Skoltech
Skolkovo Institute of Science and Technology

Thesis Changes Log

Name of Candidate: Radmir Karamov

Double PhD Program: Mathematics and Mechanics in Skoltech, Engineering Science in KU Leuven

Title of Thesis: Machine learning enhancement of micro-CT based micromechanics of composite materials

Supervisors: Prof. Ivan Sergeichev in Skoltech, Prof. Stepan Lomov and Prof. Yentl Swolfs in KU Leuven

The thesis document includes the following changes in answer to the external review process.

Reviewer 1: Prof. Christoph Heinzl

1) On page 2, it's important to clarify that CT is primarily an imaging technique, not a visualization technique.
Answer: visualisation techniques" was changed to "imaging techniques" on page 2.

2) Transitioning quickly from CT to RVE, you might consider adding a section on "Geometric modeling" as an introduction to the concept of RVE.
Answer: A short introduction to the concept of RVE was added on page 3.

3) Page 3 requires a more detailed explanation of what "periodic" means in the context of RVEs to enhance reader understanding.
Answer: Added more detailed explanations about periodicity on page 3

4) It would be beneficial to explain the rationale behind choosing RVEs over polydata for Finite Element Modeling (FEM) on page 3.
Answer: The choice of RVEs over polydata is primarily dictated by the need to accurately represent the microstructure of composite materials. In the opinion of the author, RVEs allow for a more precise and realistic depiction of the material's internal structure, taking into account factors like fiber orientation, distribution, and connectivity, which significantly influence its mechanical behavior. Polydata, on the other hand, provides a simplified representation that may not capture these intricate details, making it less suitable for accurate FEM simulations of complex composite materials.

5) Optionally, you could introduce and briefly discuss the relevance of vision transformers on page 4.
Answer: Vision transformers require a substantially larger dataset, often in the order of millions

of examples, for effective training. Regrettably, collecting and working with such extensive data surpasses the scope of this thesis.

6) A suggestion for page 5 is to consider dividing Figure 1 to prevent any potential misinterpretation.
Answer: The figure caption was changed to make it clearer.

7) An explanation of the various in-situ analysis types would be helpful on page 11.
Answer: Added a short explanation of the interrupted and uninterrupted scanning on page 12

8) To enhance clarity, consider enumerating the categories mentioned on page 16.
Answer: The categories on page 17 were enumerated

9) On page 19, it's advisable to present references without resorting to lists for improved context.
Answer: Unfortunately, it is not feasible to present the references differently on page 20, as their order aligns with their appearance in the text, ensuring clarity and coherence in the context of the subject matter.

10) Page 20 would benefit from indicating the author for all references to aid readability.
Answer: The names of authors were added were it was possible.

11) Abbreviations in titles should ideally be avoided for improved comprehension on page 24.
Answer: The matter was addressed by replacing abbreviations in titles with their full names for enhanced comprehension on page 25.

12) It's important to note that for super-resolution on page 30, there's often a trade-off between image quality and realism.
Answer: Thank you for the comment! Added a note about the trade-off between image quality and realism at page 66.

13) Page 31 should address the effects of training on a specific raw material system and explore different setups for precision.
Answer: A note about the effects of training on a specific raw material system and different setups was added on page 32.

14) In discussing the evaluation of segmentation results on page 31, it may be more concise to summarize the process.
Answer: The note about trade-off between resolution and reality and how it affects the segmentation was added in the Chapter 5 devoted to the development of super-resolution algorithm on page 69.

15) The choice of reduced resolution over full resolution and its impact on precision should be explained on page 36.
Answer: More explanation about the downgrading was added to page 37

16) On page 38, provide insights into how parameters were optimized for XCT imaging.
Answer: Insights into how parameters were optimized for XCT imaging were provided on page

37

17) Consider discussing the potential impact of different window settings on results on page 39.
Answer: the windows are the same, but from the different materials. A clearer caption is added to avoid misinterpretations on page 41.

18) Page 41 should specify the methodology for inpainting and, optionally, this section could be moved to the related works.
Answer: The methodology for inpainting is provided in the introduction of the Chapter 4.

19) On page 49, it's crucial to clarify how a specific method was adapted and its relevance to the study.
Answer: Thank you for the comment! Page 50 explains the theory about the generative adversarial networks. The clarification of how this model was adapted and how it used is explained also later in the text.

20) Page 50 should detail the experiments conducted to support the claims made.
Answer: The algorithms were tested by a number of works, but indeed it is not clear from the text. the references and some explanations are added to page 51.

21) Provide insights into the exploration of the parameter space for CNN5 and CNN9 on page 51, specifying the considered parameters.
Answer: Deeper neural networks, such as CNN9, were also under consideration; however, their substantial GPU memory requirements, coupled with hardware limitations, precluded their training during this research. The architecture with the highest complexity that could be accommodated within the GPU memory, namely CNN7. An explanation about the use of CNN9 was additionally provided on page 53-54.

22) The justification for using LeakyReLU as an activation function should be explained on page 52.
Answer: LeakyReLU is chosen as the activation function for its ability to prevent the vanishing gradient problem, promoting more stable and efficient training. The justification of LeakyReLU function usage was presented on page 53.

23) Clarify why Mean Squared Error (MSE) was chosen over other error metrics on page 54.
Answer: MSE is often preferred in GANs for its simplicity and sensitivity to small errors, making it suitable for fine-tuning the generator's output. It aligns well with the GAN objective of minimizing the discrepancy between real and generated data. A clarification about MSE metric was added on page 56

24) Explain the rationale behind opting for bicubic interpolation and provide information on training duration on page 55.
Answer: Bicubic interpolation was chosen for its superior capability to provide smooth and continuous image downscaling, which is crucial for preserving fine details when working with high-resolution CT scans. The duration of training was 24 hours for all models. More explanation about the downgrading was added to page on 37.

25) On page 56, address the stability of results under different conditions and the criteria used for selecting specific values.
Answer: The hyperparameters values on page 57 was chosen based on literature review and additional in-lab testing to ensure the stability of generative results. It was not included to the thesis, because it is not a focus of the research.

26) The reasoning behind the 24-hour training duration and the difference for CNN3 should be explained on page 58.
Answer: The decision to train for 24 hours was driven by the challenges in GAN training, as both analytical and adversarial metrics can plateau while image quality continues to improve. Additionally, to ensure an equitable comparison, an equivalent training duration was adopted for CNN3, CNN5, and CNN7, despite their distinct convergence times. Explanations on the choice of the 24-hour training were added on page 61.

27) Address artifacts in relation to RVE size on page 59 for a comprehensive understanding.
Answer: While specific evaluations of GAN performance on RVEs of varying sizes were not conducted, it is anticipated that generating larger RVEs may lead to a heightened presence of artifacts. This effect is expected to be more pronounced when using smaller neural networks compared to larger ones. The artifacts in relation to RVE size on page 63 were addressed.

28) Provide additional context for the observed errors on page 60.
Answer: Minor artifacts are present at the periphery of the generated area, resulting in a less-than-optimal smoothness in the border transition. Added more discussion on the observed artifacts on page 63.

29) On page 70, discuss why ADAM stochastic gradient descent was chosen as the optimization algorithm.
Answer: As during the training of inpainting algorithm, ADAM stochastic gradient descent was selected for its ability to efficiently handle noisy gradients, making it well-suited for the training dynamics of generative networks. Its adaptive learning rate and momentum mechanisms help enhance convergence during GAN training. The use of ADAM stochastic gradient descent was discussed in more detail on page 74.

30) Justify the use of RaGAN on page 71 and explain its relevance to the research.
Answer: RaGAN is employed in super-resolution due to its capacity to enhance the generator's ability to produce realistic high-resolution images by improving gradient flow and reducing training instability, ultimately leading to sharper and more visually accurate results. Justification of the use of RaGAN loss function is added to the discussion on page 75.

31) Discuss the influence of the SSIM metric on the research results on page 72.
Answer: In the case of this study is not the most important metric and it does not influence the results of the research.

32) Page 74 should address greyscale and contrast issues and consider discussing the nature and extent of artifacts.
Answer: The artifacts and contrast different are caused by different CT system parameters to insure the difference in the resolutions.

33) Mention any studies conducted on lined artifacts on page 75.
Answer: The presence of textured defects in SR images can be attributed to the use of convolutional layers in neural networks. While it is feasible to mitigate these defects by fine-tuning training hyperparameters, it's essential to note that, for the purposes of this research, these defects have no significant impact on the accuracy of fibre analysis results. Discussion on lined artifacts was added on page 79.

34) Provide insights into the practical implementation of super-resolution on page 76.
Answer: The possible implementation includes the ability to replace multiple post-processing techniques such as denoising and contrast enhancement, streamlining the image enhancement process and providing more accurate and visually enhanced results. The note was added to page 82.

35) Address challenges related to shape variation and artifacts on page 76.
Answer: The shape variations and artifacts are caused by the randomness nature of the neural network, and unfortunately it is not possible to avoid such variations.

36) On page 76, discuss the perceived high SSIM for HR noisy and provide training time and general performance details.
Answer: Overall, the values in Table 9 shows the difference between the original HR images and other processed images. We observe a small MSE error and a high PSNR metrics for SR images compared to other images, which imply a high visual similarity between HR and SR images. The changes were added to pages 80 and 81.

37) Explore the potential of super-resolution in improving segmentation on page 77.
Answer: The potential of super-resolution extends to improving segmentation accuracy by providing finer image detail, facilitating sharper object boundary delineation, and ultimately improving the overall quality of segmentation results. The conclusions were improved of the SR chapter on page 82.

38) On page 83, provide reasoning for the preference of specific methods over others and mention alternative metrics.
Answer: The preference for PA and IoU is due to their meaningful representation of pixel classification and spatial overlap, which are fundamental to segmentation tasks. These metrics are widely accepted in the research community for their clarity and interpretability. However, the specific requirements of a task and dataset should also be considered, and alternative metrics such as Dice coefficient, F1 score, and memory-related metrics may be relevant depending on the context. The notes and the paragraph were added to 87-88 pages.

39) Specify column names for images on page 88 and compare the developed method against manual segmentation, micrography, and CFC.
Answer: The names of the column was added tot the Figure 30. The methods were compared with the manual segmentation only since other means of micrography are not able to analyse the internal material microstructure.

40) Discuss the usefulness of conventional segmentation slice reconstructible tools on page 89.
Answer: Conventional segmentation algorithms prove especially beneficial in straightforward cases where image objects are easily distinguishable. The discussion added to page 94.

41) Address the limitations of deep learning methods on page 91.
Answer: The limitations of deep learning segmentation, compared to other methods, include a higher demand for labelled data, computationally intensive training, susceptibility to overfitting in small datasets, and the "black box" nature of deep neural networks, which can make the interpretation of results challenging. The limitations of deep learning segmentation were addressed on page 93.

42) Explain the need for new training in the context of segmentation on page 91.
Answer: All of these methods require retraining for each new dataset. This is essential because it allows the model to adapt to the different features, characteristics, and variations specific to each dataset. Training is the means by which the model learns to extract relevant patterns and structures, ensuring accurate and context-specific segmentation results for each dataset. The note was added to page 94.

43) On page 103, explain the choice of the method mentioned.
Answer: The method allows to reach the convergence of effective elastic properties on minimal microstructures considered. Also, the initial sizes of RVE account for the effects of fiber orientation, shape, and distribution on the composite material.

44) Consider using visualization to explore additional aspects on page 121.
Answer: Thank you for the suggestion. The image was updated to make it clearer to the reader.

45) Discuss why the developed models tended to underpredict material stiffness on page 122.
Answer: The main possible reason is that the input parameters used for the fibre-matrix system may not be precise enough, and an increase in matrix stiffness, for instance, could lead to higher model predictions than the predicted tensile stiffness.

46) Investigate the presence of artifacts in super-resolution on page 132.
Answer: Likewise, linear artifacts are noticeable, similar to what's observed in short fibre composite CT image super-resolution. Importantly, these artifacts have minimal impact on the results. Discussion about artifacts of SR was also added to page 139.

47) Consider future work related to speed enhancements on page 141.
Answer: Of course, one of the possible future steps is to increase the speed of training of both inpainting and super-resolution algorithms.

48) Elaborate on the concept of a universal super-resolution model on page 146.
Answer: The universal super-resolution model should be continuously trained on different CT datasets, enabling it to consistently improve the quality of CT images across different materials and scenarios. The concept of universal super-resolution model was elaborated on page 152.

Reviewer 2: Prof. Frederik Desplentere

pre-p. 4 In case this is based on micro-CT input data
Answer: A note added to page V in the abstracts.

pre-p.4 Fibre breaks is not easy to translate within a RVE with PBC’s

Answer: During the SR verification using unidirectional fibres periodic boundaries were not used, so the fibre breaks were not translated within RVEs in the SR verification case.

p.1 impart: I don't know/use this word
Answer: It is a typo, thank you! Corrected.

p.11 I wonder if this research will look for modelling of defects.
Answer: Indeed the modelling of defects is more difficult task, in this case we would need more specific micro-CT data of defects to correctly train the networks.

p. 12 Considering the size limit of 2000-4000 pixels in one dimension, the sample size should be less than 1000-2000 times smaller than the features of interest: Isn't it opposite??
Answer: Indeed, it is a typo! Thank you. Corrected in the text.

p. 22 Describe as it is shown on the figure.
Answer: Thank you! Corrected the miswording.

p.32 This material also was panel was manufactured in the shape of a flat, circular table measuring 30 cm in diameter: sentence
Answer: The sentence was unclear, rewritten to make it better.

p.32 Due to the circular shape of the plates, the orientation of the specimens was not fixed. The tests were performed: it would be nice to see an example of those plates.
Answer: The plates themselves are not documented. However, the plates are quite simple: they are just flat circular shapes from which specimens were cut for mechanical testing.

p. 33 I'm in favour of mentioning coefficient of variation (1 stdev / average value)
Answer: It is a good idea to add this characteristic to the table! Added.

p. 36 Idea of the production process.
Answer: The type of production process was added to the Figure 13 caption.

p. 102 Provide insights into determining the appropriate size of the RVE.
Answer: The RVE size was determined by following the method outlined by Singh [47]. This approach ensures robust and reliable results, more description is in the Section 6.1.3

p.145 Reflect on potential implications of the research.
Answer: The research has potential implications for advancing the understanding and application of deep learning generated structures in materials science and finite element simulations. It provides insights into improving accuracy and predictive capabilities, ultimately benefiting fields that rely on material property predictions and simulations. The conclusion on page 149 was updated.

Reviewer 3: Dr. Larissa Gorbatikh

1) It is suggested that the developed methods (for CT image processing to microstructure generation) are more efficient in comparison with the state of the art methods thanks to the machine learning capabilities. One can image that this is the case once the tools are "trained". However, the training takes significant resources and time. Could you please give your objective opinion on the efficiency of the developed tools with the training part included in calculation. In which cases will the new tools be most beneficial and in which case conventional approach may

still work very well?
Answer: Indeed, important question. The developed methods represent an initial step toward utilizing deep learning-generated models for material behaviour simulation. While the training process requires significant time and resources, these tools show promise in enhancing efficiency, particularly in scenarios with complex microstructures or limited experimental data. Conventional approaches may continue to excel in cases where simpler microstructures are involved, and well-established models are readily applicable.

2) Who are the future users of the developed tools (considering their limitations and advantages)?
Answer: In the author's opinion, the potential future users of the tools developed are primarily researchers and then engineers in the fields of materials science, engineering and industrial X-ray computed tomography. These tools offer a number of new functionalities such as improving image quality, automating defect detection and generating periodic RVEs for finite element analysis. The tools can be particularly useful for the further development of image-based or deep learning generation-based FE simulations.

3) Most composites have some amount voids. What is the potential of the inpainting methodology to the generation of microstructures with fibers and voids at the same time? What about fibers made of different materials and of diameters, like in the case of hybrid composites? How easy or difficult would it be to extend existing tools to these cases?
Answer: The potential of the inpainting methodology for generating microstructures with both fibres and voids simultaneously depends on the availability of a balanced dataset with such features. Adapting the algorithms for hybrid composites and varying fibre properties would be also feasible with a new dataset that includes these specific features. It would not be difficult to extend the existing tools to address these cases, provided the dataset is appropriately prepared.

4) Please provide justification for the use of FEM with embedded elements instead of the standard FEM.
Answer: The use of embedded elements in FEM, especially in Abaqus software, is justified due to their ease of implementation and the demonstrated comparable results to other simulation methods. This simplifies the modelling process without compromising the accuracy of the simulations

Reviewer 4: Dr. Mahoor Mehdikhani

P 63: You show that CNN7 outperforms CNN3 and CNN5. What about CNN9? Is CNN7 performance close to a plateau?
Answer: Deeper neural networks, such as CNN9, were also under consideration; however, their substantial GPU memory requirements, coupled with hardware limitations, precluded their training during this research. The architecture with the highest complexity that could be accommodated within the GPU memory, namely CNN7. An explanation about the use of CNN9 was additionally provided on page 52

P 63: Is the 3D performance of these methods evaluated? How slice-to-slice consistency compared to the 2D methods?
Answer: The networks produce 3D microstructure representations of materials, a capability beyond the reach of classical 2D inpainting algorithms. An explanation of 2D vs 3D inpainting

was added to the conclusion on page 66.

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?
Answer: This is a good question. Basically, when we generate new data, we should not rely on MSE and PSNR because the new data may not be exactly the same as the data used for training. But for SR, we need to be sure that the enhanced image is the same as the original. This is why we mostly rely on the MSE and PSNR when developing the super-resolution algorithm.

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).
Answer: Indeed, it is a good thing to compare the physical parameters as well. The comparison of fibre diameters in UD composites was added to Table 9 and Table 11 to provide the comparison of the physical parameters. Also some discussions were added to page 94 and 82.

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?
Answer: The volume fraction was calculated from the fibre mass fraction used during the manufacturing of composite materials. More explanation of the use of fibre volume and mass fraction was added on page 108.

P 105: you have applied PBC to these models. Do the models have periodic boundaries?
Answer: In this instance, the models lack periodic structure, but the implementation of PBC serves to approximate the RVE size as closely as possible to the final simulation. A note about the use of PBC for RVE size determination was added on page 111.

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?
Answer: The generated periodic structures shown in Figure 39 demonstrate that the algorithm was able to successfully generate microstructures with over 90% periodicity (pixel correlation of opposite faces), a substantial improvement compared to the original images which had approximately 50% periodicity. A note about the periodicity evaluation was added on page 119.

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
Answer: The images shown here are from the original images and serve to illustrate the initial quality of fibre identification using probability maps, as well as the method of combining probabilities across different slices. It is noted that the physical properties of the generated objects are very similar to those of the original volume on page 118, as can be seen from the inpainting in Chapter 4. It's worth noting that Figures 42 and 43 represent periodic structures, although their 3D representation may be challenging due to the inherent complexity of the microstructure.

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 possible 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?
Answer: The argument is based on the premise that the matrix properties may have been undervalued and should have been examined more thoroughly in subsequent investigations. Under such circumstances, the simulation results could potentially be higher for both the original and periodic models, with both possibly exceeding the experimental values. Therefore, in this case, the periodic simulation would already yield results that are closer to the experimental data.

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"?
Answer: The statement about the tetrahedral models being "more physical" is grounded in the observation that these models generate fewer elements with von Mises stresses exceeding the critical threshold of 5-6%. This outcome can be attributed to the structural characteristics of the voxel models, which feature a ladder-like structure with sharp edges and lack the smooth curves found in tetrahedral models. The sharp edges in voxel models can lead to stress concentrations in more elements, resulting in non-physical outcomes, such as a higher percentage of failed matrix elements. Consequently, it is on the basis of these considerations that the assertion of tetrahedral models being "more physically correct" is made. More discussion is added to page 131.

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.
Answer: Thank you for the suggestions! Indeed, during the work we considered different terminology, but chosen terminology was used in the text.

P 61: Isn't it better to present some (average) numbers of Table 6 on a graph?
Answer: we opted to display all figures with average numbers highlighted in bold. This choice was made to show all the statistics for comparison of whole volumes vs ROI reconstruction.

P 61: Table 6: What is the size of the whole volume and the ROI? Is the RIO equal to the masked volume?
Answer: The whole size of the volume is 64×64×64 pixel^3 and the size of ROI indeed equal to the masked volume 32×32×32 pixel^3. A short addition was introduced on page 63.

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
Answer: An additional image was added on page 59 for more clear understanding of metrics used

P 74: Figure 25b has a different contrast. Doesn't it influence the results? Why don't you show the original low-resolution image?
Answer: The different contrast in the images results from different CT parameters used to ensure that super-resolution is based on authentic physical data rather than generated. To the human eye, the original LR and the interpolated images appear nearly identical, with the interpolated image

having a higher pixel count. This increased pixel count is advantageous for computer-based image analysis purposes.

P76: How do the values in Table 9 relate to the original HR images? Do they show the difference with HR values?
Answer: Indeed, the table was not very clear. The table description and the table itself were corrected.

P76: “We observe a very small MSE error and a very high PSNR” what do you mean with very small and very high?
Answer: We observe a small MSE error and a high PSNR metrics for SR images compared to other images, which imply a high visual similarity between HR and SR images. To make the statement clearer, a note added about the MSE and PSNR metrics on page 81.

P104: Can you include a thresholded slice in Fig. 33?
Answer: Of course! A thresholded slice of the model was added in Fig.34.

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

P 121: what are we supposed to see in this figure?
Answer: The images supposed to show the readers the internal microstructure of the finite element models. The quality of the images was improved.

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?
Answer: Legends and labels have been included in the images as suggested. The term "non-physical stress fluctuations" refers to the observed inconsistencies between opposite faces of the model. Specifically, a significant difference is noticed between faces a) and b), which is not characteristic of a model with implemented PBC where a smoother transition is expected. In contrast, images c) and d) show much smaller differences, resulting in a more uniform transition from one face to another.

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?
Answer: Thank you for bringing this to my attention. It should indeed be "the higher error in effective properties" instead of "higher effective properties," and I appreciate your observation. The lower predicted effective properties in the voxel model can be attributed to the presence of more elements, which can result in stress concentrations not propagating as far as in the smoother model. As a result, the volume affected by stress concentrations is larger in the voxel model, contributing to the higher predicted effective properties.

Reviewer 5: Prof. Alexander Safonov

1) It is necessary to improve the style of the text. There is no dot in the titles of chapters and tables. Use the same style of tables and formulas. Check the numbering of formulas.
Answer: The dots were added to the titles of chapters and tables. The formatting for all tables was updated. The numbering of formulas was additionally checked.

2) It is recommended to add an overview of methods and algorithms for Machine learning based image processing in Chapter 1.
Answer: Thank you for the comment! The overview of the methods and algorithm for machine learning image processing is performed as separate introduction to each section. In my opinion, the separate introductions provide clear context for each case and explain the limitations of conventional methods.

3) Chapter 4 recommends justifying the choice of materials used.
Answer: The choice of a short-fibre composite with a relatively high fibre volume was motivated by the need to address the limitations of conventional methods, which struggle to generate RVEs with such high-volume fractions. Additionally, random fibre composite materials lack periodicity, making it exceedingly challenging to create accurate models for such composite materials. More explanation was added to Chapter 4.

4) Check formula (17).
Answer: Thank you! There was a typo in indexes.

5) Explain the stress designation in formula (21).
Answer: The stress designation in formula (21, 23 in the new numbering) follows the same conventions as those in equation (17, 19 in the new numbering). To enhance clarity, the stress designation was included.

6) In Chapter 6, describe exactly for which materials the results were obtained. For example, for which material the results are given in Table 14.
Answer: Chapter 6 is mostly devoted to the 1000C material, which was selected for periodic boundary generation due to its random microstructure. More notes added to Chapter 6.

7) Improve the quality of Figure 44.
Answer: The quality of Figure 44 was improved.

8) In Table 16 explain which module is meant for E22. Give values for E33.
Answer: In this research, the properties E11 and E22 were calculated to account for the prevalent orientation of the material, which exhibits almost transversely isotropic behaviour. E33, representing the property perpendicular to the prevalent orientation, was not explicitly calculated as it aligns closely with E22 due to the minimal orientation preference in the material. More notes were added on page 127.

9) It is recommended in Chapter 6.1 to make a comparison with analytical models for calculating mechanical properties.
Answer: Thank you for your comment! Indeed, adding a comparison with analytical models for calculating mechanical properties of short fibre composites is a valuable suggestion. While it was not initially part of the research plan, I will incorporate this comparison into a paper dedicated to the use of periodicity generation. This paper is scheduled for submission in 2023.

10) Add a legend to Figure 45.
Answer: A legend for the Figure was added.

11) It is recommended to describe how the results obtained can be applied in the engineering practice of designing new composite materials.
Answer: At this stage, the research results may not be directly applicable to engineering practices due to the complexities of data collection and deep learning model training. However, the developed algorithm has the potential to be integrated into existing FEM or CT software. Engineers could then use this software to obtain initial predictions of effective mechanical properties based on limited material samples, reducing the need for extensive and often costly full-scale mechanical testing at first stages of composite material development. This note was also added to the conclusion of the thesis.

Reviewer 6: Prof. Oleg Vasilyev

The organization of the thesis is a little unorthodox, mainly due to presence of multiple introduction (5.1.1, 5.2.1, 5.3.1, 6.1.1, 6.2.1) and conclusion (5.1.7, 5.2.6, 5.3.5, 5.4, 6.1.6, 6.2.5, 6.3) subsections, which is probably the artifact of the subsections being published as papers. Conclusion sections 5.4 and 6.3 read more like summary. These organizational peculiarities are not critical and do not affect the quality of the thesis. However, they are distractive to the reader to the point that I wanted to mention them in my report.

Answer: Indeed, the presence of multiple introductions was a deliberate choice, as it allows me to clearly present the specific methods and their applicability in each section without causing confusion (though it may seem distracting to some). Combining them into a single introduction could lead to a loss of focus in the thesis. The main objective of the thesis is to improve CT-based simulations of composites, and these individual introductions help to set the context for each case and explain why conventional methods cannot be used for the specific purposes. I hope that for a reader new to machine learning, the separation of these discussions will aid clarity and understanding. I appreciate your suggestions for improving the thesis. Thank you for your feedback!