Kaalen-v1.0 User guide

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1 Installation

Download and extract the $kaalen - app - windows - dist.zip$ file under Files in Zenodo. The program will open with the .exe file found inside the extracted folder.
Link to Zenodo repository: `https://zenodo.org/uploads/17038308`

If you encounter an error, you can always find the latest version on the Kaalen GitHub repository. Click the link below to go to the repository, then click on "Releases" on the right side of the page. You will find the correct file under "Assets," labeled $Kaalen - App - dist.zip$. Download and extract this file to run the program.
Link to Github repository: `https://github.com/Matheshv98/Kaalen-v1.0`

2 Getting Started

This manual will guide you through the features of the Kaalen-v1.0 application. The main interface is divided into a **Main Plots** tab and additional tabs for data analysis, such as **Global Fit**.

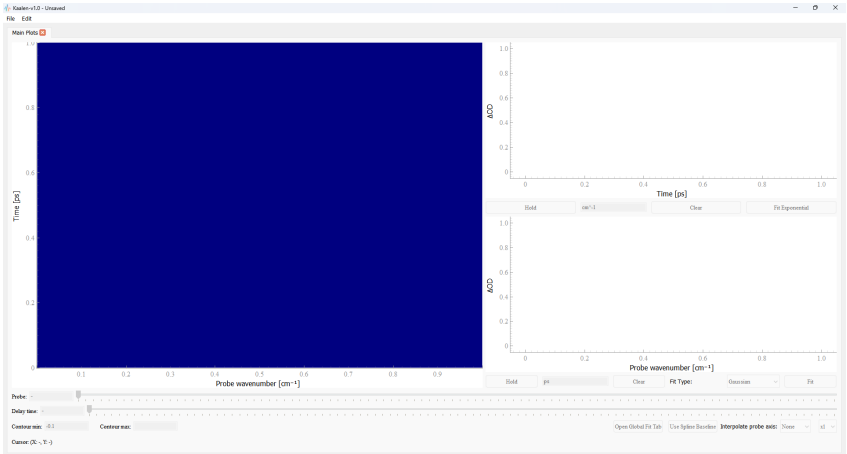
2.1 The Main Plots Tab

When you first start the application, the **Main Plots** tab is the default view. This is where you can load your data, view the 2D map, and generate time and probe slices.

2.1.1 Importing Data

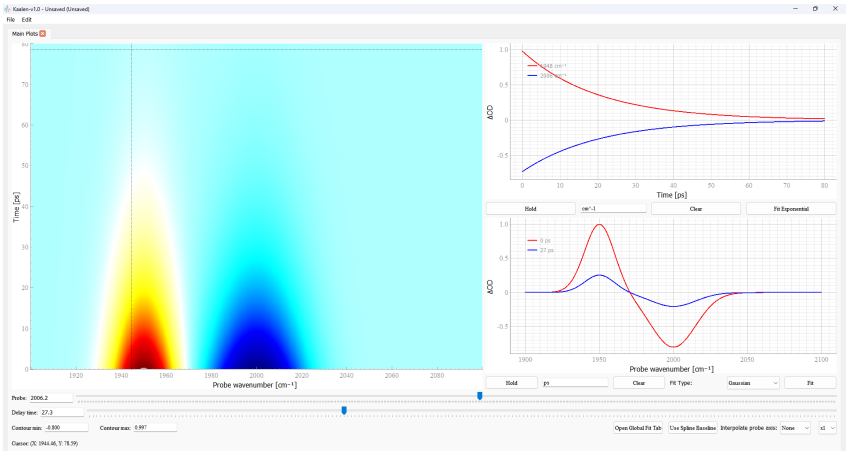
Go to **File** $>$ **Import Data...** in the menu bar. Select a file that has the preferred data format. The program expects the first row and first column to contain the probe wavelengths and time values, respectively. The rest of the data should be the signal values. The decimals should be '.' and the delimiter should be ','.

Note: You can change the labels for the plots by going to **Edit** $>$ **Edit Names...** in the menu bar. The names and units given for the 2D map will be used in all the axis labels in the later opened tabs.



2.1.2 Exploring Your Data

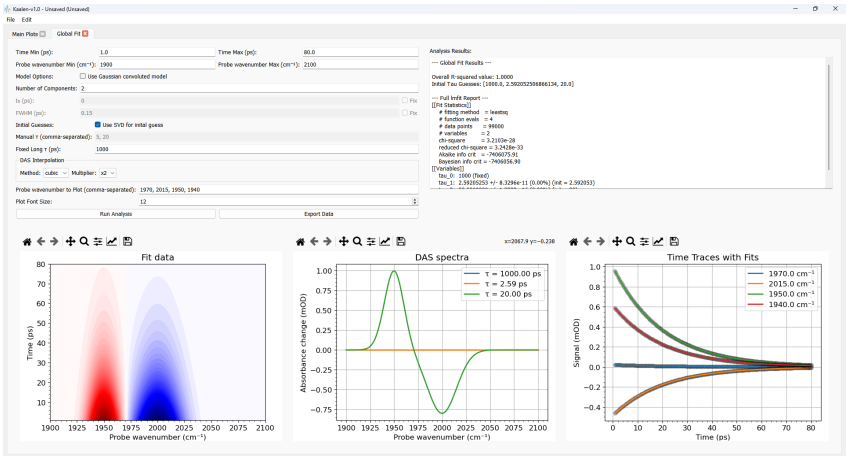
Use the sliders at the bottom to navigate the data. The **Probe** slider (X-axis) and **Delay time** slider (Y-axis) control the position of the cursor lines and slices on the 2D plot. The two smaller plots on the right will automatically update to show the corresponding time and probe slices.



- **Holding Slices:** Click the **Hold** button on either the time or probe slice plot to save a static copy of the current slice. You can hold multiple slices.
- **Clearing Slices:** Click the **Clear** button to remove all held slices from a plot.
- **Adjusting Contour Levels:** Use the **Contour min** and **Contour max** input boxes to change the colour scale of the 2D map.
- **Applying Spline Baseline Correction:** Click the **Apply Spline Baseline** button to remove a smoothly varying baseline from your data. The button text will change to **Revert to Original** once the correction is applied. The function used here is UnivariateSpline from Python with s (smoothing factor and weights, w) as 0. The spline is done on every time point and along the probe axis.
- **Interpolation:** You can interpolate the probe axis to get smoother DAS plots by selecting an interpolation method and a multiplier. The multiplier multiplies the number of points by ×2, ×3, etc. No interpolation is done for the time points.

3 Using the Global Fit Tab

The **Global Fit** tab is a powerful tool for analysing your data with a multi-exponential model. The user interface is divided into three main sections: **Input Panel**, **Analysis Results**, and **Plots**.



3.1 Getting Started with Global Fitting

To begin a global fit analysis, follow these steps:

1. **Launch the GlobalFitApp:** Click the **Global Fit** button in the main window.
2. **Set Data Ranges:** In the **Input Panel**, adjust the **Time Min** and **Time Max** values to define the time range you wish to fit. Similarly, set the **Probe Min** and **Probe Max** values to specify the spectral range for the fit.
3. **Configure the Model:**
    - **Number of Components:** Enter the number of exponential components to be included in your model.
    - **Convoluted Model:** Check the **Use Gaussian convoluted model** box to account for the Gaussian instrument response function (IRF). If selected, you can adjust the initial guess for the t_0 (time-zero) and FWHM (full width at half maximum) parameters, and choose to fix either of these values. The convolution function is adopted from J. J. Snellenburg et al. [1].
    - **Initial Guesses:** Choose between two methods for generating initial guesses for the decay lifetimes (τ): SVD-based or Manual.
    - **Fixed Long τ:** Enter a value for a fixed, long-lived lifetime. This component will always be included in the fit and its value won't be varied. The DAS for this long lifetime will be equivalent to the signals that are not decayed at the end of the measurement time.
4. **Run the Analysis:** Click the **Run Analysis** button to start the fitting process.

4 Understanding the Results

After a successful fit, the results will be automatically displayed.

4.1 Analysis Results

This section provides a detailed breakdown of the fitting process and outcomes, including:

- **Overall R-squared Value:** Indicates how well the model fits the data, with a value closer to 1.0 suggesting a better fit.
- **Initial τ Guesses:** Lists the starting lifetime values used for the fit.
- **Full lmfit Report:** A comprehensive report from the lmfit library, including the final fitted values for all parameters (τ, t_0, FWHM), their standard errors, and goodness-of-fit statistics.
- **Warnings:** Any issues encountered during the fitting process.

4.2 Plots

- **Fitted Model Plot:** Shows the 2D data map generated by the fitted global model.
- **DAS Spectra Plot:** Displays the Decay-Associated Spectra (DAS). Each curve corresponds to a specific lifetime (τ) and represents the amplitude spectrum of that exponential component.
- **Time Traces with Fits Plot:** Shows the raw experimental data as points and the corresponding fitted curves at specific probe wavelengths.

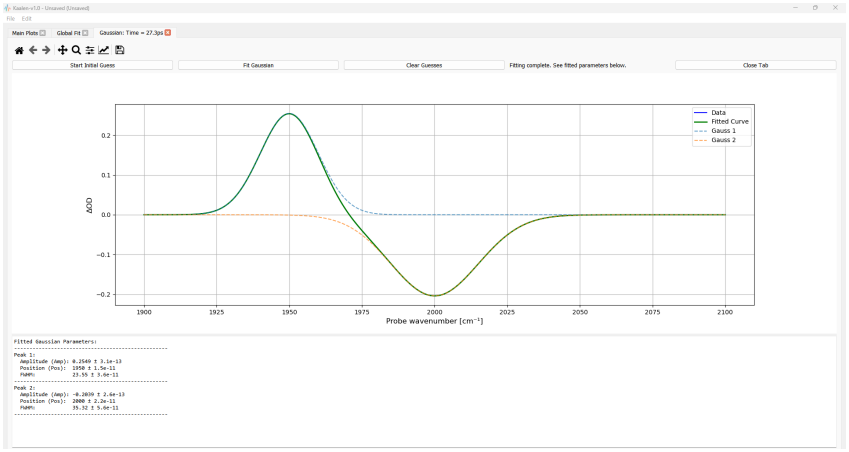
Axis labels, legends, font size etc., can be edited before saving the image. The buttons with icons above each matplotlib plots gives these functions

5 Exporting Your Data

You can export the results of your global fit by clicking the **Export Data** button. The program will generate three .csv files: [file_name]_DAS.csv, [file_name]_2D_fitted_data.csv, and [file_name]_time_traces.csv. The icons on top of each plot gives more option to save as image, zoom, edit, etc,.

6 Other Features

- **Signal Plotter:** The hold button below the slice plots open the tab for fit. This tool can perform exponential or Gaussian fits to a specific slice. The initial guesses for the slice plots are set with mouse clicks and drags. For a Gaussian fit, the first click on the screen sets the position and amplitude, and dragging the mouse while holding the click sets the FWHM. A second click on the plot will then fix the initial guess. For an exponential fit, the user can draw a sum of exponentials on top of the data in the same manner. Any number of functions can be fit by following the step mentioned.



- **Saving and Loading Projects:** You can save your entire session using **File** > **Save Project**. To continue your work, use **File** > **Load Project...**.
- **Editing Axis Names:** Change the labels for the plots by going to **Edit** > **Edit Names...**.
- **Tab title:** Double clicking the tab title gives the option to edit the title of the tabs.

References

[1] J. J. Snellenburg, S. Laptenok, R. Seger, K. M. Mullen, and I. H. M. van Stokkum, "Glotaran: A Java-based graphical user interface for the R package TIMP," J Stat Softw, vol. 49, pp. 1–22, 2012, doi: 10.18637/JSS.V049.I03.

[2] Stensitzki, T. (2021). skultrafast - a python package for time-resolved spectroscopy (4.0). Zenodo. https://doi.org/10.5281/zenodo.5713589