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## Deep learning and chemical constraints allow accurate segmentation of $\mu$ CT data from metamorphic rocks

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X-ray tomographic imaging has become a very valuable tool for the analysis of (rock) materials, both for visualising complex 3D microstructures and for imaging internal features such as damage, mineral reaction, and fluid/rock interactions quantitatively. The validity of the results derived from X-ray tomography, however, hinge on the accuracy of the image segmentation. There are many methods for image segmentation (from simple manual thresholding to machine learning and deep learning approaches), which can produce a high range of variability in the segmentation results. Accuracy of segmentation results is seldom checked and thus calling the reproducibility of the results into question. In this contribution we show how metamorphic reactions themselves can be used to constrain accuracy and highlight the benefits of deep learning methods to extend this over many large datasets efficiently.

Here, we demonstrate a methodology that uses deep learning to achieve reliable segmentation of time-series volumetric images of gypsum dehydration reaction, on which standard segmentation approaches fail due to insufficient contrast. We implement 2D U-net architecture for segmentation, and, to overcome the limitations of training data obtained experimentally through imaging, we show how labelled data obtained via machine learning (i.e., Random Forest Classification) can be used as input data and enhance the neural network performances. The developed deep learning algorithm proves to be incredibly robust, as it is able to consistently segment volume phases within the whole suite of experiments. In addition, the trained neural network exhibits short run times (<7 minutes for ~250 MB of image volumes) on a local workstation equipped with a GPU card.

To confirm the precision achieved by our workflow, we consider the theoretical and measured molar evolution of gypsum (CaSO4.2H2O) to bassanite (CaSO4.½H2O) during the dehydration. Within all time-series experiments, errors between the predicted theoretical and the segmented

volumes fall within the 5% confidence intervals of the theoretical curves. Thus, the segmented CT images are very well suited for extracting quantitative information, such as mineral growth rate and pore size variations during the reaction. To our knowledge, this is the first time an internal standard is used to unequivocally measure the accuracy of a segmentation model. Being able to accurately and unambiguously measure the volumetric evolution during a reaction enables high-level modelling and verification of the physical (hydraulic and mechanical) properties of rock materials involved in tectono-metamorphic processes.