

Title: Next-generation data management: efficient acquisition, automated processing, and extensive data interrogation tools

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The efficiency at which LA-ICP-MS setups operate depends, apart from instrumental aspects, for a large part on the software tools for data acquisition and processing available to the researcher. A plethora of software tools have been developed over the years to reconstruct elemental images from a collection of one or more files containing transient MS profile traces. With very few exceptions, these in-house build tools have limited capabilities and little to no support. Over the last 5 years, a software package for LA-ICP-MS data processing was developed at Ghent University, and deployed in many publications in the last 5 years. The package is a highly sophisticated image processing tool based around HDF5, a hierarchical, transparent, and efficient data container format with a set of features supporting complex metadata retention and data management. The package contains more than 2×10^5 lines of C, C++, and Python code, extensive functionality, and documentation. Some of the functionality includes: (non-rectangular) image reconstruction, volume-of-interest isolation, advanced background fitting, calibration, 3D image stack production, multivariate statistics, signal processing tools, matrix calculation, and spatial transformation.

The package aims to automate the data reduction process for imaging applications to a higher degree than was possible before, whilst managing the structure of the data, and is powerful enough to deal with files multiple gigabyte in size and 3D images exceeding 10^9 voxels. The semi-automation of the data processing pipeline for imaging has proven to be a multi-faceted challenge, in which all pieces of information of the laser and ICP-MS have to be brought together. For example, the laser metadata needs to be included to allow for very efficient data acquisition routines, which in turn results in significant cost and time savings. Other, less critical aspects are also significant, such as the layout of the data in the HDF5 file, which is the result of years of experience working with experimental data in this file format. Furthermore, the ability to interrogate the data using supervised and non-supervised multivariate methods can prove purposeful, as it can reveal insights in the correlation of different elemental maps relative to each other, or relative to other (multimodal) images, acquired *a priori*. Full support and integration with Teledyne Photon Machines lasers and most ICP-MS systems is present. The package is easily extensible towards data formats of manufacturers which have not been included yet. The package is currently undergoing testing in a selected number of research groups, and will be made available to the LA-ICP-MS community in the near future. In this talk, this software package is introduced for the first time. Data of various previous projects will be included in this talk, including zircon analysis and high-resolution, 3D and single-cell imaging.