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A step change in multi-dimensional zircon provenance analysis from forward registered CL, U/Pb age, and trace element data

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Morphology, internal structure, age, trace element and radiogenic isotope information of detrital heavy minerals all carry provenance information, exploitable with computerised classification schemes. These become more powerful with combined data sources (e.g., U/Pb with (U+Th)/He dates, Hf-isotopes). Incorporating ever more data for accurate provenancing poses two main challenges: (i) all data need to be spatially registered and (ii) the dimensionality of the full data needs to be reduced for intuitive exploration. We have built a new forward registration solution based on scripts that orchestrate bioinformatics and geospatial image analysis freeware and new algorithms. Here we demonstrate how researchers can interact with such data in a single data space simultaneously visualising age, geochemical and CL information of zircons from a modern river drainage system.

In the example, we reduce multi-trace element chemical systematics into 2D with a non-linear technique (uniform manifold approximation and projection). Unlike conventional PCA, the projection searches neighbouring points, calculates, and preserves the closest 2D fuzzy topological structure, reflecting local and global variance in relation to large literature datasets. The result is a map, where zircon spot data plot as clusters and branches, effectively grouping zircons from different types of source rocks. Rather than representing each zircon date as a symbol, our spatially integrated image registration shows each grain as its CL image, crucially permitting users to deploy the innate human image processing capacity (akin to a video game) for detection of interdependencies between geochemical clustering and CL appearance.

The final dimension of the cube is the $^{206}Pb/^{238}U$ date, which lifts and distributes the geochemistry clusters and branches of CL images into 3D. Researchers can now detect whether different geochemical groups of zircons contribute to the same age class (e.g., Grenville), whether discordance causes spurious age spread, and if zircons of similar CL appearance are related in age or chemistry or both. Such data cubes from sequential provenance samples can be scrutinised for the appearance or disappearance of unique clusters of grains with stratigraphy.

The forward image registration and dimensionality reduction are flexible for deployment on different target minerals and sources of image, chemical and isotope information.