

KJ: A Julia package for physics-based LA-ICP-MS data processing

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is one of the most widely used technologies for in-situ geochronology. Dozens of data reduction programs have been developed to process LA-ICP-MS data, with a small number of proprietary and increasingly closed programs dominating the market. Most of these programs (both free and paid) are based on heuristic algorithms, which are demonstrably biased [1].

KJ (which stands for 'Kasper Julia') addresses this problem. It offers the following advantages over existing LA-ICP-MS data reduction packages.

1. KJ is free and open (LGPL 3.0 license)
2. KJ uses a physics-based algorithm that solves the biases of the heuristic methods [1].
3. KJ is written in Julia, which makes it platform-independent yet extremely fast.
4. KJ provides an easy mechanism to save session logs, which can be run on other computers and thereby produce truly FAIR data flows.

KJ is proof-of-concept software, which lacks the polished user interface of commercial packages. Nevertheless, an attempt has been made to improve the user experience by providing three different ways to access KJ's functionality:

1. Using a text query based user interface (TUI, Figure 1)
2. Via the Julia-based API
3. Using GUI elements provided by the 'KTgui' extension to KJ

At the time of writing, KJ accommodates input files generated by quadrupole instruments produced by Agilent and Thermo Fisher. Importers for other instruments (including multi-collector machines) will be added later. A built-in extension mechanism provides a way to extend KJ's functionality for applications such as elemental and isotopic mapping.

KJ can be installed from <https://github.com/pvermees/KJ.jl>

Any feedback will be gratefully acknowledged.

[1] Vermeesch, P and Glorie, S (2025), A physics-based isotope ratio estimation algorithm for geochronology by LA-ICP-MS; Session 06i of this conference.

Figure 1

