

SECPlot

Processing and visualization of spectroelectrochemical data

Academic software, free of charge · Windows and Linux

SECPlot loads a three-dimensional dataset — an intensity measured for every wavelength and every frame —, shows it as a surface or a map, and takes it apart into the spectra and the time profiles of the species that make it.

A spectroelectrochemical run is thousands of spectra. SECPlot shows them at once, as a 3D surface or a 2D map, with the frame axis switched to time in one click: the switch is purely visual, the data are never modified.

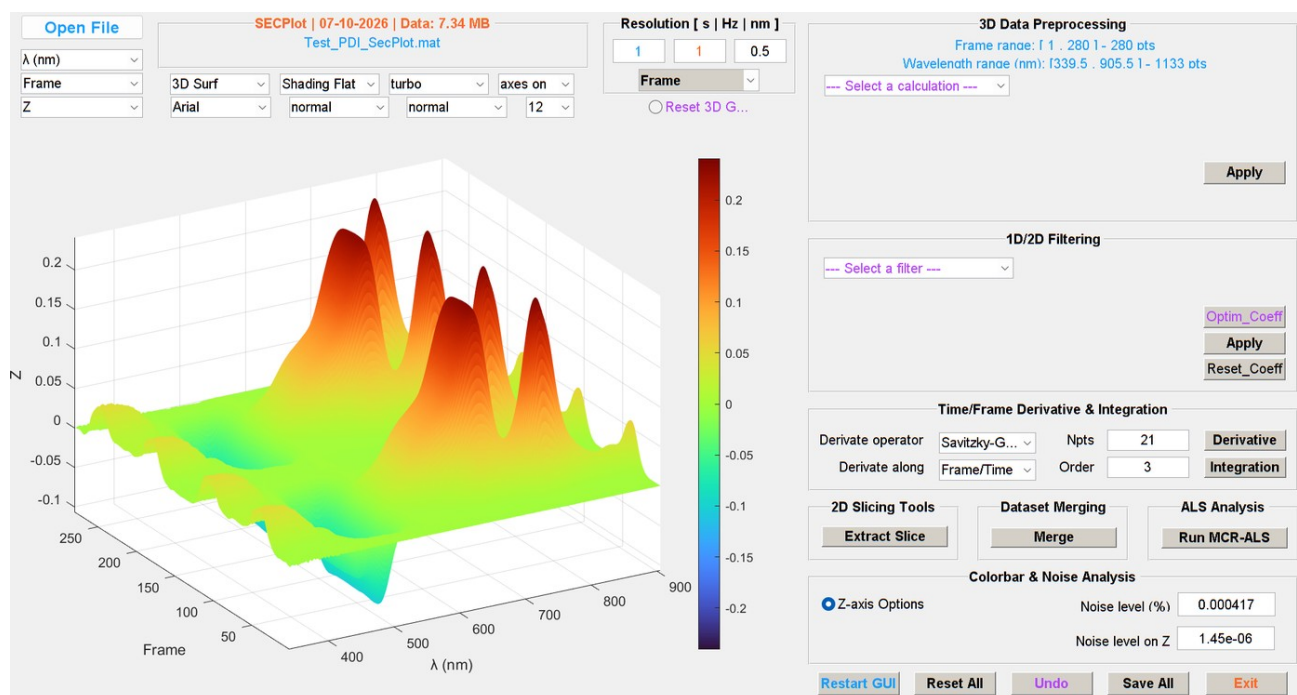


Figure 1 — The main window: a dataset of 280 frames and 1133 wavelengths shown as a 3D surface, with the processing panels on the right.

Processing

- algebraic operations and baseline corrections on the whole dataset
- 1D and 2D filters (Savitzky-Golay, Gaussian, mean, median), with the noise level measured
- derivative and integration along time or frames
- slices at a fixed wavelength (kinetics) or at a fixed frame (spectra), with peak detection
- two acquisitions merged into a single dataset, and chopped-beam measurements rebuilt
- results written as text files and to Excel

Multivariate curve resolution (MCR-ALS)

The dataset is written as a product: the concentration profiles C of a few components times their spectra S , plus a residual. SECPlot proposes the number of components from the singular values and says what it rests on; the count stays yours.

- starting profiles chosen automatically (purest variables), picked by hand or measured from presence windows
- constraints on either factor: non-negativity, unimodality, presence windows, blank frames held at zero
- processing along frames or along wavelengths, with the profiles reprojected when the axis is switched
- the outcome named: convergence, divergence, or a solution that only reproduces the singular-value decomposition

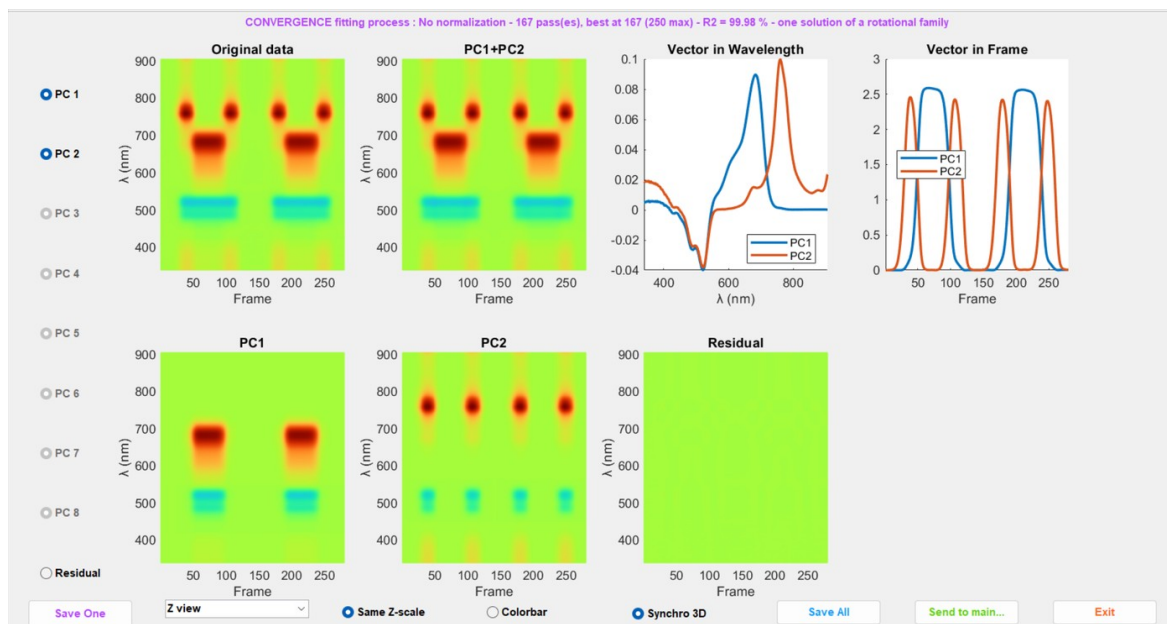


Figure 2 — Two components resolved: the data, their reconstruction, each component and the residual as maps; spectra and time profiles on the right.

Checked

Every version is compared with more than 900 recorded cases covering the file readers, the filters, the matrix operations and the resolution. A change that moves a result is either a correction, said as such, or a fault.

Getting started

A user guide in French and English explains every button and every field, and the order of work in the resolution window. No computing background is required. The interface is in English.

Free of charge for everyone

SECPlot is free of charge for everyone, students and researchers alike. It is distributed as 64-bit Windows and Linux executables that need only the free MATLAB Runtime: no MATLAB licence is required. Its licence of use, free of charge, allows it to be installed on as many computers as wished and passed on unchanged. The demo version needs no formality: everything runs and is shown, nothing is saved; the full version is granted, free of charge too, to users registered with an academic address.

SECPlot comes with absolutely **NO WARRANTY**.

To obtain SECPlot: write to the developers at echem-tools@univ-angers.fr.

Reporting a problem: Help ► Report a problem... prepares the message, which you send yourself.

Acknowledgement: if SECPlot contributes to a publication, a thesis or a funded project (ANR, ERC, a European programme...), the authors would be grateful for a mention, for instance in the acknowledgements: « The data were processed with SECPlot (O. Alévêque and E. Levillain, MOLTECH Anjou, UMR 6200 CNRS, University of Angers), software free of charge, available on request from echem-tools@univ-angers.fr. »

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