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Image registration, dimensionality reduction and semantic segmentation of combined optical and chemical images: Discoveries in an example of carbon mass-balancing in a pelagic limestone

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Superimposed high-resolution optical and chemical whole-slide imaging (WSI) stacks tie elemental to textural, structural and mineralogical properties. Experts can appreciate meaningful correlative microscopy associations of diagnostic chemical with certain optical features. However, with increasing number of chemical WSI channels, the dimensionality rapidly overwhelms the human capacity to pinpoint all relevant associations, leaving important features undiscovered.

Here, we combined optical (0.14 µm/px; 6 GB) with chemical (~1.5 µm/px; 2.5 GB) WSI from synchrotron X-ray Fluorescence Microscopy (XFM) covering an entire thin section of a hemipelagic limestone (Kaiwhata Formation, NZ). Optical WSI shows micrite, micro-fossils, burrow marks, 'dykes', micro-dissolution seams and several bedding-normal calcite vein generations. XFM maps acquired at 18.5 keV (to capture heavy elements) were selected before applying a median-filter (5x5) and principal component analysis (PCA) represented as a single false-colour RGB image. The four images (reflected, PPL and XPL, XFM PCA) were registered in the Fiji software ecosystem and imported into QuPath for agnostic annotation and semantic segmentation following [1] in a 3-hour workflow.

The segmentation revealed unprecedented level of detail, highlighting cryptic structural features from noise, separating >2 micro-fossil species, 3 types of micrite matrix, 3 vein generations (1 invisible in XFM PCA alone), 1 macro- and 1 micro-stylolite, and >5 detrital minerals. The developed segmentation approach could enable quantitative estimates of the amount of CO_2 dissolved by diagenetic micro-dissolution seams in this formation. A pilot study of the Kaiwhata limestone localised diagenetic micro-dissolution seams with XFM related to macro-stylolites [2]. The 1-D mass balance calculated that micro-dissolution seams mobilised ~10% of total carbon. Seam abundance depends on contact with fossil and detrital objects, networking of micro-dissolution seams and tectonic regime interpretation. For large datasets sampling the entire formation, an automated segmentation approach would require to recognise these features, as achieved by the bioinformatics pixel-based approach presented here for a complex sample. It will thus permit 2-D computations of diagenetic fluid flow and dissolved carbon and tracking of release pathways from carbonate mud at the ocean floor.

1. Acevedo Zamora & Kamber (2023) Minerals 13(2):156.
2. Schrank, et al. (2021) Commun Earth Environ 2 174.