PPViewer User Manual

Author: Ilya Stepanenko <ilstep@gmail.com>
23.08.2007

PPViewer is basically a viewer for two-way spectroscopic data, in particular time-resolved spectra where the first dimension is wavelength or wave number, while second dimension is time.

The main goal of the program is to provide comfortable way of displaying data and friendly user interface, which should help users to "feel" results of their measurements.

PPViewer can be used for examining a single dataset or for comparison of several datasets. PPViewer also may be used as an extension to the TIMP Package, as it allows comparison of measured datasets with a fitted model output by TIMP. The program allows for interactive data exploration that is currently difficult to implement in the R language alone (in which TIMP is based).

Managing data files

Supported input file types

PPViewer supports input files with a widely-used structure : the first line contains the real-valued wavelengths at which measurements were taken. The first value of each of the remaining lines represent the independent variable value (i.e. time) at which the spectrum contained on that row was taken. The rest of each remaining row represents a (space or tab-delimited) spectrum.

PPViewer also supports the *Wavelength Explicit* file format used in the TIMP R package and the tim Fortran codes. This file format is described at
http://www.nat.vu.nl/~kate/TIM/tim/node76.html

Adding and deleting datasets

One input file contains one dataset. To load dataset to PPViewer click **Add…** button and select input file. Its name will appear in **Datasets** list, meaning that the dataset was loaded to the viewer. Also a new curve on the graph and a new slider will appear. Notice that new filename, curve and slider have the same color, which means they correspond to the same dataset. In this version of PPViewer you can add up to 10 datasets.

You can add several copies of single dataset (it is useful, for example, when you want to view and compare transient spectra with different delay times within single dataset). To add a copy of already loaded dataset select it in the **Datasets** list and click **Duplicate** button.

To delete dataset from the viewer select it in the **Datasets** list and click **Delete** button

Data representation

Display modes

PPViewer supports two display modes of data representation. Transient spectra, which correspond to some fixed time values, are displayed on the graph in **Spectra** mode. This fixed time values are displayed in **Actual values** numeric controls and are also represented by the positions of **sliders**. The values can be interactively changed: just drag any slider or enter new value in one of the **Actual values** numeric controls.

In **Kinetic** mode kinetic curves are displayed, while fixed values, which can be interactively changed, are wavelengths. Kinetic curves are plotted in linear-logarithmic time scale (i.e. time scale is linear in range [-1;1] and logarithmic elsewhere). [in this PPViewer version marker values aren't displayed correctly outside [-1;1] range: e.g. marker value "2" really means 10^2, to be fixed]

The slider is a great interactive tool for controlling data representation as it allows seeing and feeling "dynamics" of the data.

Sometimes (e.g. while comparing measured and modeled datasets) you may want to drag two or several sliders simultaneously. To do that, drag sliders using right mouse button.

You can always change scale limits for sliders to work in the time/wavelength range of interest: just double-click the upper or lower limit on the scale of the slide, type a new value and press enter. To reset scale limits click **Reset limits** button.

Scaling

While displaying several datasets on the graph it is sometimes useful to scale certain curves. You can apply scaling to any dataset using **Scaling** numeric controls. Suppose amplitude of the curve is Y, if you enter values "A" and "B" to the controls, amplitude will change to A+B*Y. Obviously, values "0" and "1" mean no scaling.

You can also normalize all curves at some X value (e.g. normalize all spectra at some wavelength in Spectra mode). To do that, move cursor (see "Using cursors" section) to the corresponding X value and click **Normalize at cursor** button. If you want PPViewer to preserve normalization while you drag sliders, enable **Auto normalize** switch.

To reset all scalings and normalizations click **Reset** button.

Using the Graph Palette

Use the graph palette to interact with a graph.

With the graph palette, you can move cursors, zoom, and pan the display. The graph palette contains the following buttons, in order from left to right:

- **Cursor Movement Tool**—Moves the cursor on the display.
- **Zoom**—Zooms in and out of the display.
- **Panning Tool**—Picks up the plot and moves it around on the display.
- **Scale Y**—Click this button to adjust scales to fit all plotted data. You can also press **Space** button on your keyboard to get the same result.

Click a button in the graph palette to enable moving the cursor, zooming the display, or panning the display. Each button displays a green LED when it is enabled.

Graph can automatically adjust its horizontal and vertical scales to fit the plotted data. This behavior is called autoscaling. Right-click the graph and select **AutoScale X** or **AutoScale Y** from the shortcut menu to turn autoscaling on or off.

Using Cursors

Cursor is a useful tool e.g. for measuring and estimation of exact positions of features on the curve. To move cursor use **Cursor Movement Tool** from graph palette or directly type values in cursor legend.

To add cursor to a Graph right-click anywhere in the cursor legend, select **Create Cursor**, and select a cursor mode from the shortcut menu. The cursor position is defined by the cursor mode. The cursor includes the following modes:

- **Free**—Moves the cursor freely within the plot area, regardless of plot positions.
- **Single-Plot**—Positions the cursor only on the plot that is associated with the cursor. You can move the cursor along the associated plot. Right-click the cursor legend row and select **Snap To** from the shortcut menu to associate one or all plots with the cursor.

Right-click the cursor legend row and select from the following options from the shortcut menu to customize the cursor:

- **Snap To**—Locks the cursor to a plot. When the cursor mode is **Single-Plot**, you can snap the cursor to one or all plots.
- **Attributes**—Customizes the appearance of each cursor, such as color and shape.
- **Bring to Center**—Centers the cursor on the graph without changing the x- and y-scales.
- **Go to Cursor**—Changes the x- and y-scales to show the cursor at the center of the graph.

Exporting data

To export plotted data click **Export…** button and select appropriate option.
PPViewer can export an ASCII file or an image.

"Multiple X columns" option for ASCII file means that two columns (X and Y) will be written to file for each curve.

"Single X column" means that the only X column will be the first and it will be common for all following Y columns. Because X column values can differ from one dataset to another, resampling may be applied in this case to create unified X column for all datasets.

Images are exported in vector EMF format.

Exlamples
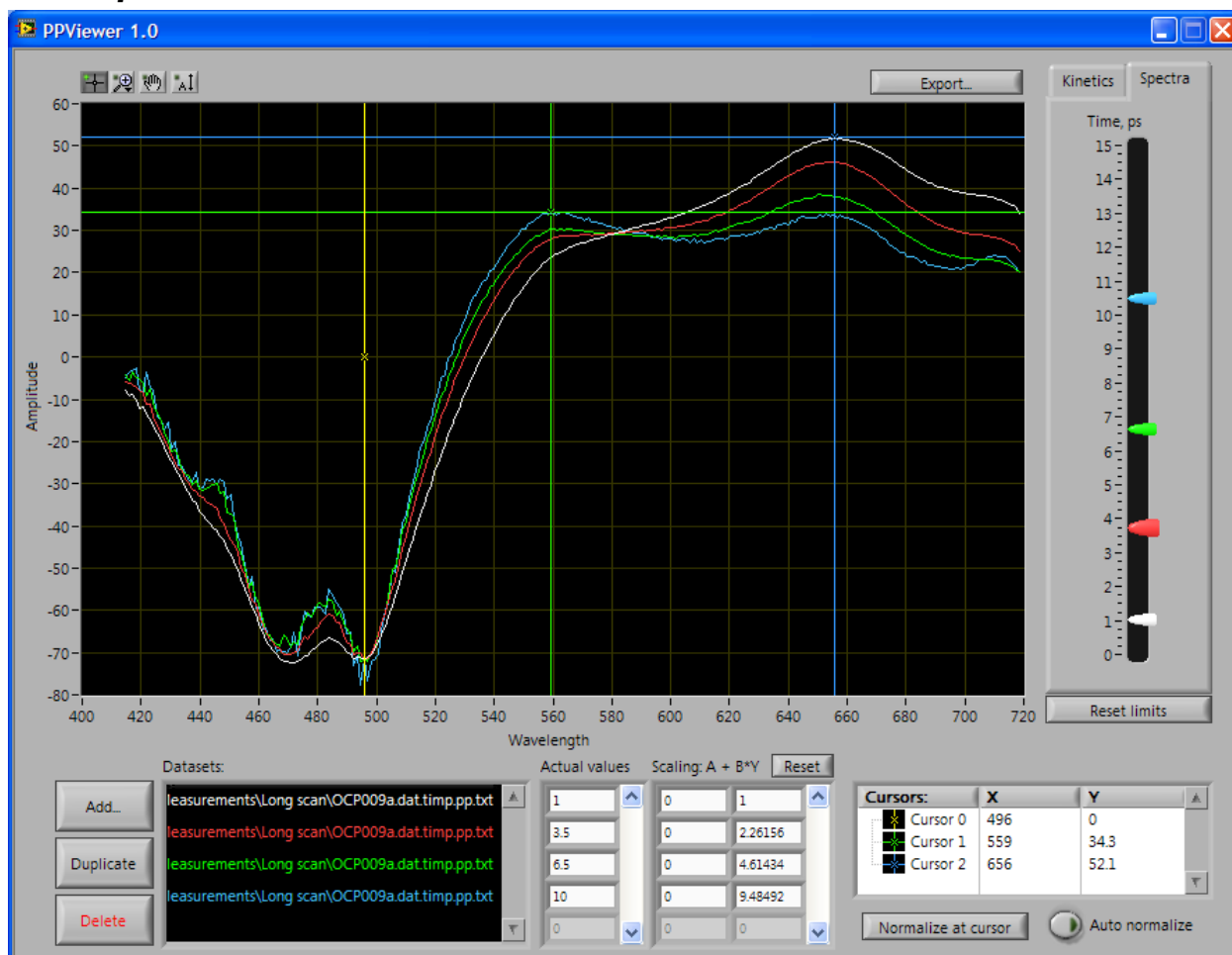
Four copies of single dataset loaded. Displaying transient difference spectra at four delay times
(1 ps, 3.5 ps, 6.5 ps, 10 ps). Spectra are normalized at ground state bleaching (496 nm).
Evolution of 559 nm and 656 nm bands can be observed.
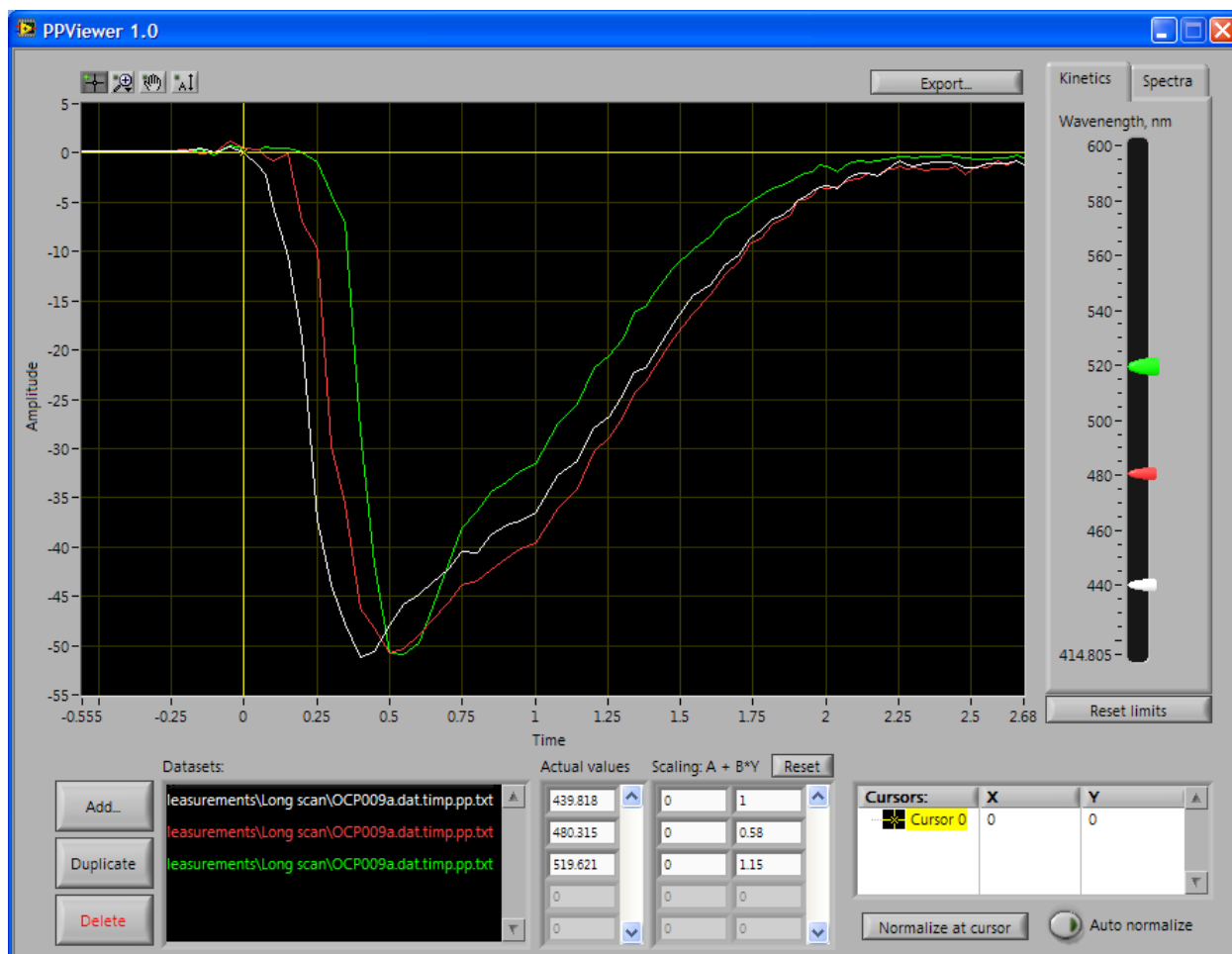
The same dataset, three copies loaded. Displaying kinetic curves corresponding to different wavelength. Graph can be used to approximately estimate IRF location and its dependence on wavelength.
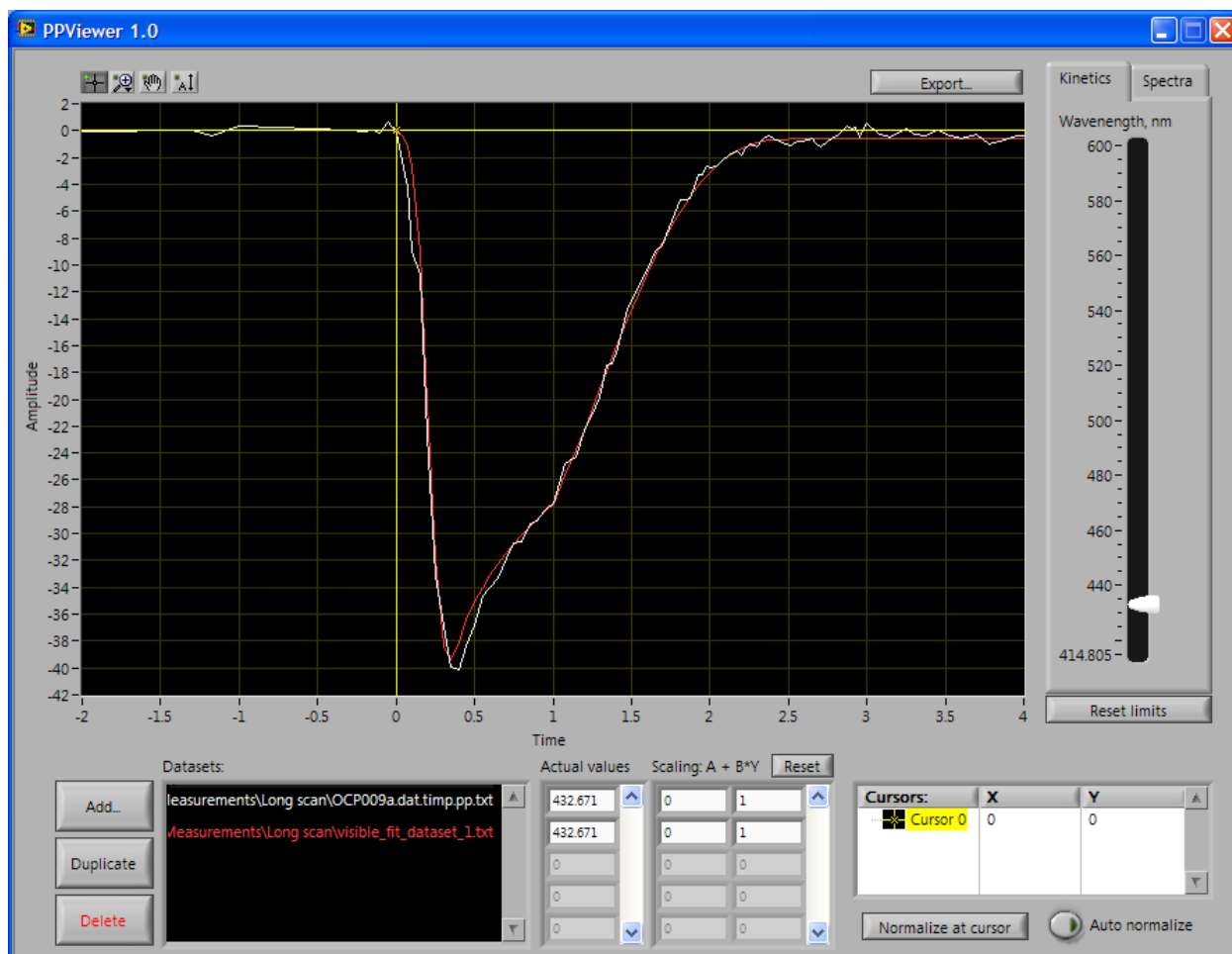
Two datasets loaded: measured data (white) and data modeled in TIMP (red). Displaying kinetic curves. Dragging slider with right mouse button allows comparison of datasets in different wavelength.