIST and Mechanical MNIST Fashion datasets, respectively. See [3] for details.

Crack Path Prediction

Our trained model achieves a mean F1 score of 0.893 on the continuous path group, 0.693 on the discontinuous path group, and 0.870 overall. Qualitatively, we consider 78.77% of the predictions as "Correct," 9.84% as "Plausible Alternative Paths," and 11.39% as "Incorrect." See [3] for details.

Future Directions

In our future work, we plan to: (1) continue developing open source datasets of complex mechanical behavior, and (2) continue exploring different metamodeling techniques for capturing these behavior. In particular, we are interested in building on this work to predict the time evolution of full field behavior with boundary conditions as a model input parameter.

References

[1] Emma Lejeune. Mechanical MNIST: A benchmark dataset for mechanical metamodels. Extreme Mechanics Letters, 36:100659, 2020.
[2] Saeed Mohammadzadeh and Emma Lejeune. Mechanical MNIST crack path extended version, 2021. (https://doi.org/10.5061/dryad.rv15dv486)
[3] Mohammadzadeh, S., & Lejeune, E. (2021). Predicting Mechanically Driven Full-Field Quantities of Interest with Deep Learning-Based Metamodels. ArXiv, abs/2108.03995.

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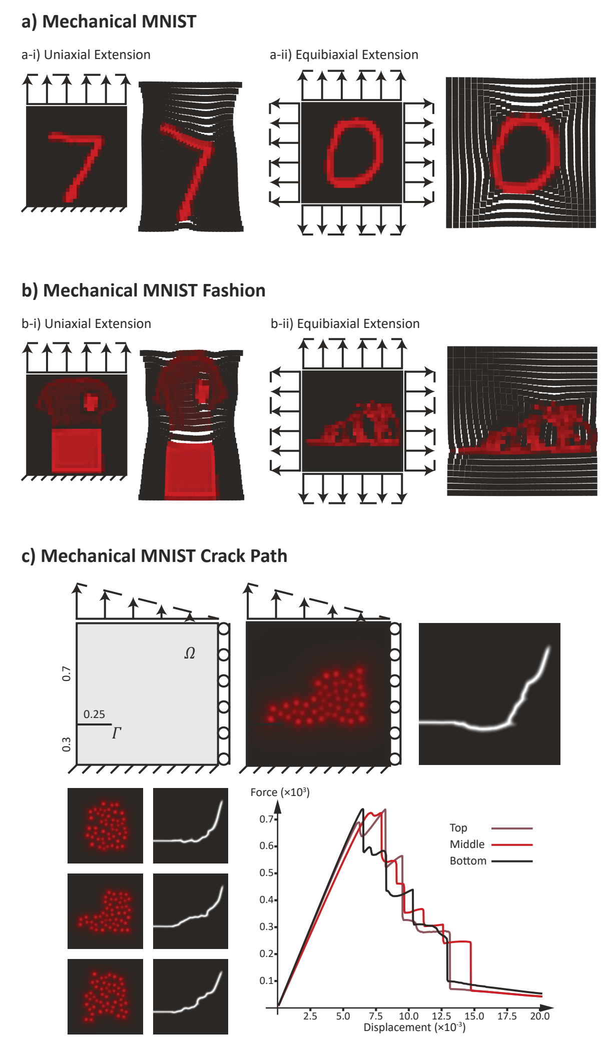
The **Mechanical MNIST Crack Path** dataset, an extension to the original **Mechanical MNIST** dataset, enables full field **crack path prediction** and provides a benchmark for Mechanics-based metamodeling of full field quantities of interest. The **MultiRes-WNet** metamodel architecture performs well on these data.

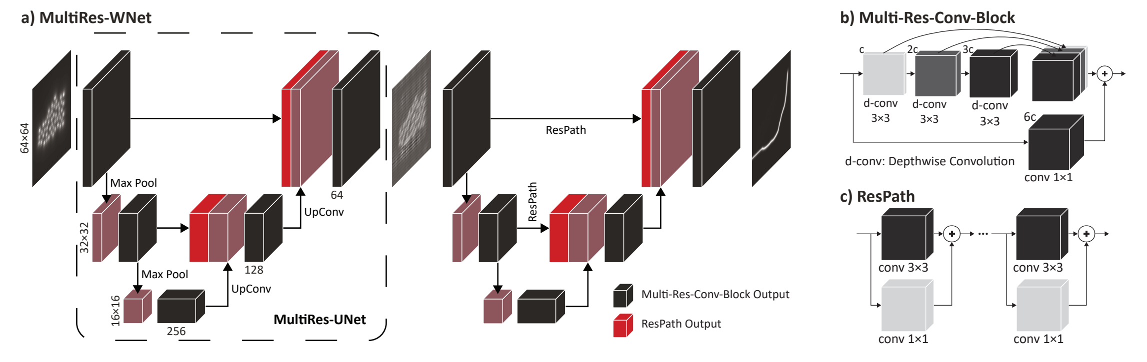
Data

Code

1. Datasets



2. Metamodel



3. Metamodel Performance on the Test Dataset