

Developing scientific open-source software - Lessons learned from SpecXY, MinPlotX and other little helpers

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To deal with the enormous amount of data that is produced, processed and visualized in science today, special software tools are essential. Unfortunately, many software solutions used in Earth Sciences are proprietary and closed software for which the code cannot be accessed, reviewed or modified. Closed research software is a barrier for innovative developments with missing transparency, unsuitable for reproducible and accessible science.

This contribution will give an overview on how to get started, especially as an early-career scientist, the different design aspects and important steps to develop accessible open-source research software that can be used by a wide audience. These steps are explained based on experience gained from the development of the spectroscopy software SpecXY [1] the mineral formula recalculation and compositional plotting program MinPlotX [2], a mass spectrometer data reduction software ICP-Base (Stumpf et al., this meeting) and other little helpers and tools.

Lessons learned on this journey are:

- Different approaches and levels of complexity require specific considerations, strategies and approaches (small tools vs. complex software environments).
- With a broad user base with diverse computer skills, the software should ideally be easy-to-use via a graphical user interface (GUI), whilst at the same time providing an application programming interface (API) and an accessible data structure for sophisticated customization.
- Open research software for a broad audience should be cross-platform compatible, easy to install, without additional dependencies, and ideally work offline as many lab computers are not connected to the internet.

This contribution is intended to spark new ideas, hopefully lead to new developments and improve collaborative open research software projects.

[1] Gies N. B., Lanari P., Hermann J. (2024) A workflow and software solution for spatially resolved spectroscopic and numerical data (SpecXY). *Computers Geoscience* 189:105626. <https://doi.org/10.1016/j.cageo.2024.105626>

[2] Walters, J. B. & Gies, N. B., (2025). MinPlotX: A powerful tool for formula recalculation, visualization, and comparison of large mineral compositional datasets. *Mineralogia*, 56, 13-22. <https://doi.org/10.2478/mipo-2025-0003>