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Gaining a deeper understanding of multi-dimensional nanoparticle data using UMAP and HDBSCAN

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The advent of time-of-flight (TOF) mass spectrometry for inductively coupled mass spectrometers has enabled the elemental and isotopic dimension specifically for fast transient signals. Other commonly used mass selectors such as the quadrupole can only detect isotopes sequentially making it impossible to detect multiple isotopes within a few milliseconds. The advantages that TOF enable are especially important for nanoparticle analysis, where each nanoparticle arrives at random times and the signal durations are in the low millisecond range.

As opposed to the detection of scanning mass spectrometers, TOF allows for the detection of not only single isotopes but the composition of particles. While the advantages gained can be applicable in many areas of current research such as forensic or environmental analysis, the data analysis can be a complicated task due to the multi-dimensional datasets. Many algorithms have been used to tackle similar problems in other areas of computer science, but their applicability to SP-ICP-TOF-MS needs to be examined and understood.

In this talk we will discuss the use of Uniform Manifold Approximation and Projection (UMAP)[1] for data reduction and Hierarchical Density-Based Spatial Clustering of Applications with Noise (HDBSCAN)[2] for unsupervised clustering on nanoparticle samples acquired on a Vitesse TOF-ICP-MS to differentiate and examine various clusters of particles separately. The results give a deep insight into the total population of all particles detected from which interesting insights can be drawn.

[1] McInnes, L, Healy, J, UMAP: Uniform Manifold Approximation and Projection for Dimension Reduction, ArXiv e-prints 1802.03426, 2018

[2] McInnes L., Healy J., Astels S., *hdbscan: Hierarchical density based clustering* In: Journal of Open Source Software, The Open Journal, volume 2, number 11. 2017