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MatCHMaker
Materials Characterisation & Modelling

MATERIALS CHARACTERISATION OF MICROSTRUCTURES WITH MACHINE LEARNING

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Questions & Answers

1. WHY DO WE CARE?

Microstructure is the cornerstone of our understanding of materials properties and strategy for performance optimisation. To characterise quantitatively microstructures is therefore of critical importance for materials scientists.

2. WHAT IS NEW?

The development of machine learning (ML) algorithms for image analysis has not yet been imported in our field. The literature dedicated to electron microscopy and image analysis for materials still relies mostly on lengthy histogram-based, morphological and spectral operations.

3. WILL IT WORK?

Our preliminary work on cement pastes is promising. Clustering algorithms allowed us to better understand the kinetics of carbonation, thus helping us to optimise carbon capture.

4. WHAT IS NEXT?

a) Convolutional neural networks and autoencoders will be implemented to further segment and analyse electron microscopy images.
b) From the segments, the porosity and PSSD of each mineral phase can be recovered and plugged into micro-mechanical models to predict material strength.
c) Uncertainty estimations algorithms will be implemented.

Motivations & challenge:

Materials science aims at bridging the gap between materials elaboration processes and their macroscopic properties through an understanding of the key microstructural features. To understand the process – microstructure – properties relationships then enable to predict and optimise materials performance. The microstructural origin of compressive strength of cement pastes is for example dictated by the porosity and mechanical properties of each constituent phase [1]; in metals, the mechanical properties depend on the grain sizes [2, Chapter 2]. To characterise microstructures precisely is therefore a critical task. Scanning electron microscopy (SEM) is one of the workhorses of materials scientists. SEM generates a variety of images that need to be analysed to yield relevant information. **→ Answer 1.**

Despite the importance of SEM image analysis, there does not yet exist a related textbook that takes advantage of machine learning (ML) techniques. The three references closest to SEM image analysis may be [3], [4] and [5]. These textbooks focus on traditional image analysis techniques that rely on geometrical, morphological and spectral operations; only very recent ones ([5] published in 2023) include a chapter on deep learning. According to Merchant [5], **the main bottleneck is the absence of an available wide dataset of labeled SEM images** [5, p449]. **→ Answer 2**

[1] Pichler, B., Hellmich, C., & Eberhardsteiner, J. (2009). Spherical and acicular representation of hydrates in a micromechanical model for cement paste: prediction of early-age elasticity and strength. *Acta Mechanica*, *203*(3-4), 137.
[2] Ashby, M. F., Shercliff, H., & Cebon, D. (2018). *Materials: engineering, science, processing and design*. Butterworth-Heinemann.
[3] Wojnar, L. (2019). *Image analysis: applications in materials engineering*. Crc Press.
[4] Heilbronner, R., & Barrett, S. (2013). *Image analysis in earth sciences: microstructures and textures of earth materials* (Vol. 129). Springer Science & Business Media.
[5] Merchant, F., & Castleman, K. (Eds.). Second edition (2023). *Microscope image processing*. Academic press.

Preliminary results: carbonation of cement pastes

Preliminary results on cement pastes are promising. Clustering algorithms like the K-Means extract the phase assemblage of cement pastes from SEM (figure 1). The clustered picture (figure 2) shows that the kinetics of carbonation does not happen in one single step: there is not one but two main carbonated phases (red and white clusters). This is important knowledge to optimise carbon capture. **→ Answer 3.** Furthermore, the particle size and shape distribution (**PSSD**) of each cluster can be recovered. The PSSD + mechanical properties of each phase (obtained by nano-indentations done at TU-WIEN-IMWS) is inputted into a micro-mechanical model to predict the overall compressive strength. **→ Answer 4 b).**

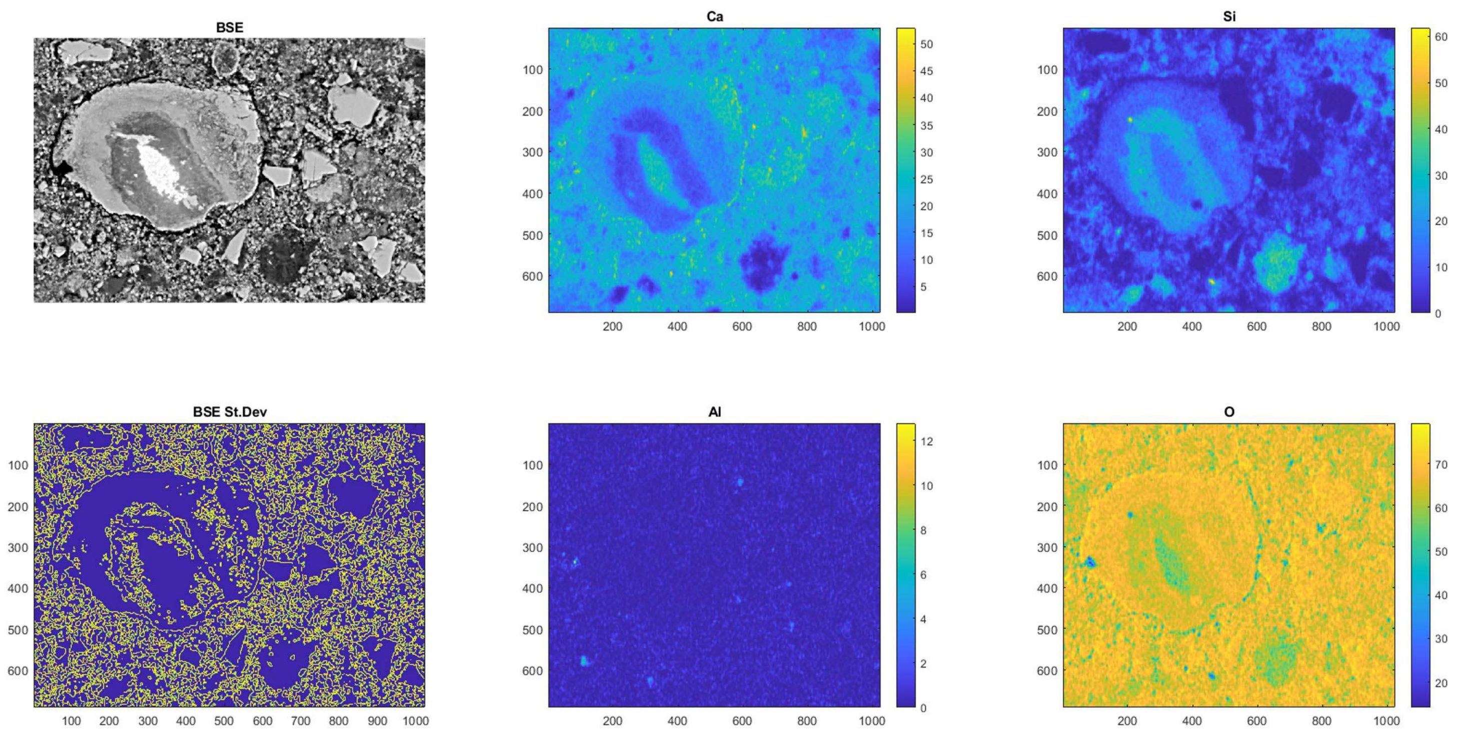
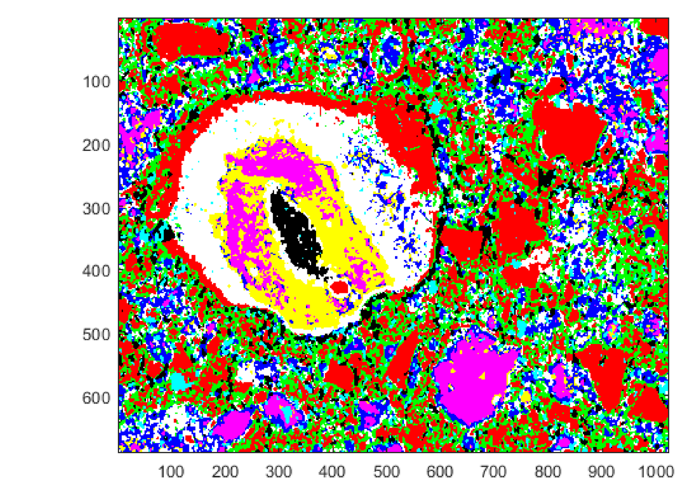


Figure 1: SEM images of a carbonated cement paste. Top left: BSE, bottom left: corresponding Sobel edge detector. Middle and right columns: SEM-EDX atomic concentration in Calcium, Silicon, Aluminum and Oxygen.



Cluster	Surface Area	Calcium	Silicon	Oxygen
Red	26 %	3	3	69
White	18 %	2	10	67
Pink	7 %	25	26	60
Yellow	6 %	23	20	64

Figure 2: K-Means clustered image of figure 1 and corresponding table of cluster properties (all in [at. %]).

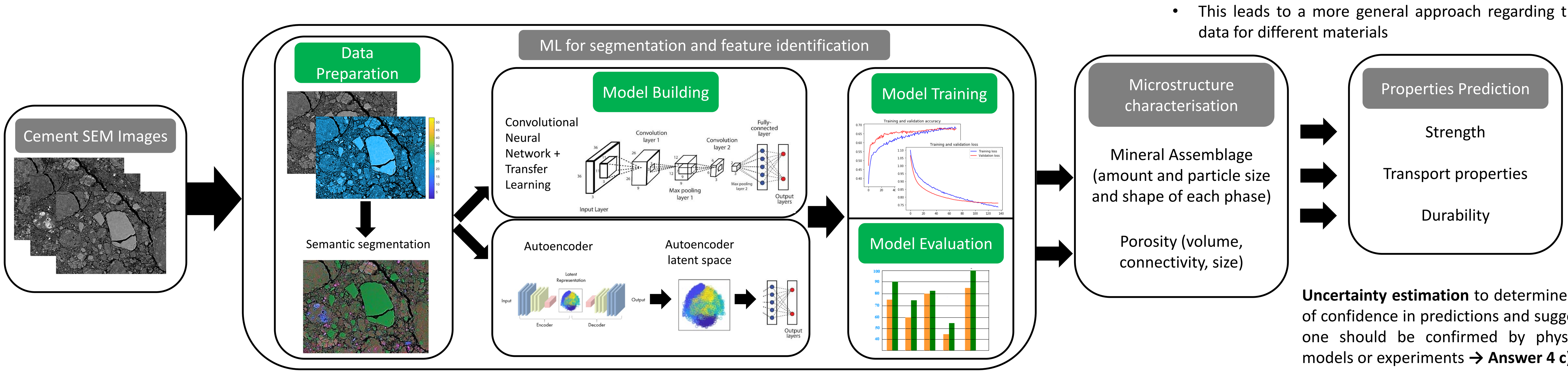
Next steps: Convolutional neural networks, auto-encoders & uncertainty estimation

Data preparation:

- Use of different unsupervised learning (e.g., k-means) to identify phase clusters in the SEM images and extract relevant information
- Raw data and segmented data are to be used both or separately to feed a Deep Neural Network for image analysis and properties prediction

Model building (Main difficulty: low amount of labelled data)

- 1st approach: Transfer learning with CNN
  - Train a CNN on a large database of images, preferably SEM images
  - Freeze the first layers of the pre-trained CNN and only train the last layers for properties predictions in our specific use case
- 2nd solution: Autoencoders
  - Reduce dimensionality by using unlabeled data on SEM images of different materials
  - Work in the latent space to predict the properties, the necessary amount of labelled data is expected to be lower in this low dimension space
  - This leads to a more general approach regarding the SEM input data for different materials



Uncertainty estimation to determine the level of confidence in predictions and suggest which one should be confirmed by physics-based models or experiments **→ Answer 4 c).**

We look for partnerships and synergies with other European projects to build case studies and transversal algorithms for all classes of materials: metals, polymers, ceramics, geomaterials, etc.
In a first step, we simply need to build a database of images: come discuss with us over a coffee ☺.

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