

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

Member of the examination committee: Christoph Heinzl

The thesis presents a novel application of deep learning algorithms for processing CT images of composite materials. The author develops and evaluates several algorithms for structure generation, image quality enhancement, segmentation, and periodic RVE generation. The algorithms are verified by comparing them with existing techniques and by demonstrating their potential for material characterisation and modelling.

Here are some minor comments that came up during the review of the thesis (most of which are just thoughts, not recommendations for action):

- 1) On page 2, it's important to clarify that CT is primarily an imaging technique, not a visualization technique.
- 2) Transitioning quickly from CT to RVE, you might consider adding a section on "Geometric modeling" as an introduction to the concept of RVE.
- 3) Page 3 requires a more detailed explanation of what "periodic" means in the context of RVEs to enhance reader understanding.
- 4) It would be beneficial to explain the rationale behind choosing RVEs over polydata for Finite Element Modeling (FEM) on page 3.
- 5) Optionally, you could introduce and briefly discuss the relevance of vision transformers on page 4.
- 6) A suggestion for page 5 is to consider dividing Figure 1 to prevent any potential misinterpretation.
- 7) An explanation of the various in-situ analysis types would be helpful on page 11.
- 8) To enhance clarity, consider enumerating the categories mentioned on page 16.
- 9) On page 19, it's advisable to present references without resorting to lists for improved context.
- 10) Page 20 would benefit from indicating the author for all references to aid readability.
- 11) Abbreviations in titles should ideally be avoided for improved comprehension on page 24.
- 12) It's important to note that for super-resolution on page 30, there's often a trade-off between image quality and realism.
- 13) Page 31 should address the effects of training on a specific raw material system and explore different setups for precision.
- 14) In discussing the evaluation of segmentation results on page 31, it may be more concise to summarize the process.
- 15) The choice of reduced resolution over full resolution and its impact on precision should be explained on page 36.
- 16) On page 38, provide insights into how parameters were optimized for XCT imaging.
- 17) Consider discussing the potential impact of different window settings on results on page 39.
- 18) Page 41 should specify the methodology for inpainting and, optionally, this section could be moved to the related works.
- 19) On page 49, it's crucial to clarify how a specific method was adapted and its relevance to the study.

- 20) Page 50 should detail the experiments conducted to support the claims made.
- 21) Provide insights into the exploration of the parameter space for CNN5 and CNN9 on page 51, specifying the considered parameters.
- 22) The justification for using LeakyReLU as an activation function should be explained on page 52.
- 23) Clarify why Mean Squared Error (MSE) was chosen over other error metrics on page 54.
- 24) Explain the rationale behind opting for bicubic interpolation and provide information on training duration on page 55.
- 25) On page 56, address the stability of results under different conditions and the criteria used for selecting specific values.
- 26) The reasoning behind the 24-hour training duration and the difference for CNN3 should be explained on page 58.
- 27) Address artifacts in relation to RVE size on page 59 for a comprehensive understanding.
- 28) Provide additional context for the observed errors on page 60.
- 29) On page 70, discuss why ADAM stochastic gradient descent was chosen as the optimization algorithm.
- 30) Justify the use of RaGAN on page 71 and explain its relevance to the research.
- 31) Discuss the influence of the SSIM metric on the research results on page 72.
- 32) Page 74 should address greyscale and contrast issues and consider discussing the nature and extent of artifacts.
- 33) Mention any studies conducted on lined artifacts on page 75.
- 34) Provide insights into the practical implementation of super-resolution on page 76.
- 35) Address challenges related to shape variation and artifacts on page 76.
- 36) On page 76, discuss the perceived high SSIM for HR noisy and provide training time and general performance details.
- 37) Explore the potential of super-resolution in improving segmentation on page 77.
- 38) On page 83, provide reasoning for the preference of specific methods over others and mention alternative metrics.
- 39) Specify column names for images on page 88 and compare the developed method against manual segmentation, micrography, and CFC.
- 40) Discuss the usefulness of conventional segmentation slice reconstructible tools on page 89.
- 41) Address the limitations of deep learning methods on page 91.
- 42) Explain the need for new training in the context of segmentation on page 91.
- 43) On page 103, explain the choice of the method mentioned.
- 44) Consider using visualization to explore additional aspects on page 121.
- 45) Discuss why the developed models tended to underpredict material stiffness on page 122.
- 46) Investigate the presence of artifacts in super-resolution on page 132.
- 47) Consider future work related to speed enhancements on page 141.
- 48) Elaborate on the concept of a universal super-resolution model on page 146.

Overall, the thesis is well-written, comprehensive, and original. I recommend it for defence.