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Clustering spICP-ToF-MS data for nanoparticle detection

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Single-Particle Inductively Coupled Plasma Time-of-Flight Mass Spectrometry (spICP-ToF-MS) is a powerful analytical technique that can be used for the characterization of nanoparticles (NPs), such as their mass distribution, number concentration and elemental composition. However, evaluating the large amounts of data generated can be challenging and requires the development of advanced data processing methodologies. We here propose a novel machine-learning approach to blindly explore spICP-ToF-MS data and automatically characterize NP populations.

We first perform a template-matching analysis on the raw spICP-ToF-MS data, by evaluating the similarity between automatically-defined templates and a sliding window of the continuous time-based record. This allows for the identification of many NPs of various types. We finally apply an unsupervised learning technique to identify sub-populations (clusters) of NPs within a sample thanks to their elemental composition. To validate this approach, we tested it on spICP-ToF-MS data obtained from a sample of gold NPs alone and then mixed with silver as well as silver shelled gold NPs. The results showed that our new approach is able to identify and group together individual NP types, and to distinguish between different sub-populations of NPs based on their elemental signature. Moreover, applied to geostandards, this methodology allowed us to identify the presence of small populations of NPs that were undetected using conventional methods of data analysis.

In conclusion, our approach turns out to be a powerful tool for the analysis of spICP-ToF-MS data. This approach has the potential to significantly improve our understanding of the behavior and properties of nanoparticles, and to contribute to the development of new applications for spICP-ToF-MS in the field of nanogeochemistry.