LaserTRAM-DB: An open-source Time Resolved Analysis Module for the complete reduction of laser ablation inductively coupled plasma mass spectrometry data

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With a wide array of applications, laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is now a commonplace tool for gathering in situ trace element data from solid materials. Raw data output from LA-ICP-MS, however, is in the form of isotope counts per second, not elemental concentrations. Furthermore, as LA-ICP-MS data in geologic samples frequently have multiple phases, chemical zoning, inclusions, and other fine-scale compositional complexities that do not represent the material of interest, user interaction is required to filter unwanted signals out of the total ablation signal. These observations necessitate a data processing pipeline that should not be automated. Currently there are several proprietary and open-source graphical user interfaces (GUIs) for LA-ICP-MS data reduction to accomplish this: SILLS (MATLAB GUI), Iolite (proprietary GUI), LAtools (Python scripting), Termite (R GUI), GLITTER (proprietary GUI), and countless other in-house spreadsheets. All have their strengths and weaknesses, however, there has yet to be a powerful, browser-hosted GUI utilizing the increasingly popular scientific Python stack of tools.

Here we introduce the theory, workflow, and structure of LaserTRAM-DB: an open-source dashboard for the complete processing pipeline of LA-ICP-MS spot data in complex materials such as geologic samples. Like other aforementioned tools, LaserTRAM-DB allows the user to filter which portion of the ablation peak is utilized in calculating concentrations. Unlike many tools, however, it allows for the processing of both individual spot analysis data and a line of spots gathered in rapid succession (e.g., data signals do not reach background levels between each spot), reducing the time required for data reduction while preserving spatial definition and still ensuring data quality. Furthermore, it also gives the user the ability to output processing decisions along the way (e.g., analysis intervals, mass spectrometer drift correction sensitivities, internal standard concentrations) such that re-processing using different internal standard analytes or calibration standard reference materials can be done efficiently and in a reproducible manner.

