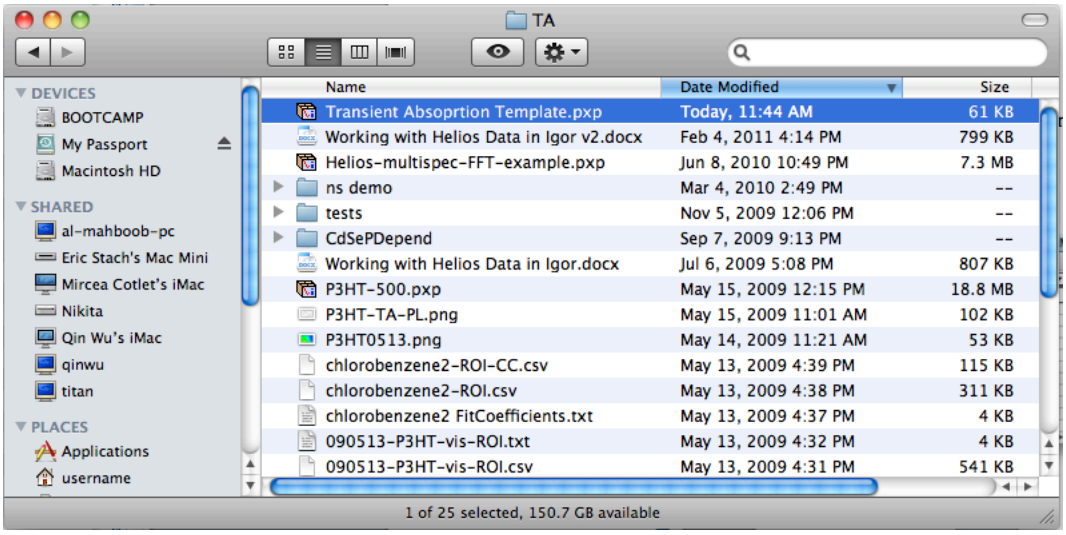
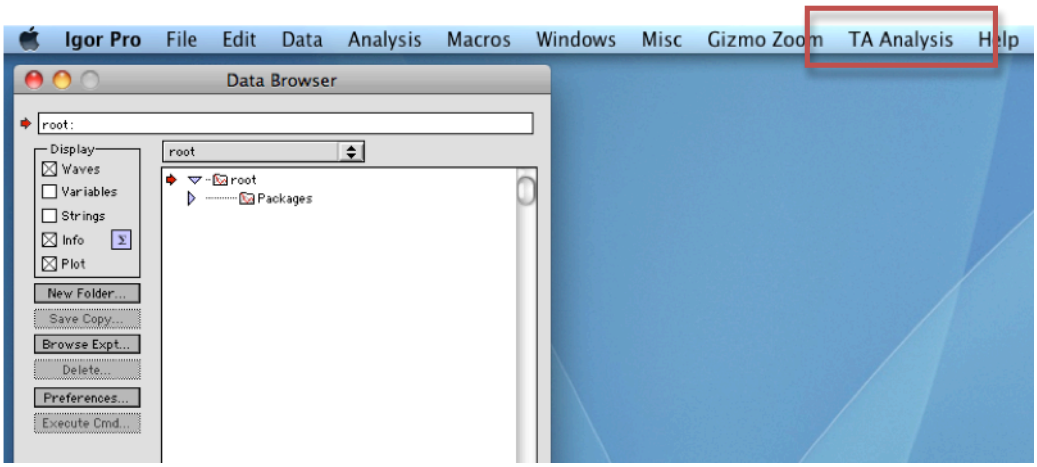
Working with Helios Data in Igor v. 6:
v.3 February 11, 2011

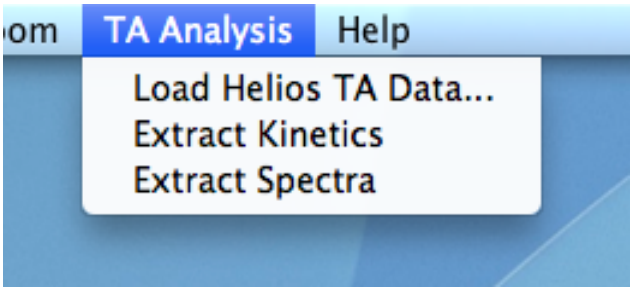
1) Open the Igor Packed Experiment file named "Transient Absorption Template.pxp"

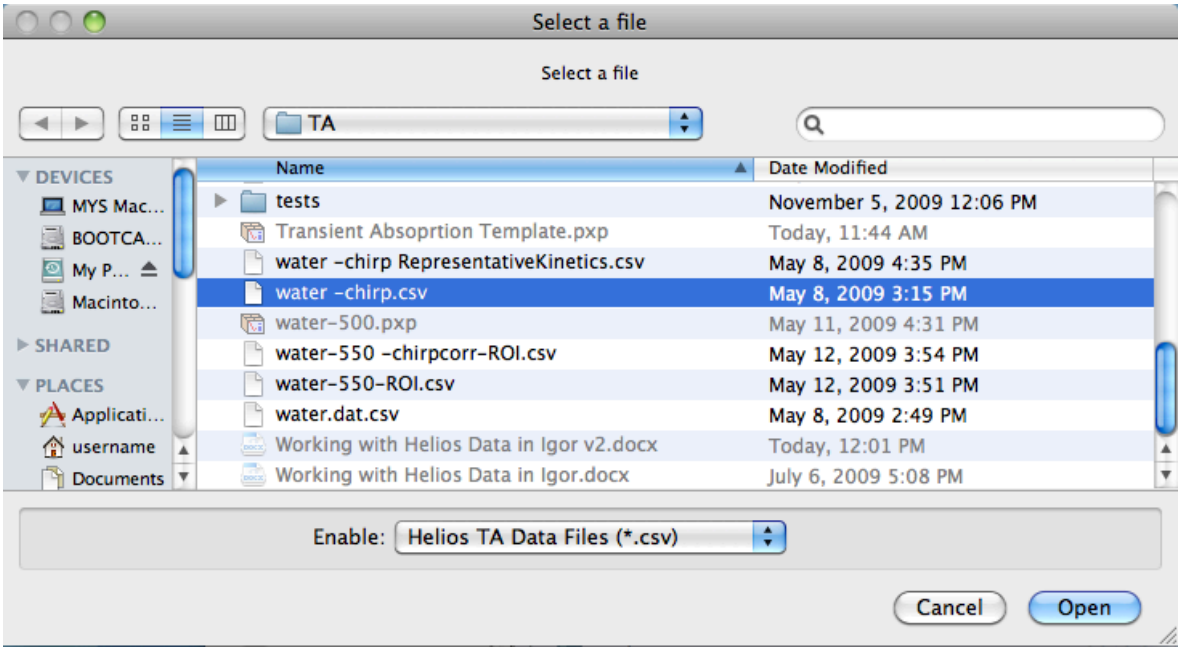


2) A blank experiment will open which automatically includes and compiles the necessary procedures. A new menu will appear on the task bar entitled, "TA Analysis."



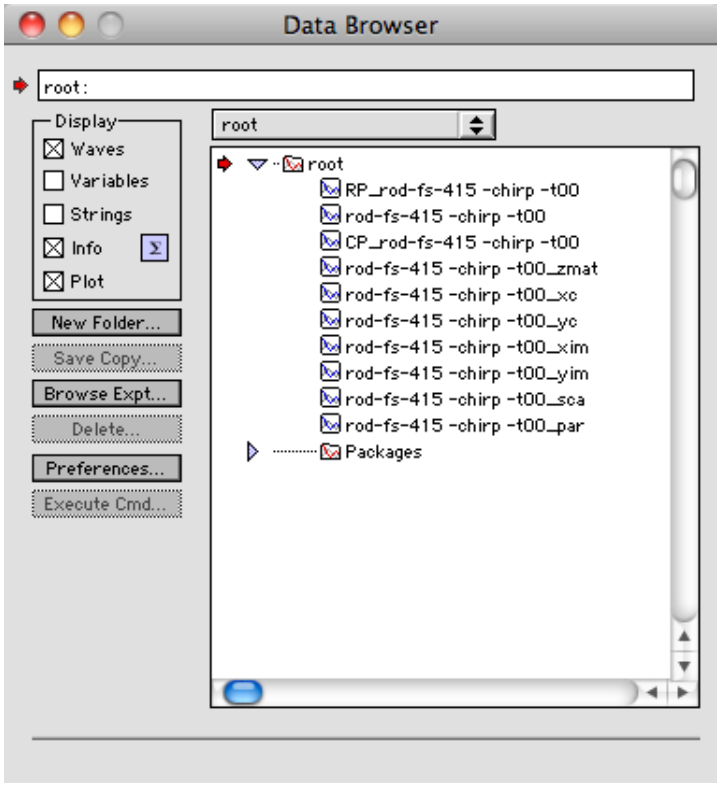
3) Open your saved transient absorption data (.csv files) using the appropriate menu option:
TA Analysis → Load Helios TA Data . . .



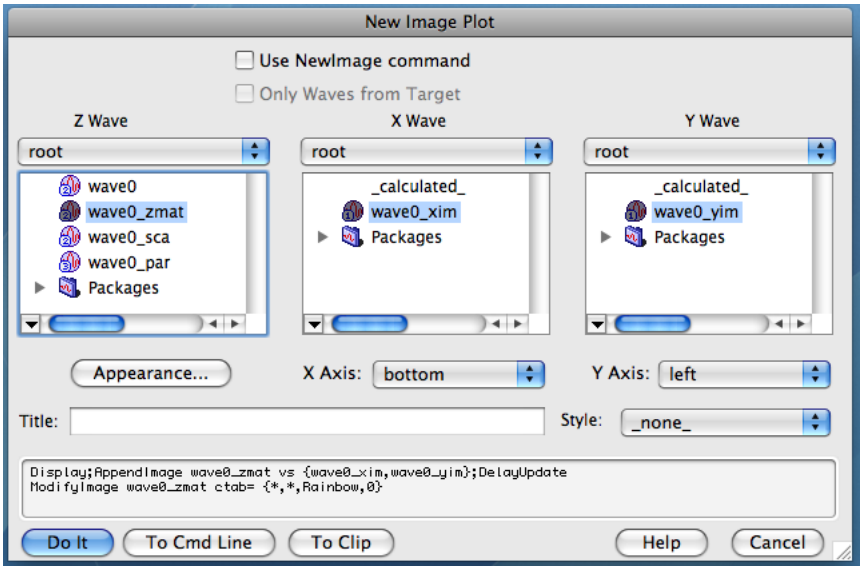


4) This procedure loads the original data in *filename* with the corresponding wavelength (RP_*filename*) and time (CP_*filename*) information. It creates a new set of these waves (*filename*_zmat; *filename*_xc; *filename*_yc), with all the NaNs and Infs in the files replaced with 0, and deletes extra rows (> 512). It also creates several additional waves for graphing puposes:

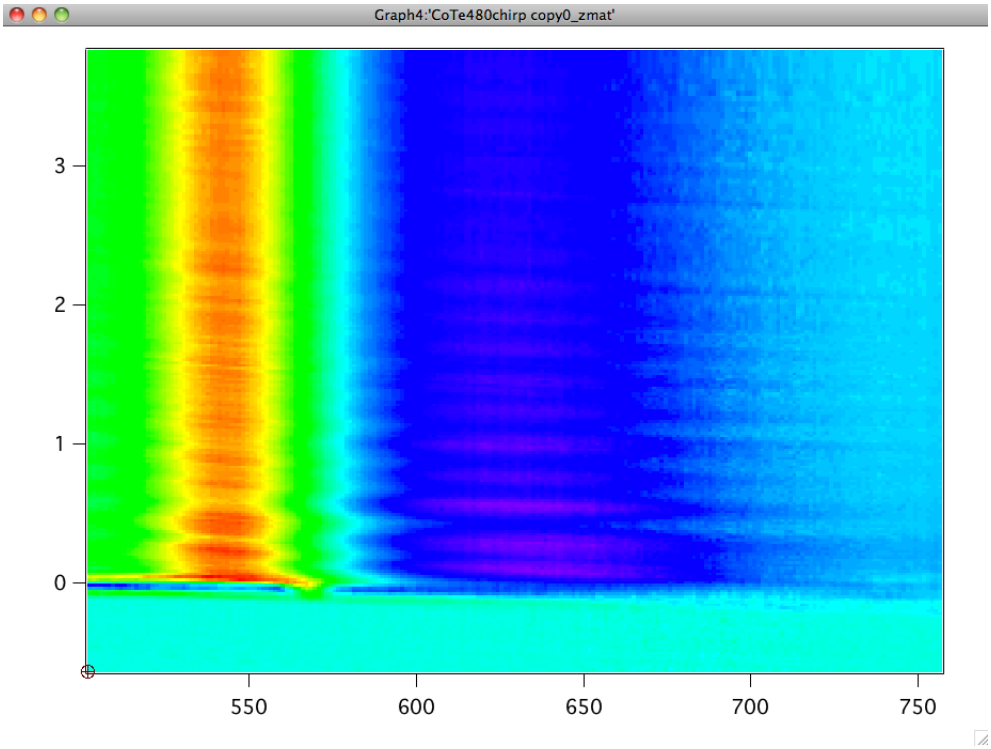
RP_*filename* (wavelength labels for row data in nm)
filename (original uncorrected matrix in ΔOD)
CP_*filename* (time labels for column data in ps)
*filename*_zmat (corrected matrix)
*filename*_xc (processed row values)
*filename*_yc (processed column values)
*filename*_xim (x values for image plot)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



5) 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

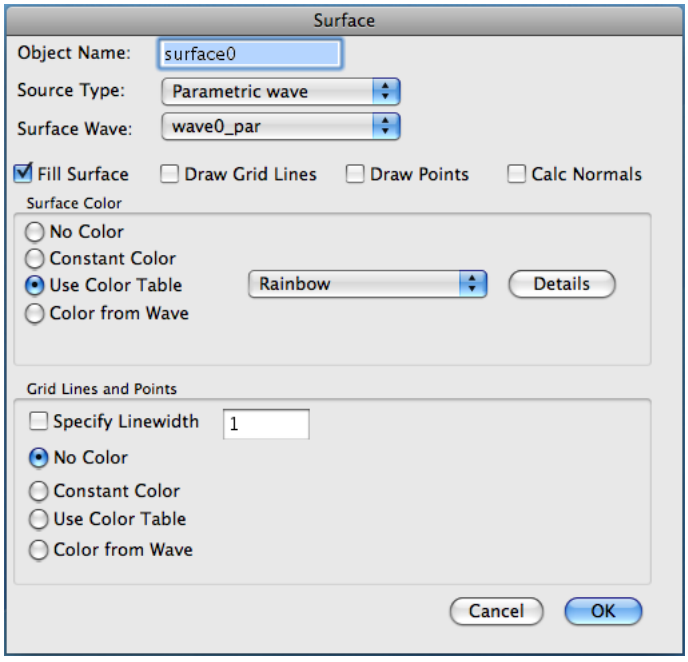


Click the "Appearance" button to generate a color image.

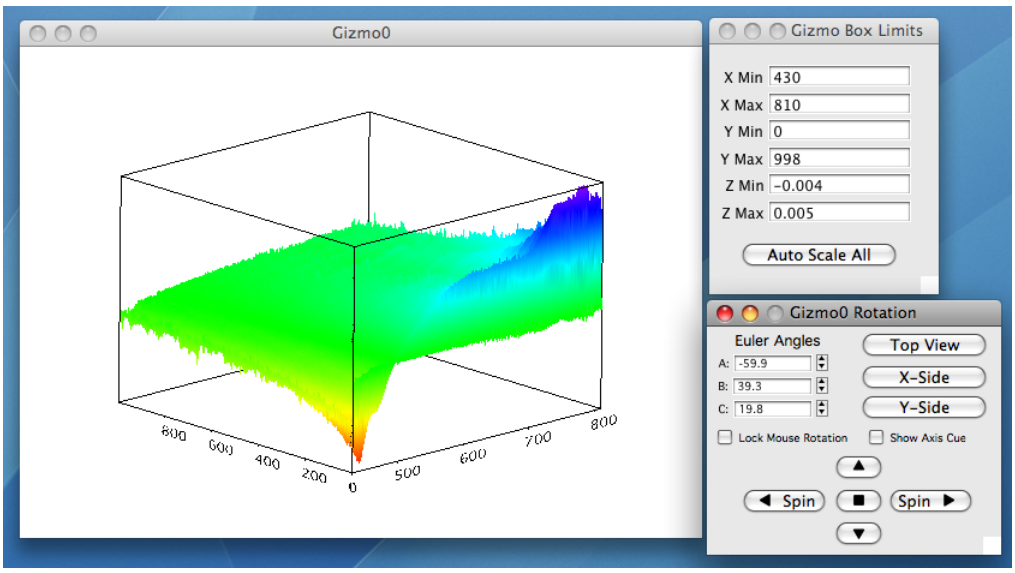


Use the CTRL-I (CMD-I for Mac) key sequence to manually show the cursors.

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

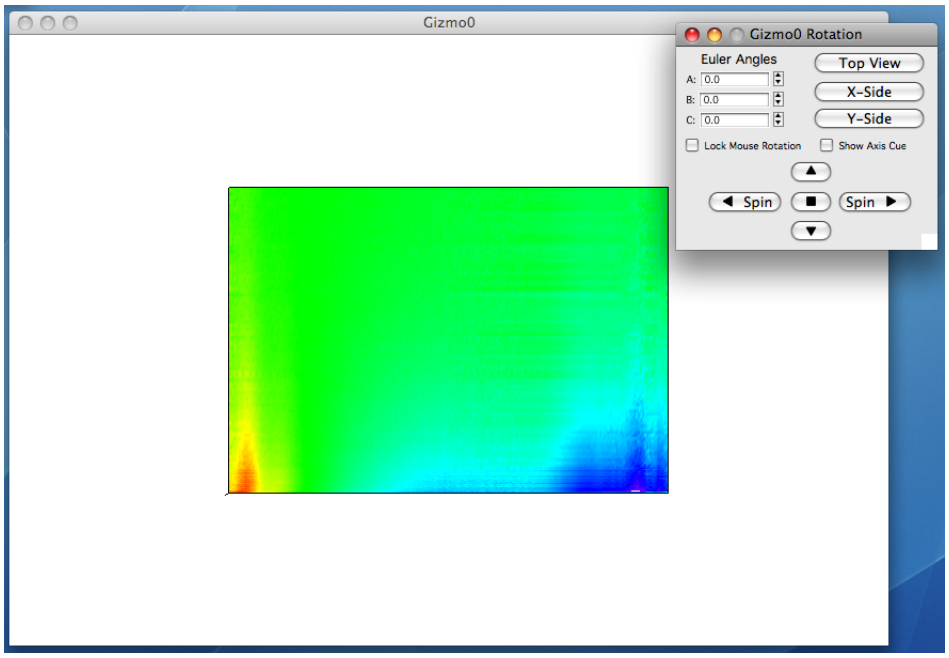


Modify as appropriate:
Gizmo -> Axis Range
Gizmo -> Rotation

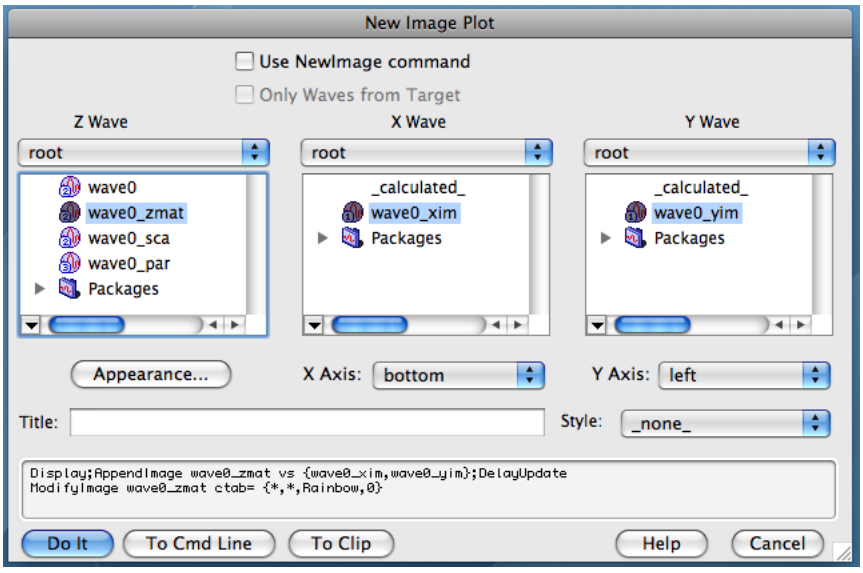


7) Similar procedures can be used to create 3D scatter plots and 2D contour plots.

8) 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

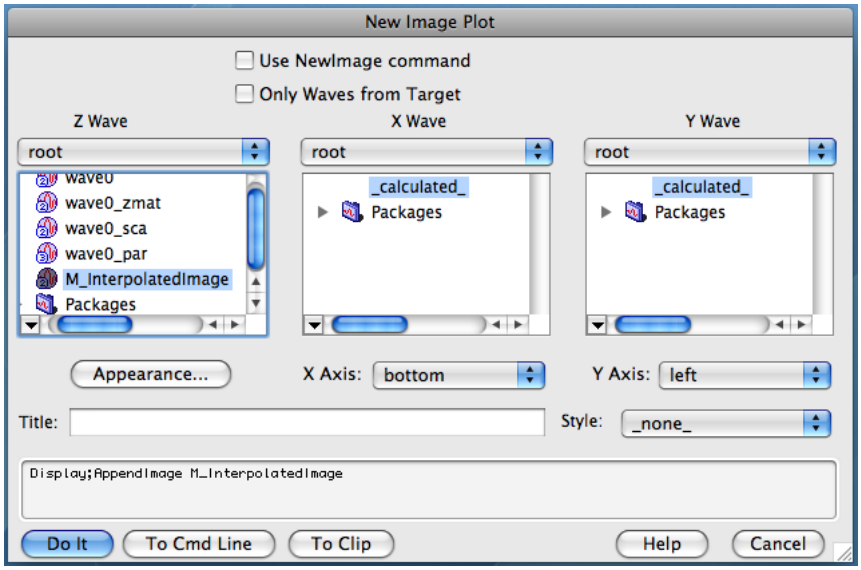


Click the “Appearance” button to generate a color image.

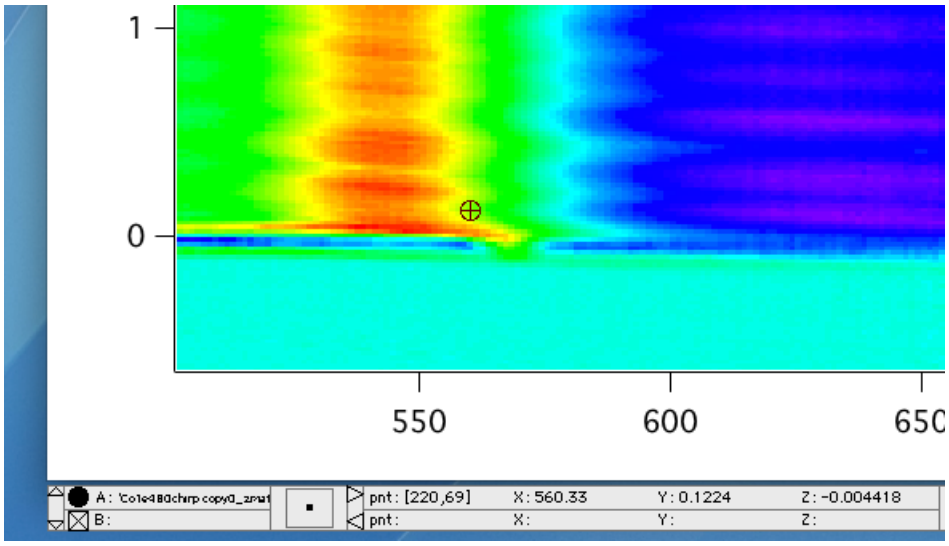
C. Interpolate a particular region of interest. Image interpolation can take several minutes depending on the image size and the mesh. An example command would be:

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

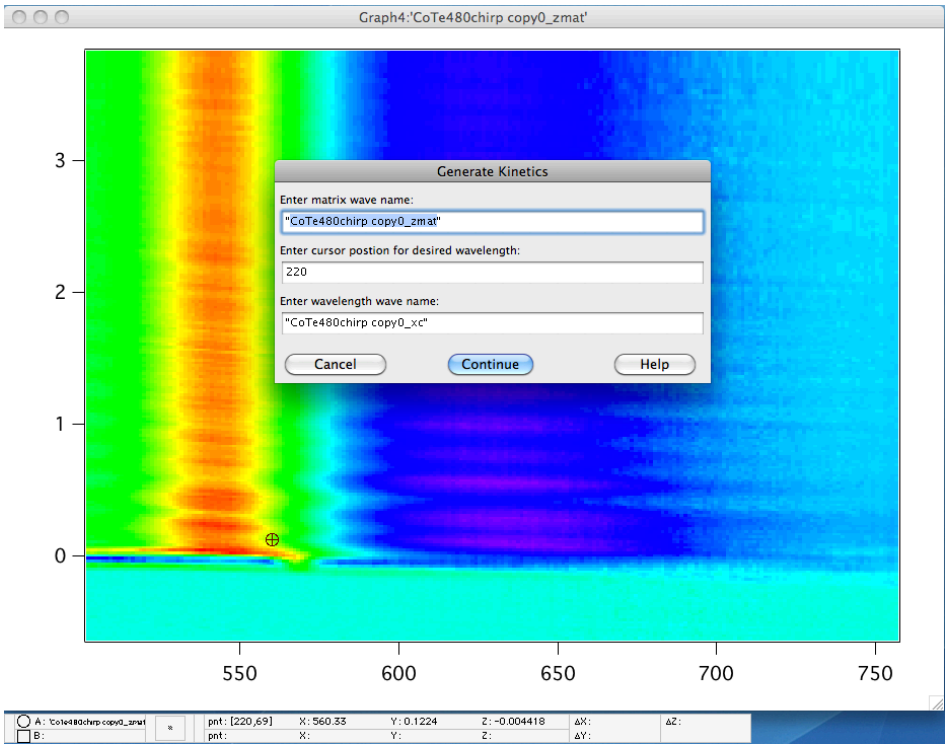
This will generate an interpolated image over the spectral range 600 – 800 nm (1 nm mesh) and time range from 0 – 10 ps (100 fs mesh). On a 2.5 GHz Intel Core 2 duo processor with 4 GB of RAM, this command takes ~ 9 minutes on an original XYZ data set that contains 109056 rows.



9) 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



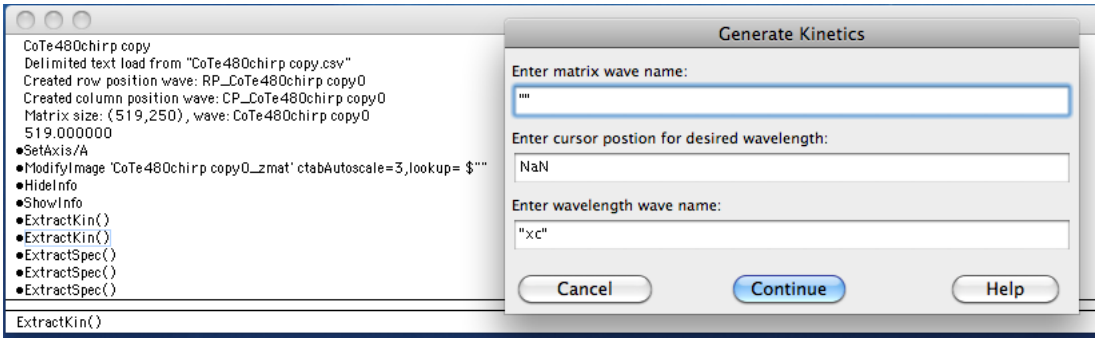
The procedure will attempt to auto-fill these values for you:
Matrix wave name: filename_zmat
Cursor position: element n [m] for (n,m) matrix for kinetics [spectra]

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

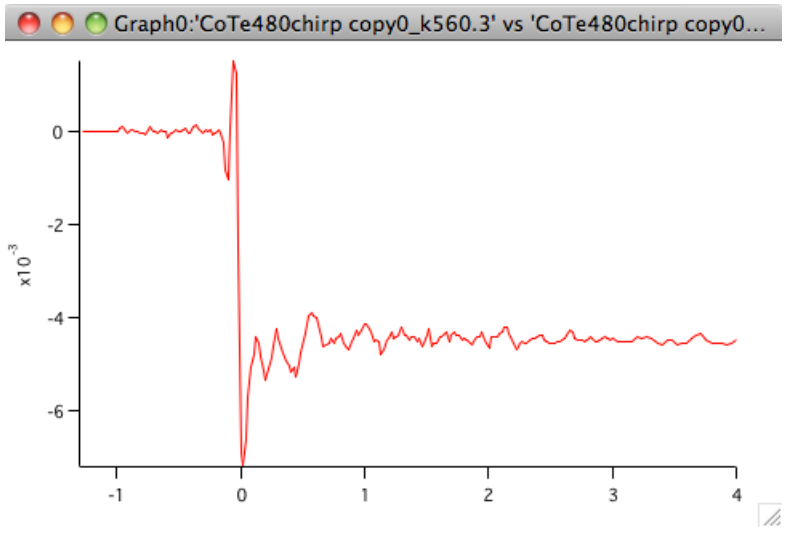
Wavelength [Time] wave name: typically *filename*_xc [*filename*_yc]

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

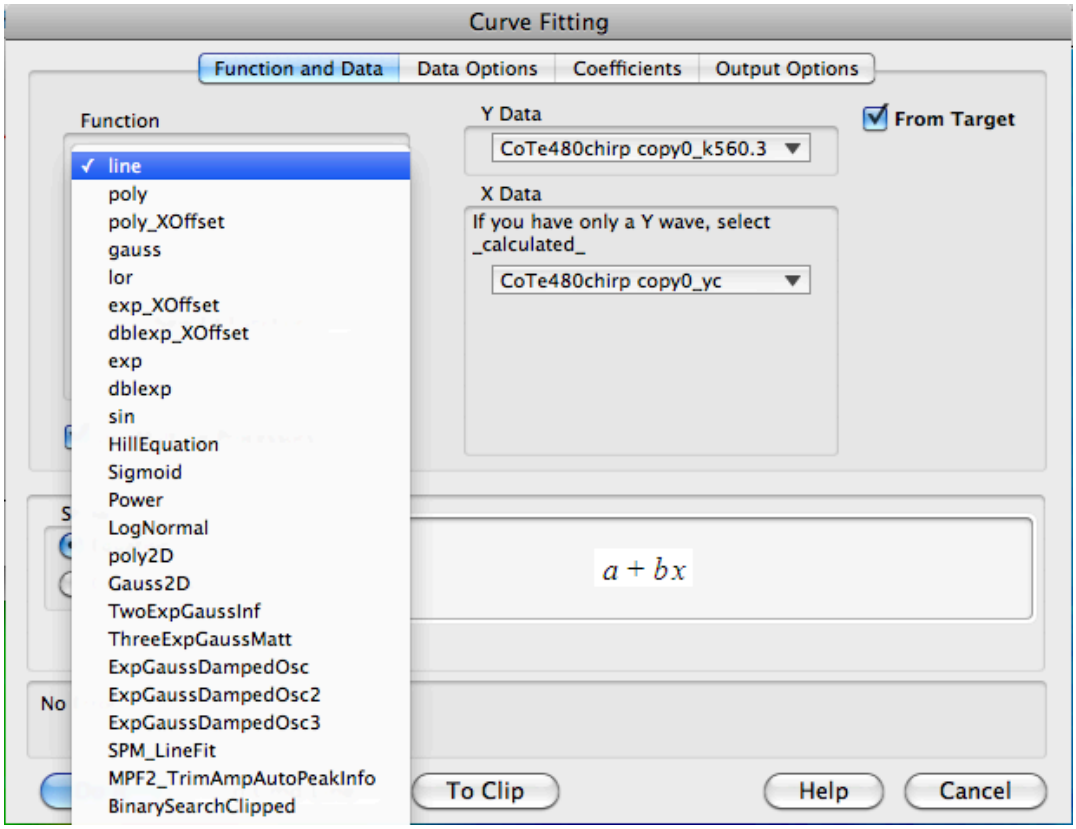
Alternatively, the functions can be called directly from the command line and the matrix information can be entered manually using the guideline above.
ExctractKin()
ExtractSpec()



New waves will be generated with the suffix _k*wavelength* or _*stime*. 1D plots will be generated automatically if the expected file structure exists.



10) 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.

11) 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.