Using Igor to Plot Trajectories

Tutorial for students in Chem 499
Step-by-step instructions with images
When Igor is opened there is a default data table. You can copy and paste columns of data into the table.
Ultraedit is one convenient program to use. If you read the data, select it and use control <c>. You can copy the data directly into Igor.
The data are automatically given the names wave0 and wave1 by Igor.
You may then rename the data columns using the rename command.

Type the command in the bottom of the box. The commands are recorded in a history.
Using the display command you can make a plot of the data. Igor calls each data column a wave. The “display” command Has the syntax >display y-wave vs x-wave.
You may bring up this menu by clicking on the border of your plot.
Change the font size. Size 14 font is recommended for publications.
Note that you may change the axis to be modified.
Here we are changing the font size for the left axis.
Using the “axis label” tag you can obtain a menu for entering the axes.
To change the x-axis so it is in units of nanoseconds, you need to divide by 2000. Note that the command is `tt/=2000`. 
To append another trajectory (continuation) you scroll to the bottom of the data column and select both columns.
Open the next trajectory and obtain the data.
Paste the data
Fix the x-axis using the Command tt=x.
Now you have plotted two successive dcd files back-to-back. In this case it is a total of 4 nanoseconds.