Combining Stochastic Geometry and Neural Models of Electron Matter Interaction for the Simulation of Electron Imaging of Porous Materials

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ABSTRACT

We introduce a neural surrogate model that approximates Monte Carlo simulations used in scanning electron microscopy (SEM) imaging of porous materials. These materials are important in practice, but their SEM images often contain artifacts, particularly where the electron beam enters pores and interacts within them. Due to these artifacts, synthetic back-scattered electron and secondary electron images are valuable for both verifying image interpretation and training machine learning models for classification and segmentation. However, Monte Carlo simulations of electron interactions are computationally expensive.

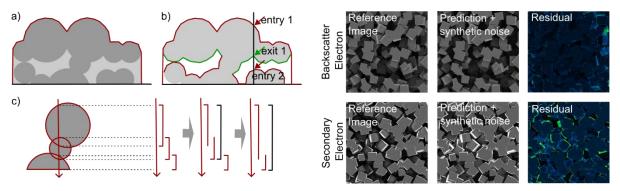


Figure 1. Left: Primitive lists are converted to a network-friendly representation. a) Heighfields are suitable for convolutional networks, but can not represent pores. b) Extended heightfields allows to remove this restrictions. c) A GPU-friendly algorithm computes the extended heightfield and resolves the constructive solid geometry of simultaneously. Right: Results of the neural model for backscatter electron and secondary electron contrast.

As an alternative, we present a hybrid approach that combines statistical geometry modelling with an encoder network. The model accepts 3D microstructure data in the form of primitive lists, converts it into a neural network-friendly representation, and uses a convolutional architecture to generate 2D back-scattered and secondary electron images in a single forward pass. This approach offers a performance boost of 4-5 orders of magnitude over conventional simulations and works well on arbitrary microstructures, even those of cubes, despite being trained only on sphere and cylinder-based structures.

Extending over previous results, we show here that very deep residual network architectures with 101 or 152 layers can further improve the simulation accuracy, but require very long training to avoid overfitting. A python package including the trained networks is released as open source.

REFERENCES

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