Feedback on the PhD manuscript “Machine learning enhancement of micro-CT based micromechanics of composite materials” by Radmir Karamov

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This thesis introduces deep learning techniques to improve the analysis of composite materials using X-ray computed tomography (CT). It presents algorithms for enhancing CT images, segmenting materials and generating periodic representations. These methods hold promise for advancing composite materials research.

Asked questions during the pre-defence:

P 63: You show that CNN7 outperforms CNN3 and CNN5. What about CNN9? Is CNN7 performance close to a plateau?

P 63: Is the 3D performance of these methods evaluated? How slice-to-slice consistency compared to the 2D methods?

P76: on P 61 you state that “When considering image-related metrics such as MSE and PSNR, it is worth noting that the simplest neural network architecture demonstrated the lowest error values (as shown in Table 3). This can be attributed to the fact that in a simple neural network, the discriminator is unable to provide meaningful feedback during the training process.” → Now, here you are relying on the small MSE error and a high PSNR. How can you make sure that what has happened for inpainting is not occurring here?

P77: are those two cases of visual comparison and image-based parameters enough to draw a conclusion on SR? Isn’t it better to also compare some physical parameters (like what you did for inpainting)? Same comment for segmentation (P 87).

P 104: “To ensure that the properties of each material in the RVEs were accurately captured, the threshold was determined by analysing the fibre volume fraction of the entire CT scan.” → how did you measure the ground truth Vf?

P 105: you have applied PBC to these models. Do the models have periodic boundaries?

P 113: “The generated periodic structures shown in Figure 38 demonstrate that the algorithm was able to successfully generate microstructures with a periodic structure.” → how do you make this evaluation? Is it enough to conclude on the periodicity of the RVE?

P 116: should/is this image periodic? Do the physical properties of this generated image represent those of an original image (fiber volume fraction, orientation distribution, etc.)? Also for figure 42 and 43

P 122: “The results suggest that the periodic RVE model exhibits a larger discrepancy from the experimental value compared to the original RVE model. This observation may be attributed to the relatively large size of the RVE used in the study, which could have minimized the effect of stress/strain fluctuations at the edges. It is plausible that the differences between the two models would favour the periodic RVE model if a smaller RVE size was employed. Furthermore, it is po98ssible that the input parameters used for the fibre-matrix system were not precise, and an increase in matrix stiffness, for instance, could lead to higher model predictions than the predicted tensile stiffness. Consequently, the periodic RVE model would perform better than the original RVE model.”

→ We can accept that because the RVE is large the edge effect may be small and hence PBC does not improve the results, but this cannot explain why PBC degrades the results!

And about the second argument, both models have the same possibly-imprecise input properties. Why do you think this affects only the periodic models?

P 125: "The analysis revealed that the tetrahedral models produced fewer elements with von Mises stresses above the critical value of 5-6%, compared to more than 20% for the voxel models, indicating more physical behavior" → how do you know which one is "more physical"?

Terminology consideration: physical descriptors (instead of features) of composite materials, stress fluctuation (instead of concentration), defect (instead of damage), morphology or structures (instead of microstructure), property jumps, deep learning vs machine learning, etc.

Not asked

P 61: Isn't it better to present some (average) numbers of Table 6 on a graph?

P 61: Table 6: What is the size of the whole volume and the ROI? Is the RIO equal to the masked volume?

P 62: the defined parameters are not clear to me. Can you explain (maybe with a figure) what they are? Orientation tensor, Degree of orientation, Cosine similarity

P 74: Figure 25b has a different contrast. Doesn't it influence the results? Why don't you show the original low-resolution image?

P76: How do the values in Table 9 relate to the original HR images? Do they show the difference with HR values?

P76: "We observe a very small MSE error and a very high PSNR" → what do you mean with very small and very high?

P104: Can you include a thresholded slice in Fig. 33?

P 108: Is the periodic inpainting GAN something fully developed by you? If not, references should be cited.

P 121: what are we supposed to see in this figure?

P 123: Fig. 45: firstly, it needs a legend and labels for a to d. Secondly, how do you see "non-physical stress and strain fluctuations"? Thirdly, why the displacement on the edges is not uniform?

P 124: "Also, the higher effective properties of the voxel model can be attributed to these stress fluctuations." → Table 16 shows that E is lower for the voxel models. And have you checked whether false stress concentrations are there for the voxel models too?

I recommend the thesis for defense.