Quantification and Optimization of 2-Phase Microstructures using Generative Deep Learning

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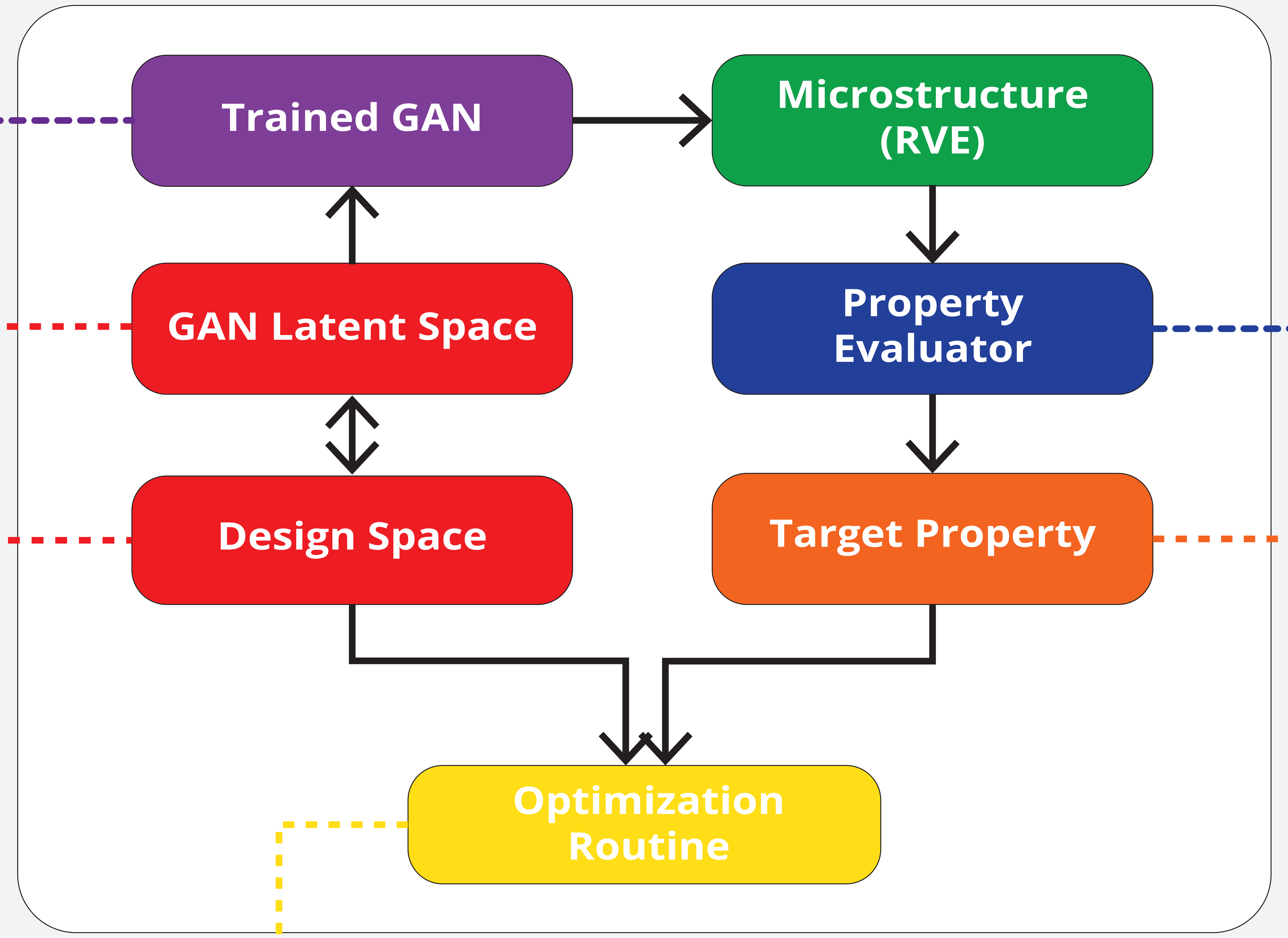

Generative Adversarial Networks

-Consists of 2 **Convolutional Neural Networks**: a Generator that takes in a low dimensional vector as input and generates the microstructure (or RVE); the Discriminator that takes in a microstructure as input, and predicts whether it is real or fake.
-Both the Generator and Discriminator are trained simulatenously, with the Discriminator minimizing and Generator maximizing the same loss (error) function.
-A StyleGAN2[1] with ADA has been used in the present study.

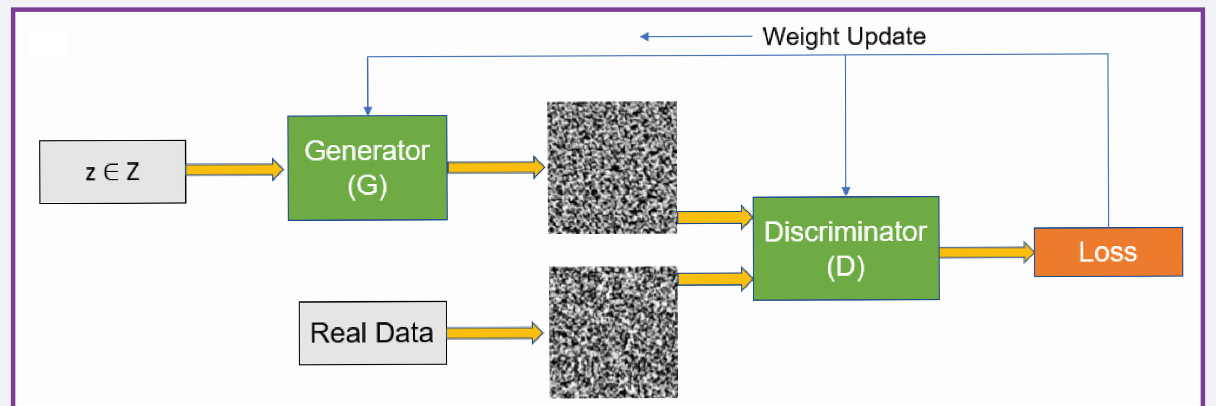

Figure 1: A schematic showing the GAN training process. Both Generator and Discriminator are trained simulateneously, and effectively "learn from each other's mistakes" by the means of a common loss (error) function.

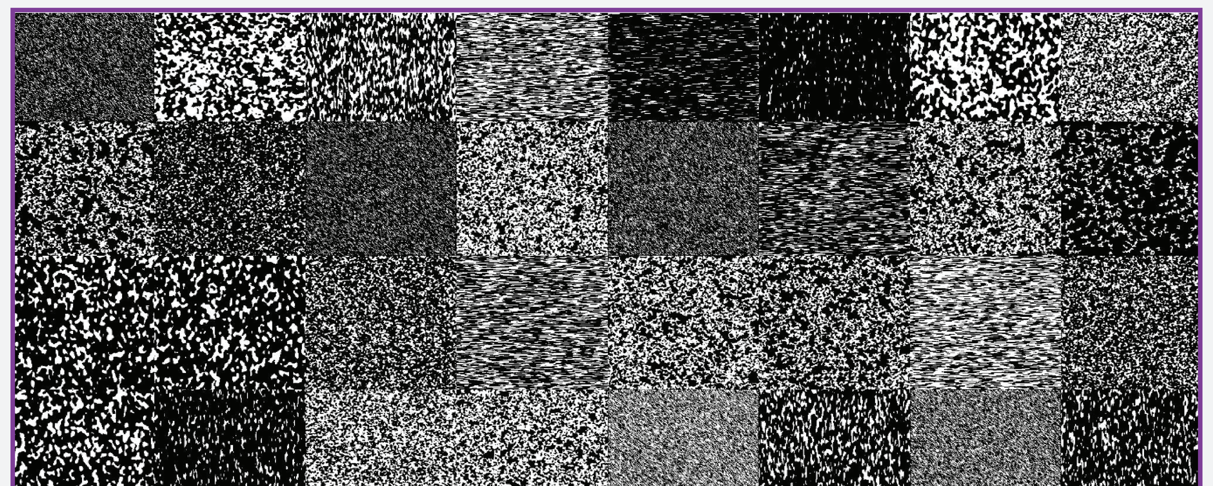

Figure 2: A look at some of the RVEs used to train the GAN. There are a total of 70 classes (or morphologies) of microstructures in the dataset.

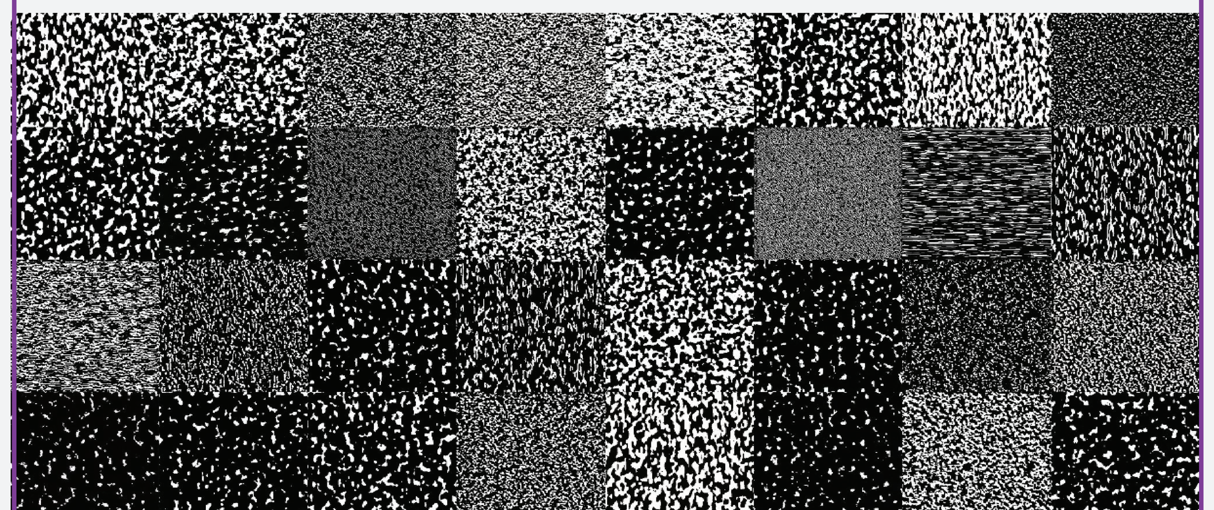

Figure 3: A look at some microstructures generated by the trained GAN.

Learned Latent Space (Design Space)

-The GAN's learned latent space has **512 dimensions**, hence 512 numbers are sampled to generate the RVE using the GAN.
-We can reduce this by performing a **Principal Component Analysis (PCA)** of the latent space, and then use the PCs as the basis vectors.
-Given an initial vector **W**, denoting the PCs as **V_i**, we can write any transformed vector **W'** in this space as[2]:

W' = W + $\Sigma a_i V_i$ = W + a*V

-It was shown in [3] that all 512 components aren't needed to describe the latent space. Hence, the problem is estimating the reduced design variable (a_is) given a target RVE.

Key References

[1]: Karras, Tero et al. 2019 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR) (2019): 4396-4405.
[2]: Rameen Abdal, Yipeng Qin, Peter Wonka; Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV), 2019.
[3]: Härkönen, Erik et al. ArXiv abs/2004.02546 (2020)
[4]: Raj, M., Thakre, S., Annabattula, R.K. et al. ntegr Mater Manuf Innov 10, 444–460 (2021).
[5]: Isola, Phillip et al. 2017 IEEE Conference on Computer Vision and Pattern Recogntion (CVPR) (2017): 5967-5976.

Morphology Reconstruction

-Problem statement: **Generate more (statistically similar) microstructural representations of a particular morphology using the GAN, given the RVE of the target morphology.**
-The morphology of a microstructure can be quantified using the 2-point correlation map (for 2-phase materials).
-We use **Bayesian optimization** with an upper limit on the number of function calls allowed (here, 50) to estimate a_is here.
-By using the PCs as the basis vectors, we can reduce the search space further. Consider the cases of using 1 and 10 PCs as the basis, leading to 1 and 10 design variables.
-As can be seen below, even the first **10 PCs** out of the 512 in total are sufficient to capture the morphology of the micrsotructures really well.

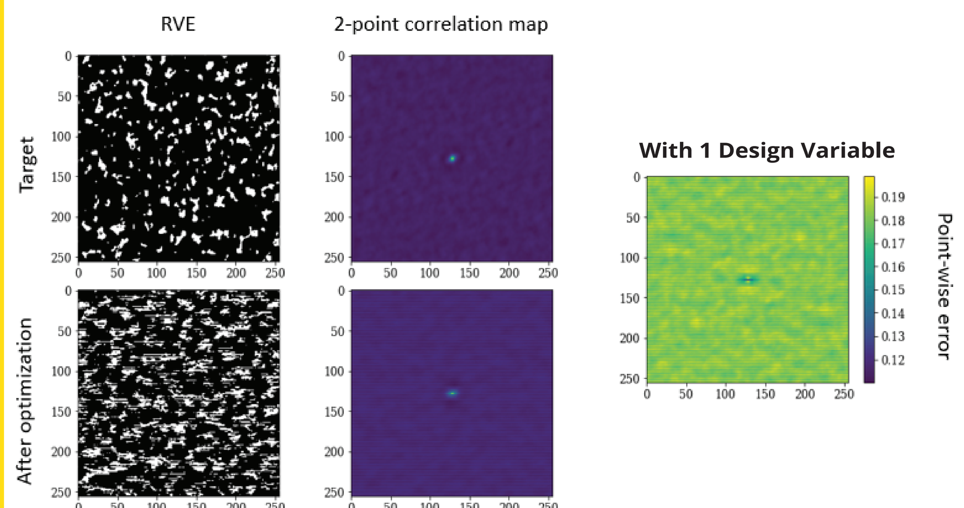

Figure 5: Results after morphology optimization using the proposed framework, with 1 PC as the basis.

Target Properties

-Fraction of stress concentration sites: A site is labelled as such if the local stress at that site is >2x mean stress in RVE.
-Mean and max stress (compressive or tensile) in the RVE.

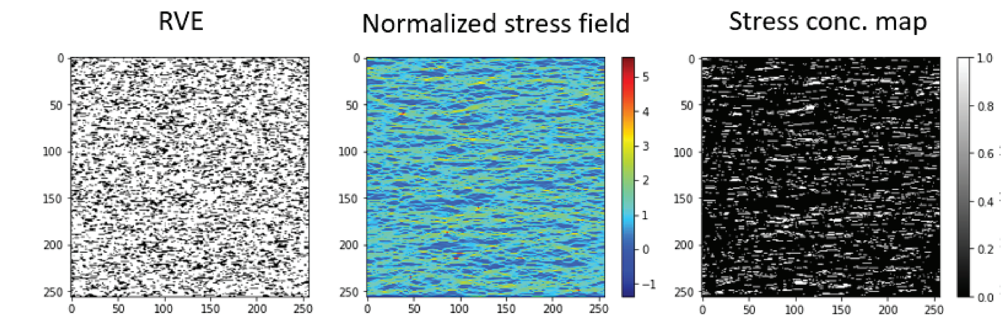

Figure 4: A sample RVE (left), and the same after normalizing all entries with the mean stress of the RVE (center). Using the criteria for defining stress concentrations, the stress concentration map (right) is obtained.

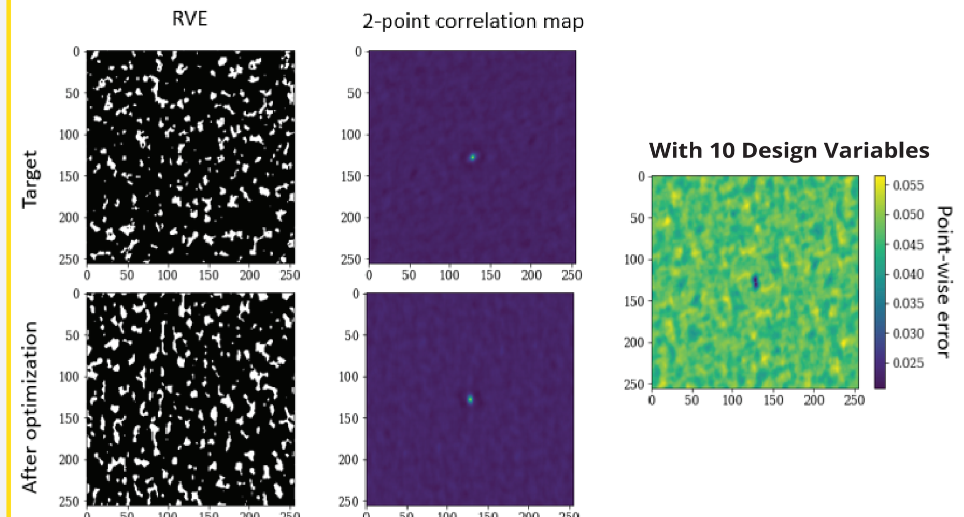

Figure 6: Results after morphology optimization using the proposed framework, with 10 PCs as the basis.

Finite Element Analysis of RVEs

- **FEM simulations** were performed in Abaqus for 2-phase RVEs, to mimic a tensile test by fixing left edge and pulling right edge.
-8000 samples in total were generated in the dataset, where each sample was a pair of RVE and the corresponding local stress field.
-Each stress field was normalized to range of (-1, 1), and the RVE has its entries as 0 or 1 depending on the phase.

U-Net to Predict Local Stress Fields

-A U-net[4] is a Convolutional Neural Network that takes in the RVE (X) as input and predicts the stress field (Y) as output, as shown below.

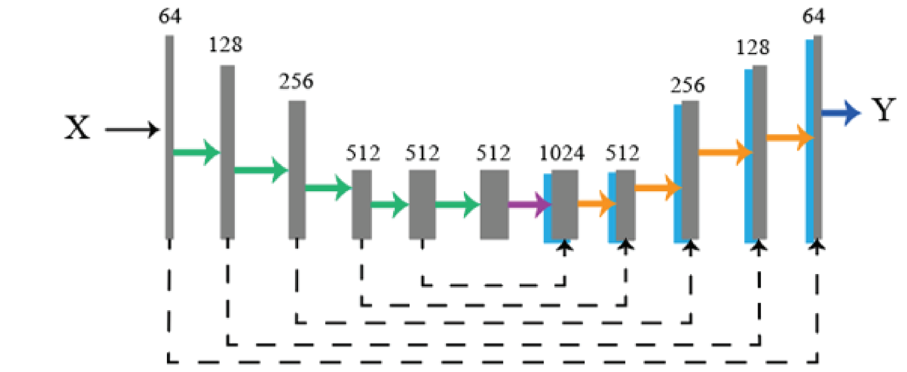

Figure 7: A schematic showing the "U-shaped" architecture of the U-net.

Pix2Pix to Predict Local Stress Fields

-The U-net is now extended to a GAN, by introducing an additional term in loss function[5]. This can also be thought of as a GAN with a U-net based Generator network.
-The additional GAN loss quantifies the "realness" of the predictions made by the U-net generator. Training objective for the model is now: $\arg\min_G \max_D \mathcal{L}_{cGAN}(G, D) + \lambda \mathcal{L}_{L_1}(G)$

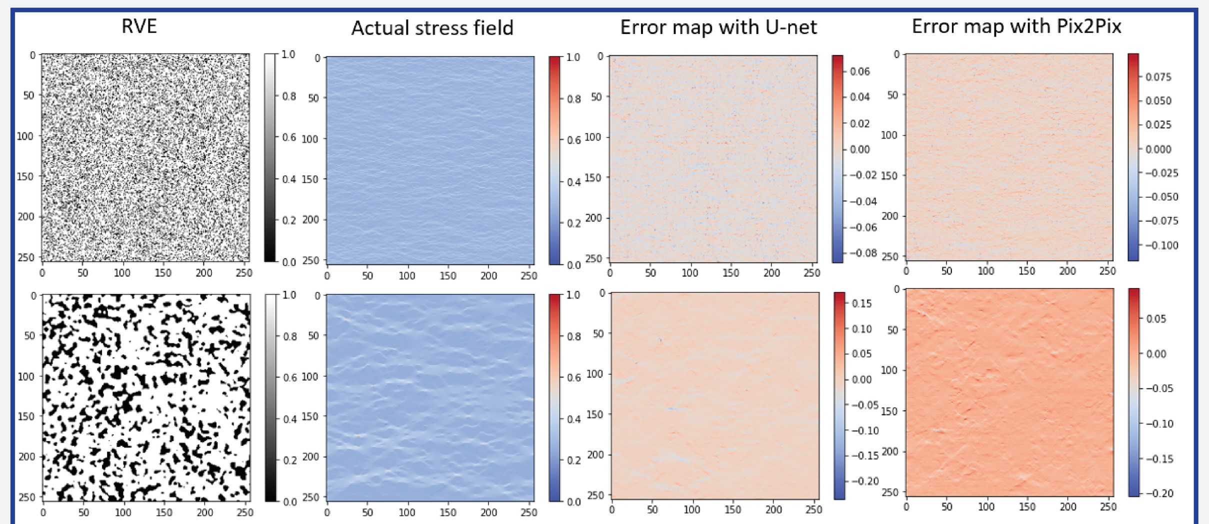

Figure 8: Local stress field predictions using the trained U-net and Pix2Pix models for 2 randomly selected RVEs from the test (validation) dataset.

R2 Scores for Target Properties	U-Net		Pix2Pix	
	Train	Test	Train	Test
Mean Stress	0.98286	0.98125	0.9962	0.9944
Fraction of stress conc. sites	0.93599	0.85853	0.9059	0.8927

Figure 9: R2 Scores of the predictions made by the trained DL models.

Outcomes

A part of this work has been submitted to the journal "Computational Materials Science", and is presently under review under the title "*Quantification of similarity and physical awareness of microstructures generated via Generative models*" by Sanket Thake, Vir Karan and Anand K Kanjarla.

Acknowledgements

This work was performed as part of the YRF Program (2021-22 cohort) at IIT Madras. I'm grateful to the YRF team to give me this opportunity. I'm also thankful to Mayank Raj (Batch of 2021, ME and IDDD DS) who helped me set-up the FEM simulations, and also Sanket Thakre (Research Scholar, MME) for his constant support while I struggled with training the GAN and his expertise in analyzing the trained GAN's RVEs statistically.