Working with Broadband Transient Absorption Data in Igor Pro
v. 4.0beta May 4, 2011

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Starting Igor Pro

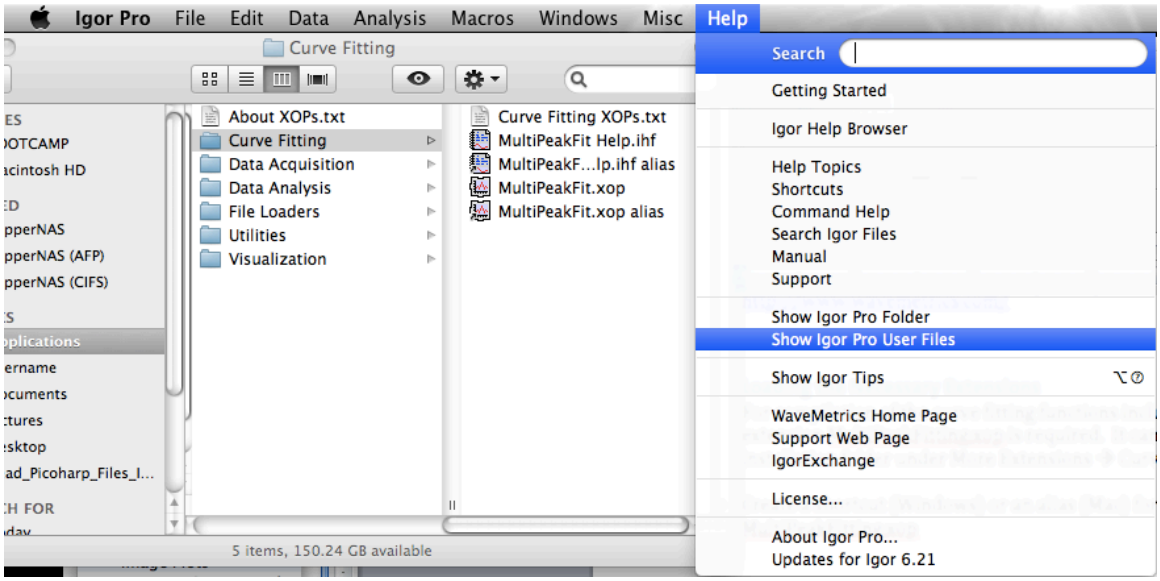
Version Requirements

These procedures require Igor Pro version 6.2 or later. Igor Pro is written by Wavemetrics, Inc. More information can be found at:
http://www.wavemetrics.com/

Loading the Necessary Extensions

For compilation of the curve fitting functions included in the procedure, the optional extension MultiPeakFit.xop is required. It can be found in the Igor Pro installation folder under More Extensions → Curve Fitting → MultiPeakFitting.xop

Create a shortcut (Windows) or an alias (Mac) for the files:
MultiPeakFit.xop
MultiPeakFit Help.ihf



From the Igor Help menu, choose, "Show Igor Pro User Files." Add these shortcuts to the Extensions folder in the User files directory.

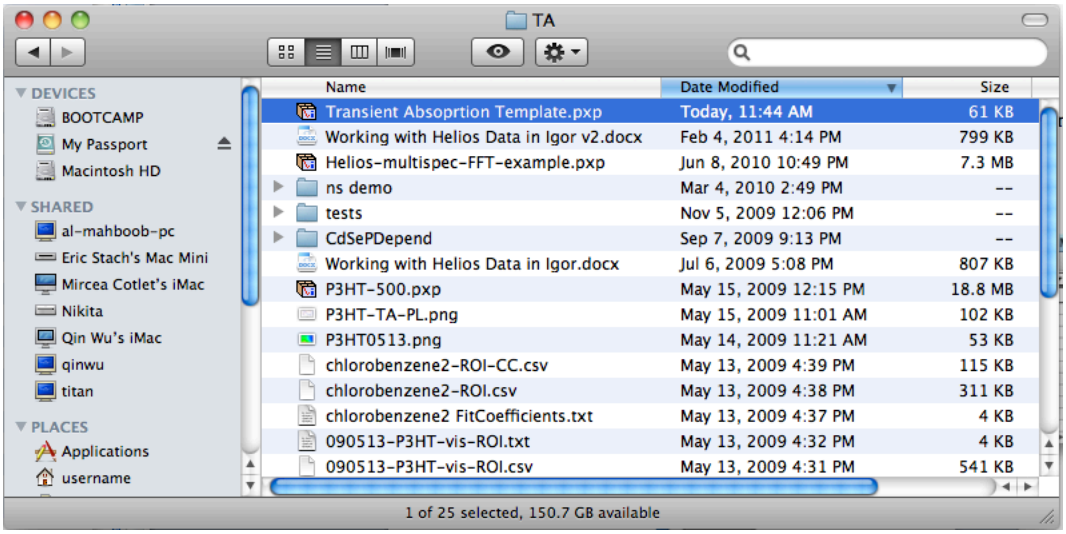
If Igor is already running, then it must be restarted for these changes to take effect.

Importing Transient Absorption Data into Igor Pro

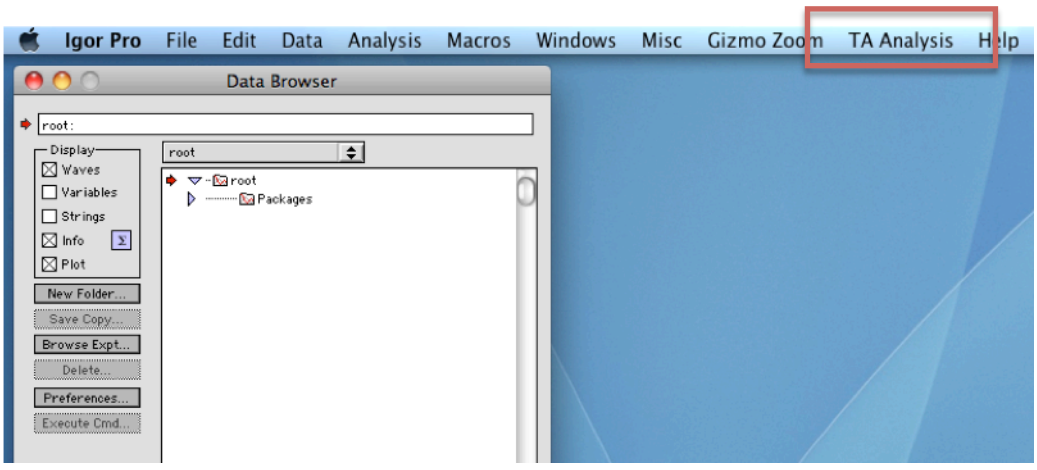
Open File

1) Load and compile the appropriate procedures into a new Igor Pro experiment, using the appropriate menu options.
   File → Open File → Procedure . . .
   TAData_Analysis_vX.XX.ipf
   TAData_CurveFitting_vX.XX.ipf

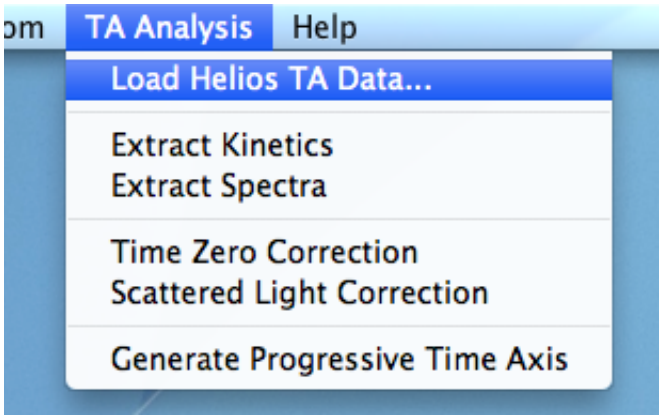
2) Alternatively, open the Igor Packed Experiment file named "Transient Absorption Template.pxp". Note that this makes upgrading to a new procedure file more difficult.

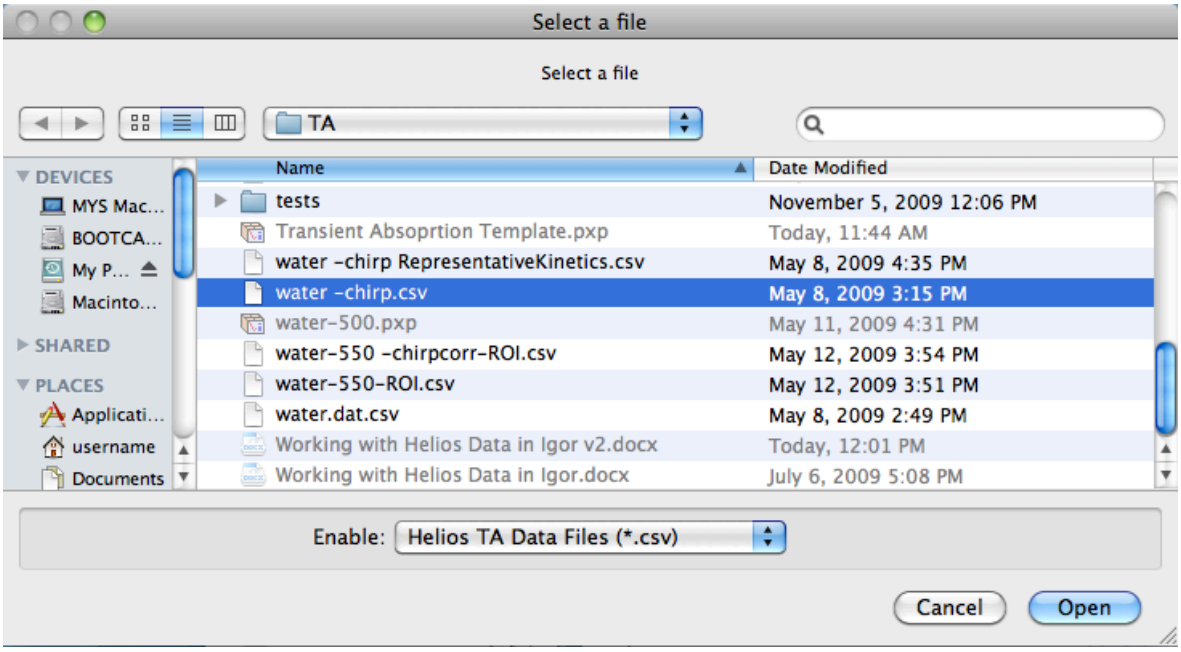


3) A blank experiment will open which automatically includes and compiles the necessary procedures. A new menu will appear on the task bar entitled, "TA Analysis."



4) Open your saved transient absorption data (.csv files) using the appropriate menu option:
TA Analysis → Load Helios TA Data . . .

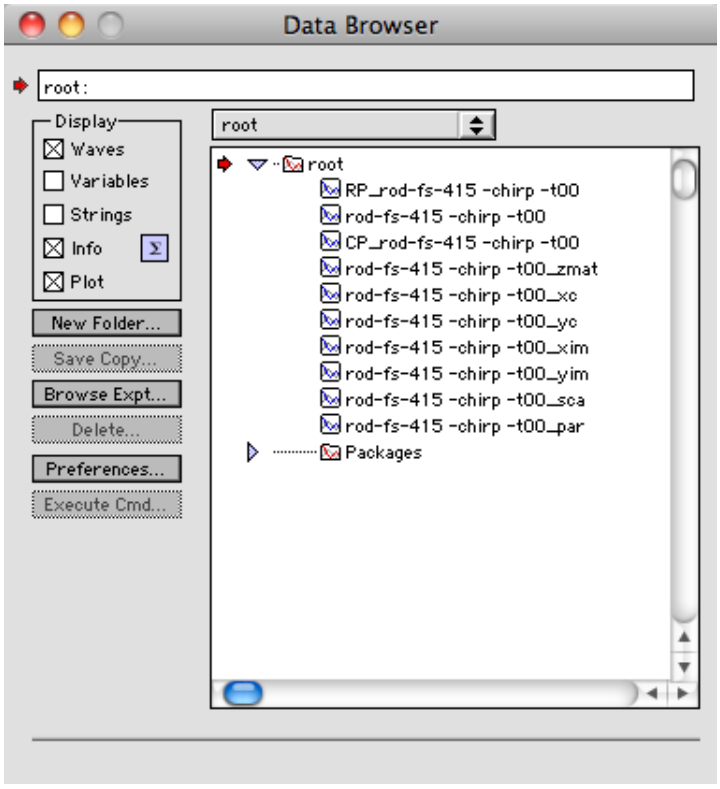




Wave Format

5) This procedure loads the original data in *filename* with the corresponding wavelength (RP_*filename*) and time (CP_*filename*) information. It creates a new set of these waves (*filename*_zmat; *filename*_xc; *filename*_yc), with all the NaNs and Infs in the files replaced with 0, and deletes extra rows (for which the spacing is non-monotonic). It also creates several additional waves for graphing puposes:

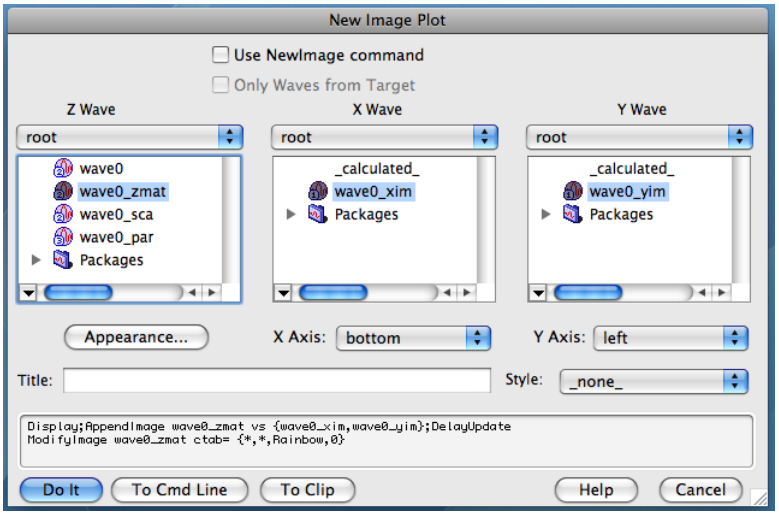
RP_*filename* (wavelength labels for row data in nm)
filename (original uncorrected matrix in ΔOD)
CP_*filename* (time labels for column data in ps)
*filename*_zmat (corrected matrix)
*filename*_xc (processed row values)
*filename*_yc (processed column values)
*filename*_xim (x values for image plot)
*filename*_yim (y values for image plot)
*filename*_sca (xyz wave for scatter plot)
*filename*_par (3D parametric wave)



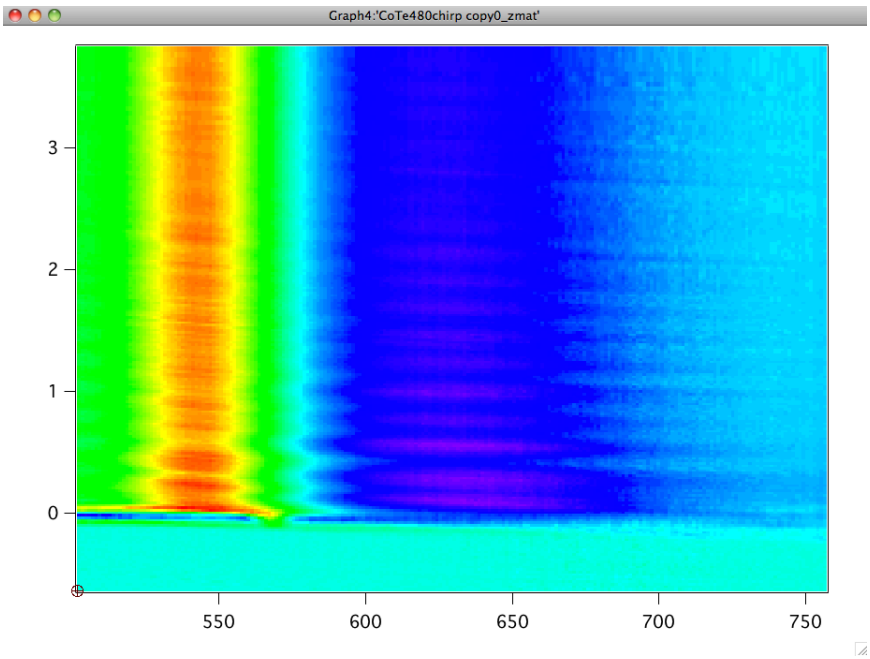
Plotting TA Data

Automatically Generated Plots

1) An image plot of your data will be automatically created with a visible cursor. This plot can be generated manually in the following way, using *filename*_zmat, *filename*_xim, and *filename*_yim:
Windows → New → Image Plot



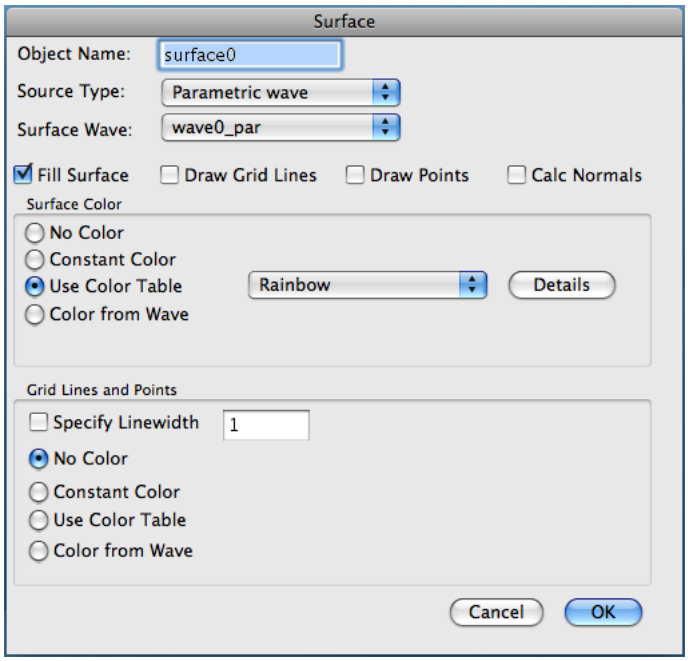
Click the "Appearance" button to generate a color image.



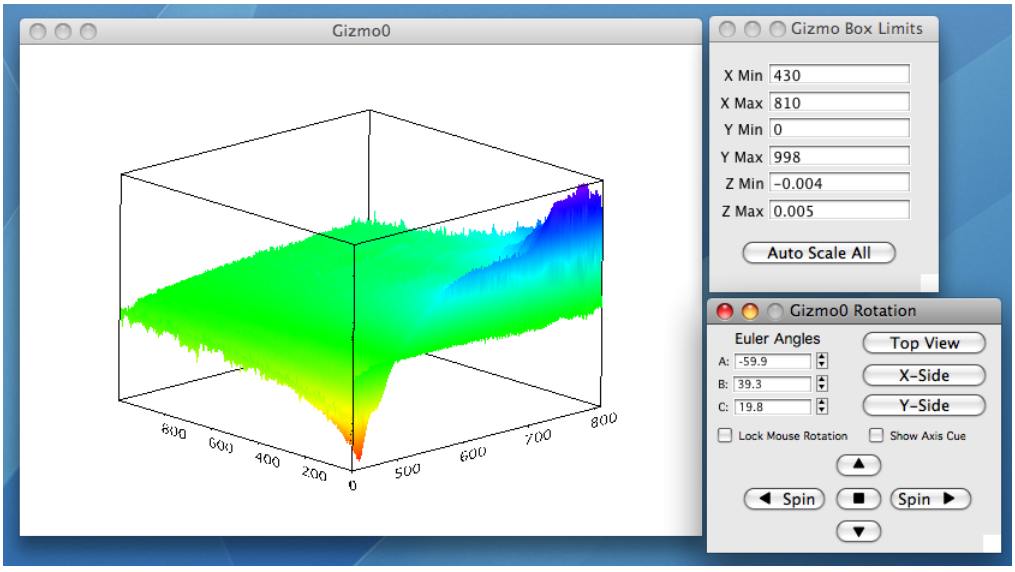
Use the CTRL-I (CMD-I for Mac) key sequence to manually show the cursors.

3D Surface Plots

2) To generate a 3D Plot of your data:
Windows -> New -> 3D Plots -> Surface Plot



Modify as appropriate:
Gizmo -> Axis Range
Gizmo -> Rotation

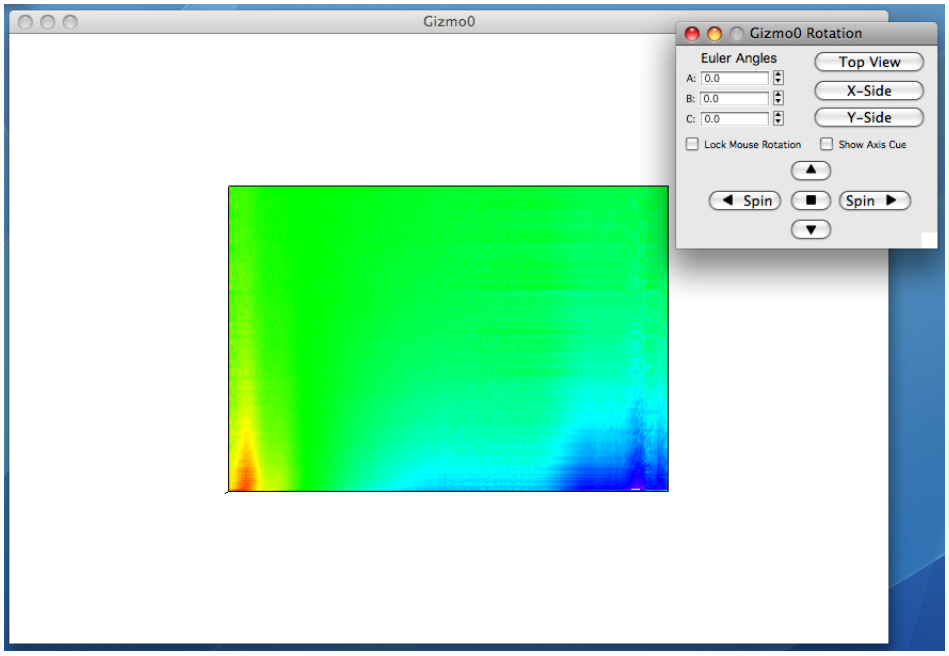


Scatter and Contour Plots

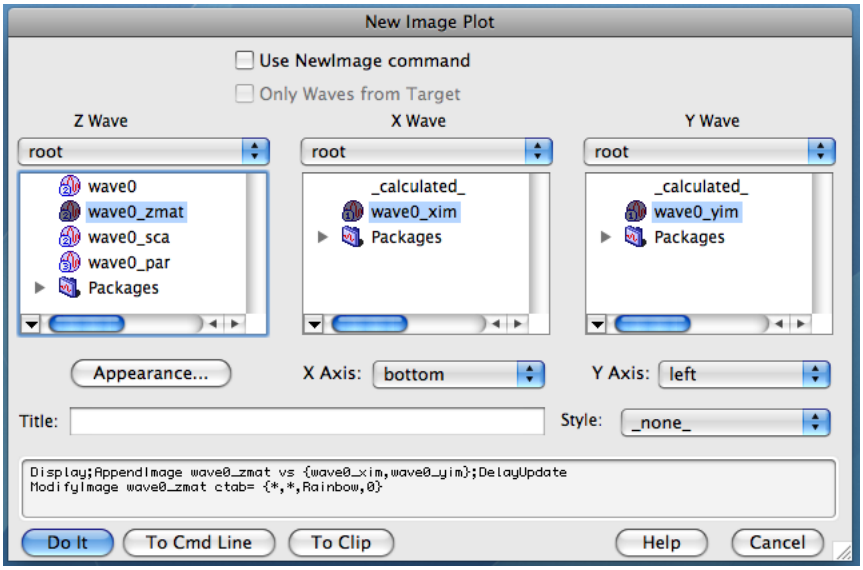
3) Similar procedures can be used to create 3D scatter plots and 2D contour plots.

Image Plots

4) Image Plots can be generated in one of the following ways:
   A. In the Gizmo rotation panel, click "Top View."



B. The ProcessTA procedure generates axes which are *approximately* scaled to generate an image (N -> N+1 points with no interpolation).
Windows → New → Image Plot

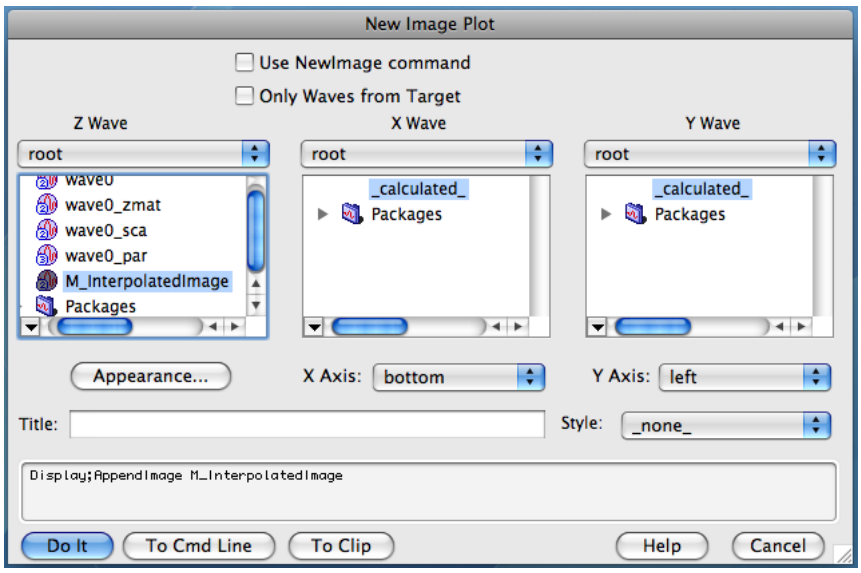


Click the “Appearance” button to generate a color image.

C. Interpolate a particular region of interest. Image interpolation can take several minutes depending on the image size and the mesh. An example command would be:

ImageInterpolate /S={600,1,800,0,0.1,10} Voronoi wave0_sca

This will generate an interpolated image over the spectral range 600 – 800 nm (1 nm mesh) and time range from 0 – 10 ps (100 fs mesh). On a 2.5 GHz Intel Core 2 duo processor with 4 GB of RAM, this command takes ~ 9 minutes on an original XYZ data set that contains 109056 rows.

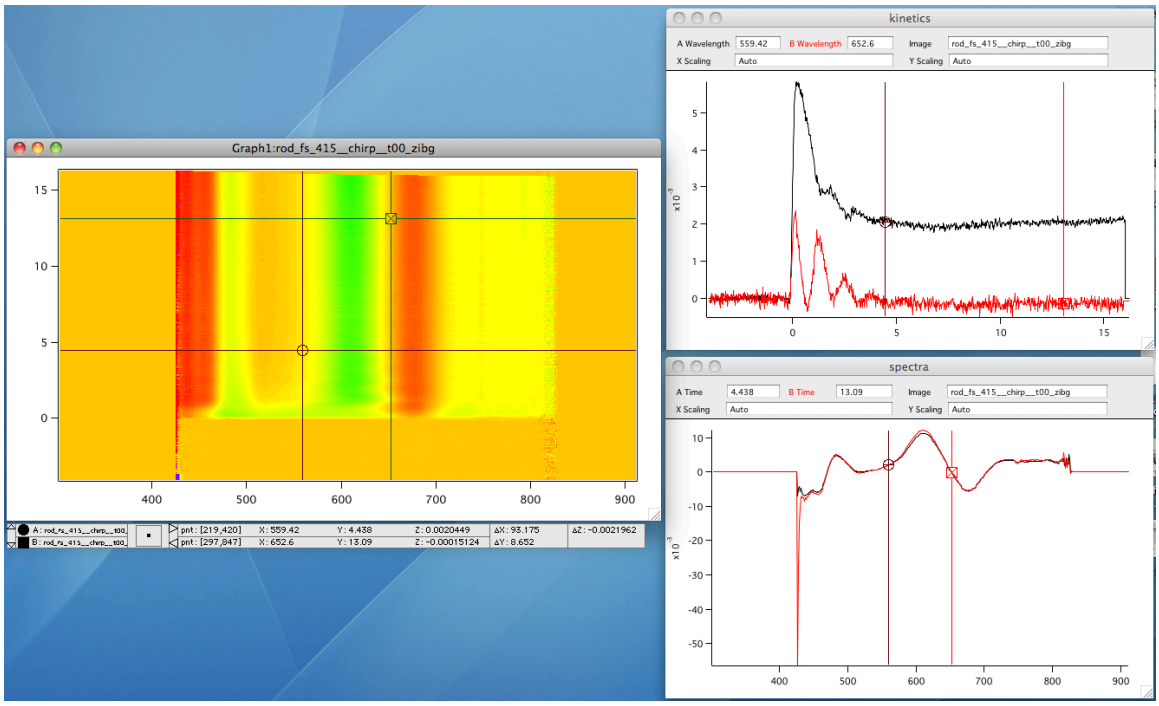


Visualizing Spectra and Kinetics from an Image Plot

Quick Visualization Using the Data Inspector

Spectra or kinetic data can be visualized through a set of windows that are automatically created when an image file is loaded or generated via one of the built-in processing functions.

The windows are named “kinetics” (vertical slices) and “spectra” (horizontal slices). Cursors A and B can be used to look at your data at a fixed point in time or wavelength.

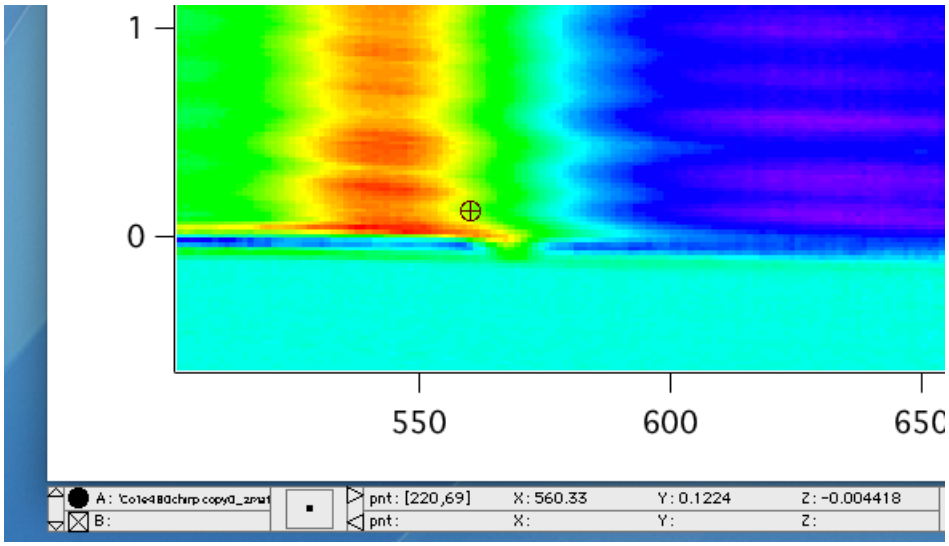


The information displayed in these windows is automatically updated when the cursors are moved or when a different image plot is activated.

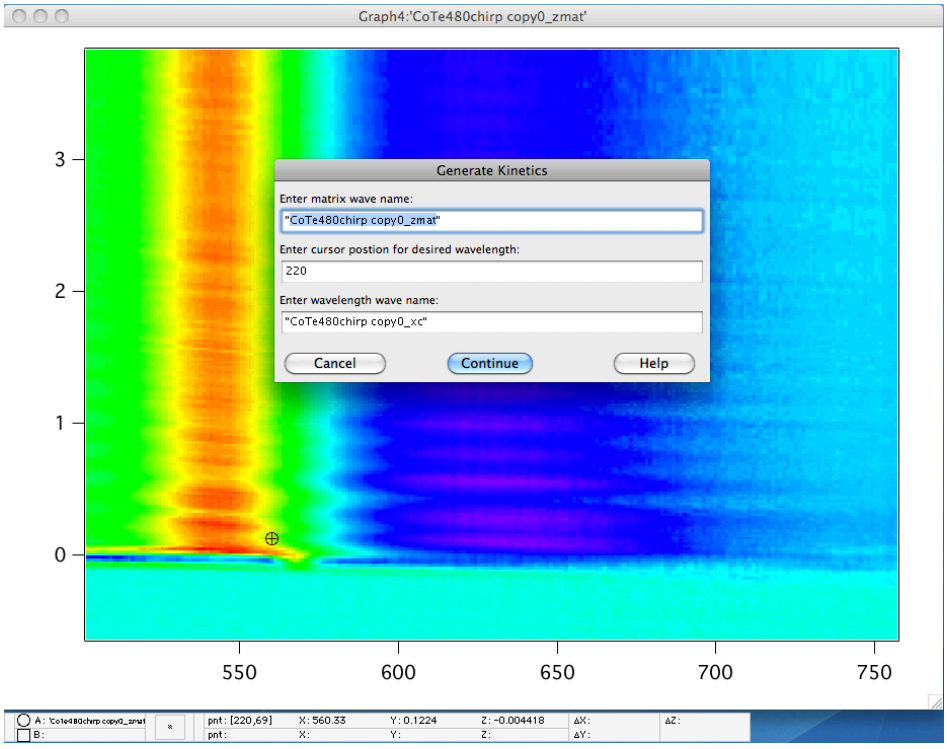
Data in these windows should not be fit or manipulated directly. Use the “Extract . . .” functions described in the next section to save regions of interest.

Extracting 1D Data for Fitting and Plotting

1) Extract Spectra and Kinetics from an image from *filename*_zmat.
The simplest way is to use the automatically generated image plot. Place the cursor in the spot where the data is to be extracted:



Select the appropriate function from the TA analysis menu:
TA Analysis → Extract Kinetics
TA Analysis → Extract Spectra



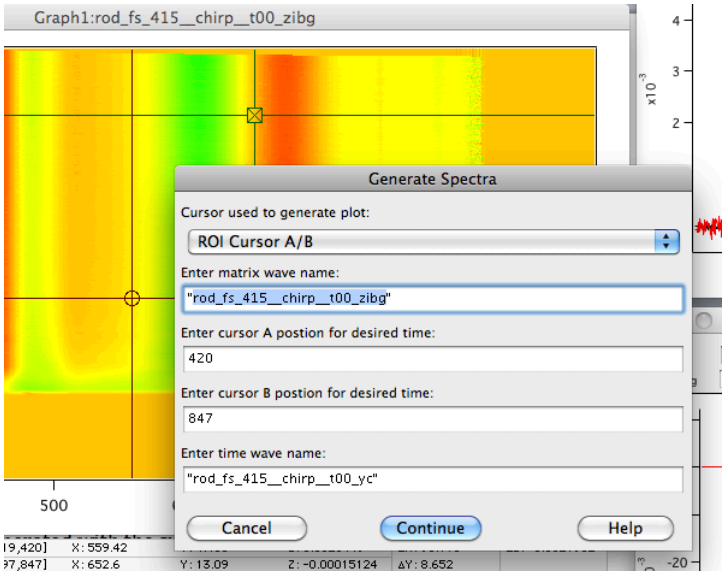
The procedure will attempt to auto-fill these values for you:
Matrix wave name: filename_zmat
Cursor position: element n [m] for (n,m) matrix for kinetics [spectra]

- note: this is not the actual wavelength or time value

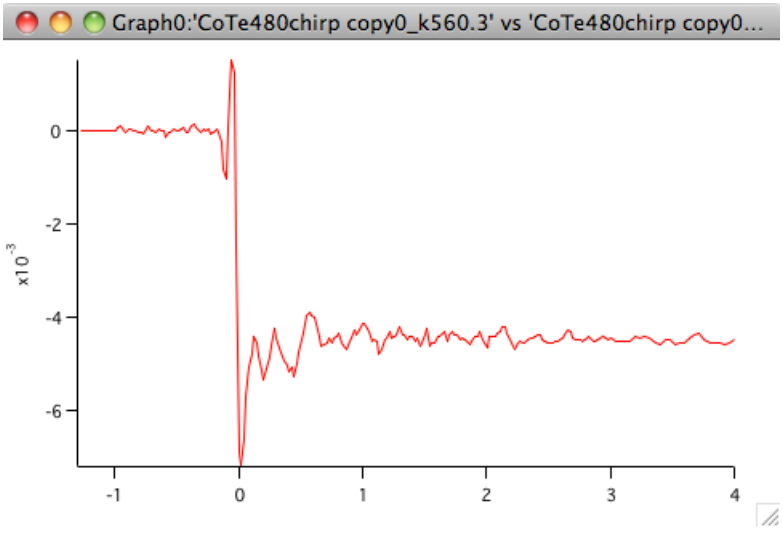
Wavelength [Time] wave name: typically *filename*_xc [*filename*_yc]

- note: this is not the waves used generate the image plot (which contain N+1 points rather than the desired N)

If both Cursors A and B are on the graph, you will have the option of extracting the data at either position or averaging between them:

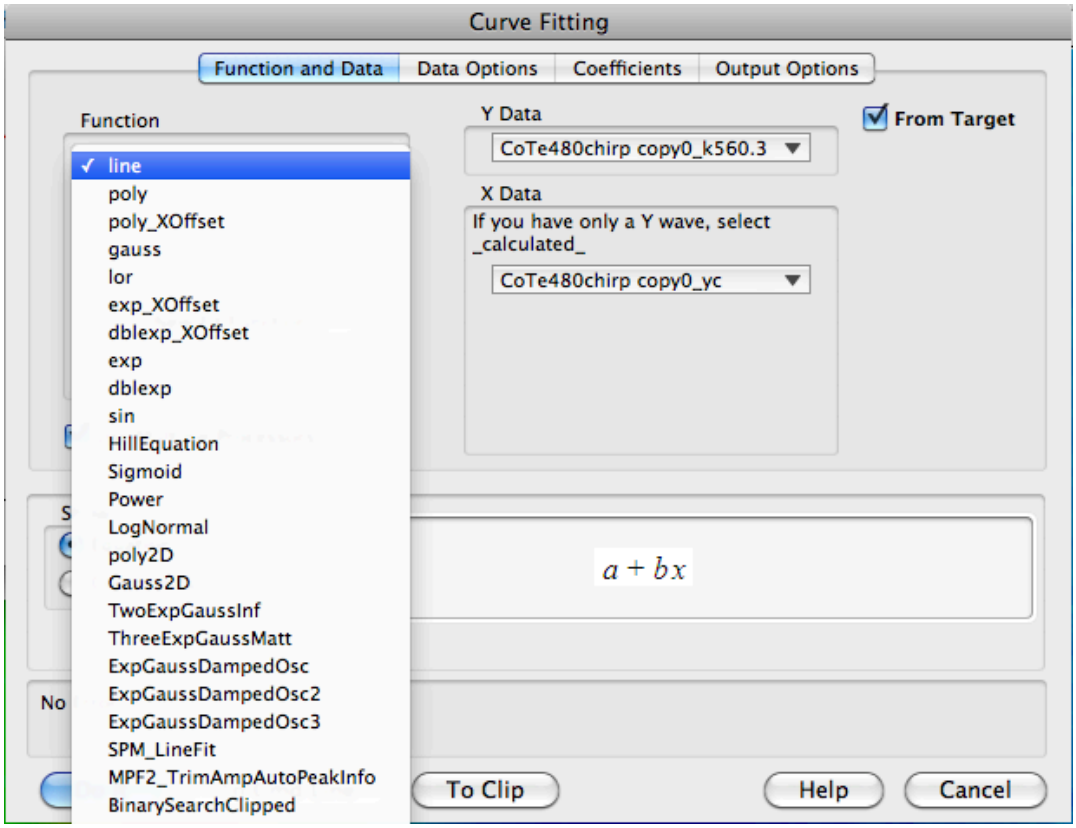


New waves will be generated with the suffix _k*wavelength_pix* or *stime_pix* (pix: number of pixels in the average of A and B cursors). 1D plots will be generated automatically if the expected file structure exists.



Curve and Peak Fitting

1) Fits of the kinetic data can be made using the built in Curve Fitting functions. Analysis → Curve Fitting →



A few special fitting functions are added in this experiment:

TwoExpGaussInf
ThreeExpGaussMatt
ExpGaussDampedOsc[2,3]

These use the built-in ExpGauss function to convolute the effect of impulsive excitation and exponential decay. The only difference is that a common pulsewidth and time zero is used for all exponentials.

Parameters for ThreeExpGaussMatt are entered in the Coefficients tab:

y0: constant y offset, usually fixed at 0 during fitting
amp1: amplitude of first exponential decay
t0: time zero (time of impulsive excitation)
pw: pulsewidth can be usually set to .12 for initial guess.

- Note: This is the standard deviation of the Gaussian used to approximate the laser pulse, not the FWHM. The conversion is FWHM ~ 2.355*pw.

G1: the rate of the first exponential decay component

- Note: This is equal to the inverse of the lifetime

amp2: amplitude of the second exponential decay component
G2: the rate of the second exponential decay component
amp3: amplitude of the third exponential decay component
G3: the rate of the second exponential decay component

The parameters for TwoExpGaussInf are identical with amp3 now called Ainf and G3 being automatically set to 0. This is used when the last decay component if effectively flat over the time range being fit.

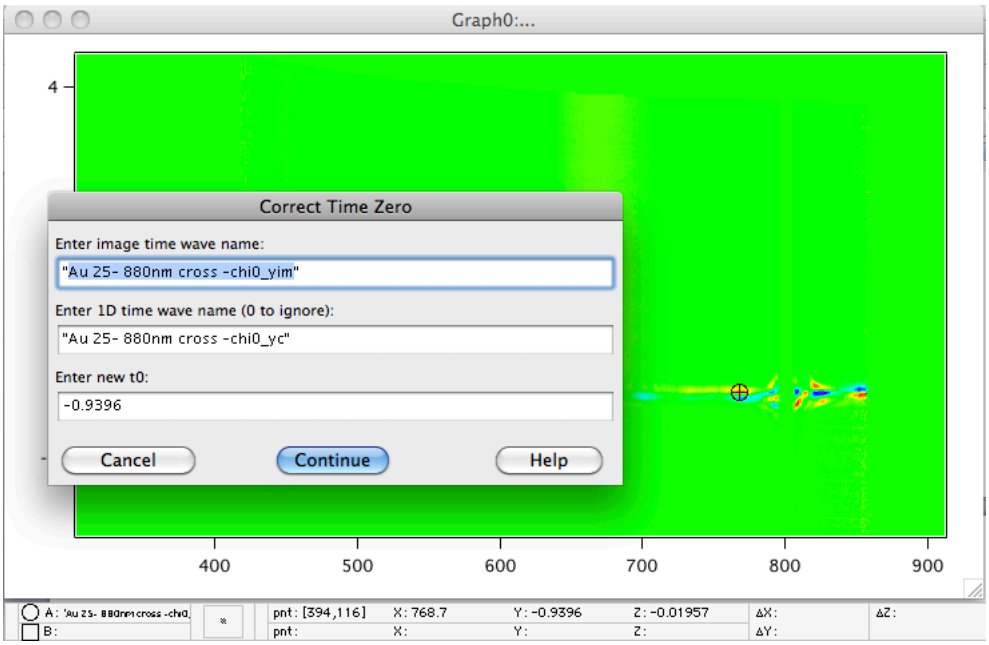
2) Transient spectra can be fit using the Multi-peak fit dialog.
Analysis → Multi-peak Fit → Start New Multi-peak Fit

More information can be found in the Igor Help Browser.

Data Processing Procedure

Time Zero Correction

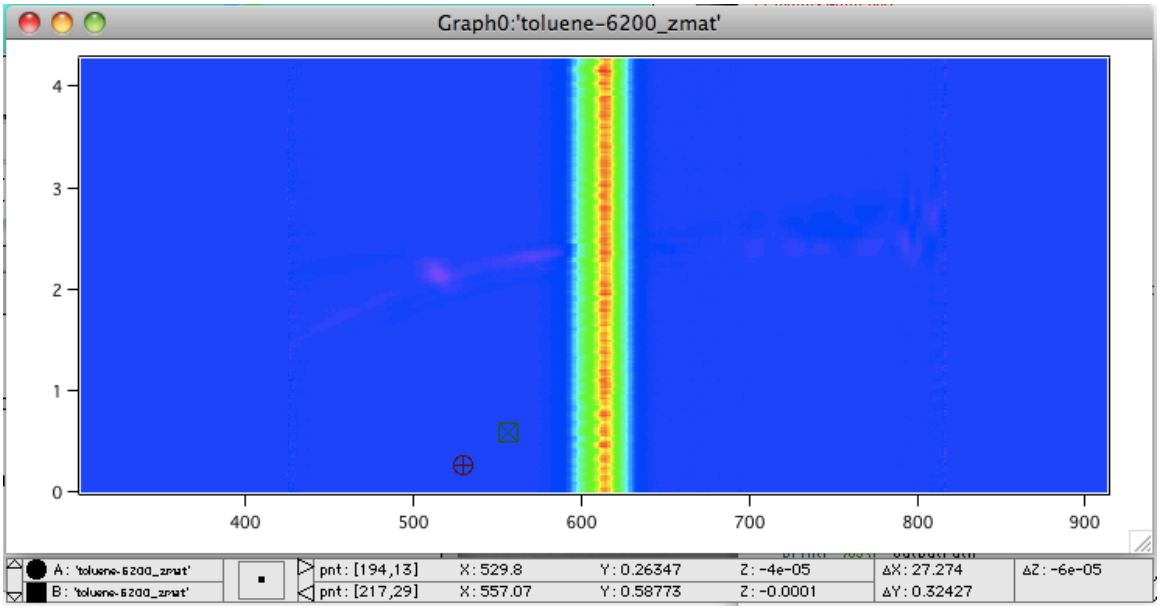
1) Use this procedure to correct your image and spectra for an absolute time zero. Place cursor A on your image at time zero and choose:
   TA Analysis → Time Zero Correction
2) This procedure attempts to automatically pick the correct time files and will choose the cursor position as the new time zero. These can be modified from the dialog prompt:



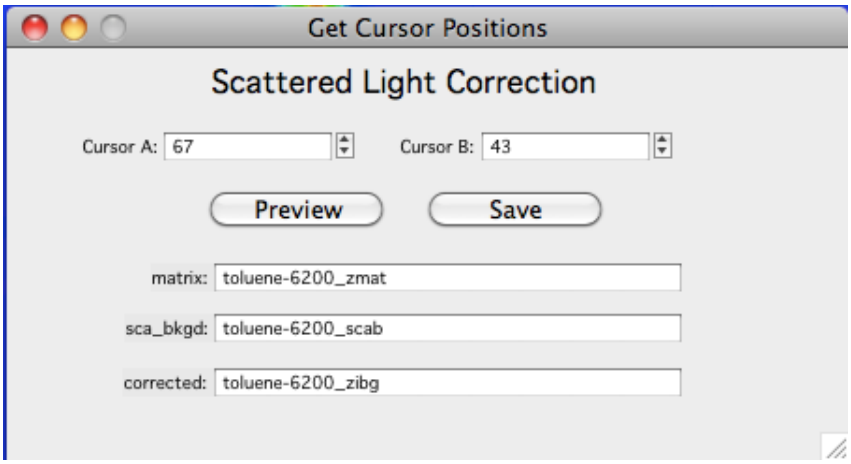
3) The first wave name, *filename*_yim is the y axis for the image plot (N+1 point) and the second, *filename*_yc, is the y axis for extracted kinetics (N points). To leave the kinetic plots undisturbed, enter "0" in this field. To choose a different value for the new time zero, manually enter it into the appropriate field.

Scattered Light Correction

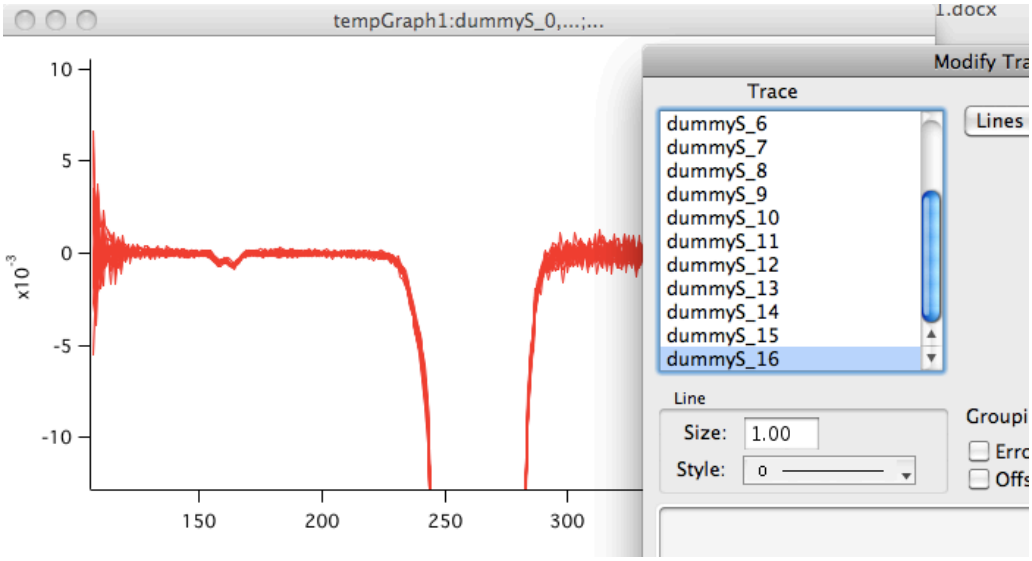
1) Scattered light collected by the array detectors can be automatically removed using the "Scattered Light Correction" procedure. The easiest way to do this is to use an image plot of your data.
2) Place cursor A and cursor B on the image to select a range to be averaged for the correction. Both of these cursors should be in the t<0 regime. Avoid early times that contain empty pixels (due to chirp correction).



3) Choose the appropriate procedure from the TA Analysis menu:
TA Analysis → Scattered Light Correction



4) Click the preview button to view the set of curves that will be averaged to make the correction file. The locations of the cursors will be sent automatically, as will the wave names.



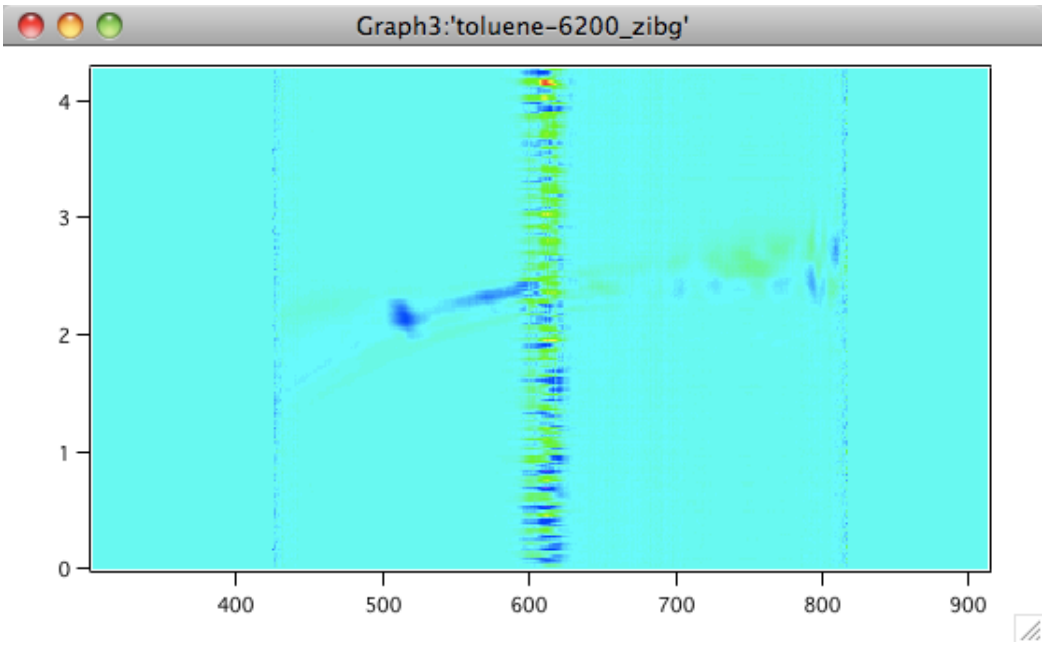
5) If this range is acceptable, close the window to return to the correction dialog box and click "Save." Make sure that the image file is the top graph, i.e., click on it again to bring it to the front before clicking "Save."

Alternatively, these procedures can be run from the command line interface. The syntax is:
PreviewSLC(*filename*_zmat, *imin*, *imax*) for Preview
ApplySLC(*filename*_zmat, *imin*, *imax*) to apply SLC

where *imin* and *imax* are the indices of the time positions to be averaged.

6) A new matrix is produced with the wave name *filename*_zibg along with a copy of the averaged t<0 file used for the correction (*filename*_scab).

   A new image plot is produced with the corrected wave file. The "Extract Spectra" and "Extract Kinetics" routines will also work with the new image file.



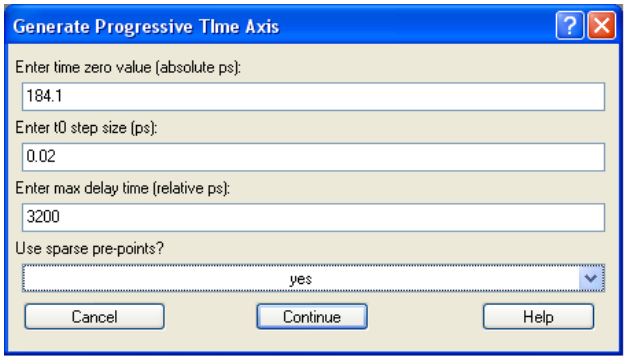
Export a Progressive Time Axis for Data Acquisition

This procedure generates a set of measurement times in a 1D row format for use with common TA acquisition software. It uses an exponentially increasing spacing, similar to Megerle et. al., *Applied Physics B* 96 215 (2009).

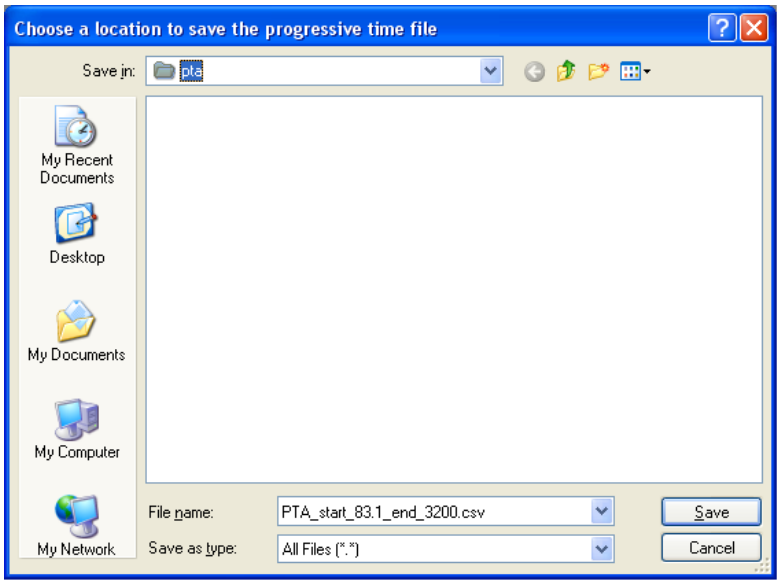
1) Choose the procedure from the TA Analysis Menu:
   TA Analysis -> Generate Progressive Time Axis

2) Enter the value of absolute time zero location in the dialog box. This value is referenced from the position of smallest delay on you mechanical stage, in units of ps.

3) Enter the value of the step size for the time window from -1 ps to +1 ps (relative delay to t_0). In this range the step size is constant. From 1 ps until the end of the scan (entered into dialog box in relative ps) the number of points is reproduced over each order of magnitude in time (1 – 10 ps, 10 - 100 ps, etc.). The sparse pre-points option will insert 10 data points in the 100 ps before time zero if desired for display and baseline determination.



4) The procedure will automatically generate a dialog box so that the file can be saved in the correct format (.csv). It will automatically be given a name that defines the start and stop points (absolute and relative time respectively) based on the input parameters.



5) Load the file into the appropriate data acquisition software. The name of the file will give you the appropriate start and end points. If sparse pre-points are used, this will be 101 ps before time zero. Otherwise, it will be 1 ps.