

Tutorial: Using Grace to produce graphs for Physics Labs

Contents

Introduction	1
Saving and Opening an Xmgrace File	2
The First Graph	2
A. Entering Data into the spreadsheet of Grace	3
B. Issue: xmgrace seems locked up	4
C. Tuning a graph in Grace	4
D. Linear Fit: Regression analysis	4
E. Axis Labels	5
F. Slope and intercept: Rounding and quoting \pm error	6
G. Slope and intercept: units.	6
H. Adding Error Bars and Calculations in xmgrace	6
I. A Few Hints for xmgrace	8
Second Graph: More Calculations Using Grace's data set operations	8
Additional Advice for Using xmgrace	11
J. Greek Letters	11
K. Extending the line of best fit.	11
L. Importing Multicolumn Data From other Sources.	11
M. Plotting a function in xmgrace	11
N. Removing or Selecting some data from a Set	12
1. In the Spreadsheet	12
2. By Formula	12
O. Placing Additional Text and Other Objects on a Graph	12
Error Bars Again	12
Graph 3: Nonlinear Curve Fitting	13
Graph 4: Another Linear Plot	13
Instructions for Graph 4	14
Graphing with xmgrace: Quick Reference Guide	14
Importing graphs to L^AT_EX	15
Running Grace in Windows OS	15
P. QtGrace for Windows	15
References	16

Introduction

After collecting data it is usually necessary to display and analyze it. A two dimensional plot of the variables measured will show the relationship between them. Regression analysis will show the quality of fit and the degree of dependence of one variable on the other. There are many software packages available for this. One of the better ones available is called Grace, which has a home page <http://plasma-gate.weizmann.ac.il/Grace/>. It is available for many common operating systems at no charge, and widely used in scientific publications. The following tutorial will give you an introduction to using Grace for your physics labs. You will produce three plots of data and hand them in for marking.

Saving and Opening an Xmgrace File

Xmgrace's save file dialog has two fields that must be understood to avoid confusion. The top field is named 'Filter'. In that field will be the directory xmgrace was started from, usually the home directory of the user. In addition, the end of the filter has *.agr tacked on. This means the files list only shows files that end in .agr which is graces default file extension. Leave this as is.

To save a file, you type in the filename in the 'Selection' field. Do not remove the sub-directory names that are present, for example. /home/gary. To save the file as test_graph1.agr in your home directory, you should have /home/your_login_name/test_graph-1.agr. Then click ok.

Opening a files makes use of the filter as well. By default, only .agr files are shown in the 'Files' list. If your file is not present, you can remove the .agr in the 'Filter' field and press enter. Leaving the * means all files will be shown in the 'Files' list.

The First Graph

Log into Linux and start the Grace program. The executable is called xmgrace (entered into a command line shell) and may also be in the menu under "Education" or "other".[1] This will present you with the main window of Grace as shown in figure 1. There are a few buttons on the left side of the main window. The most used ones are:

- A_S = auto-scale all points to appear in the plot area.
- Draw = redraw the plot

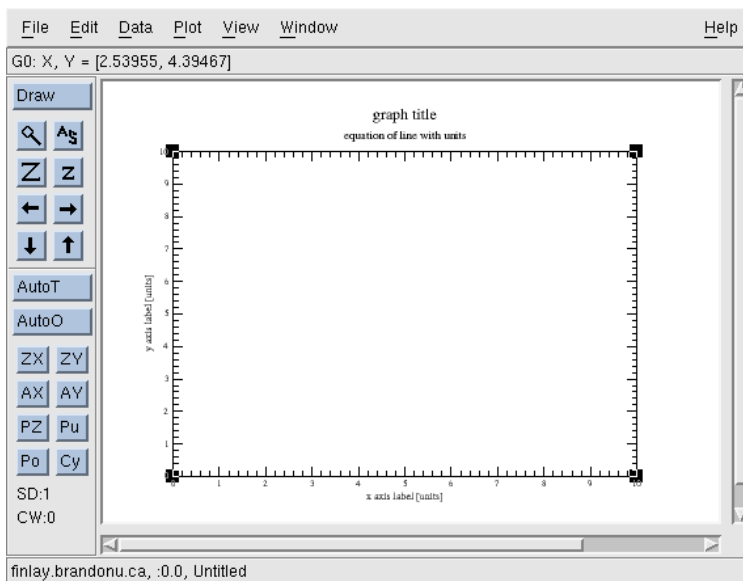


Figure 1: Grace's main window

The process of creating a graph will take the following general steps:

1. Choose which data is for the x-axis and which is for the y-axis. Error bars can be calculated or entered directly
2. Enter the data into the appropriate columns in the spreadsheet contained in Grace. Calculations on this data may be necessary and can be performed within Grace.
3. Save the file periodically; use the .agr extension on the filename.
4. Produce a scatter plot with Grace. This type of plot is one with just the data points showing. Remove the "join-the-dots" line and execute the best-fit (regression) analysis. Use the subtitle field to report the best fit equation with errors and units.

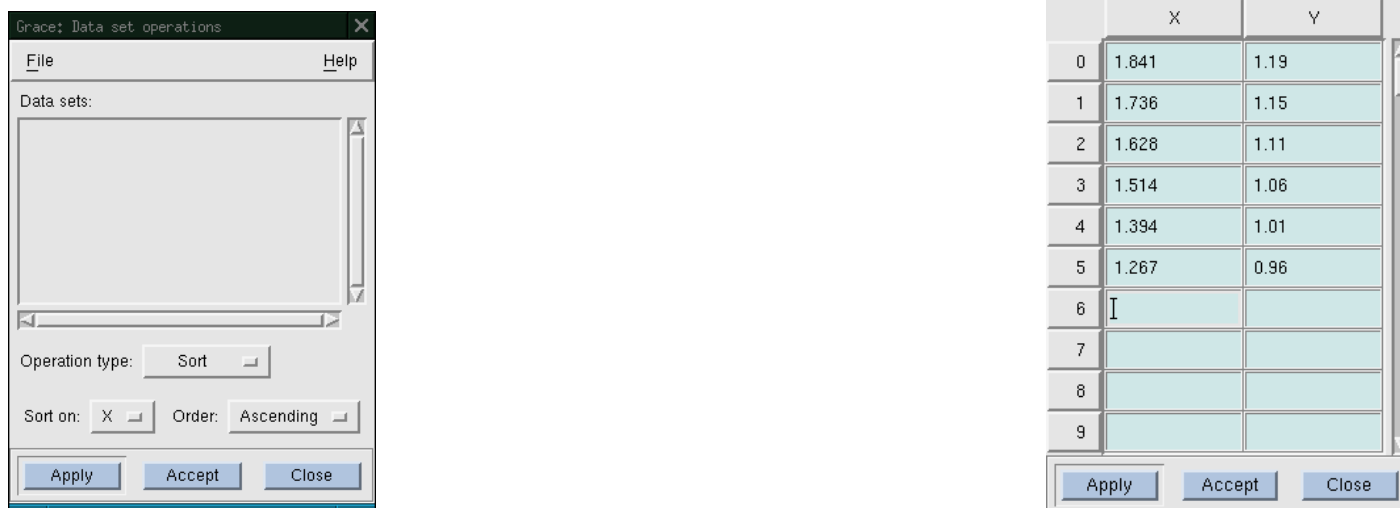


Figure 2: Dialog windows for data entry. The left window is used to create the window on the right. Using tab after entering each data/number is helpful. Tab out of the last cell so that the value is parsed and not set to zero.

5. Scale the graph as appropriate. The reader must know ahead of time if the the y-intercept or both intercepts should be shown. If only the slope is used in future calculations then, then showing the intercept(s) may not be necessary.
6. Perform a linear regression or arbitrary curve fit on the data. Use the fit results to specify the constants of the fit.
7. Label the x and y axes with the variable plotted and its units.
8. Put a title on the graph.
9. Print the graph or export it to an image file for importing into a report as required.

A. Entering Data into the spreadsheet of Grace

The Lab Instruction Book will ask that you graph two variables to produce a plot of your data. One of the first questions that arises is which variable goes on the x-axis and the y-axis. *Instructions for producing graphs are phrased in the form 'plot y as a function of x'. In other words you will always put the first variable (could be time, temperature, etc) on the y-axis and the second variable on the x-axis.* So if you are asked to 'plot phase shift as a function of temperature', phase shift values are on the y-axis and temperature is on the x-axis. This follows from the idea that the independent variable is plotted on the x-axis, the dependent variable goes on the y-axis: y is a function of x or $y(x)$.

The following example is to produce a plot of time T as a function of the square root of the sum of two distances $(s+L)[2]$.

1. **Data Set Operations:** To bring up the spreadsheet, click on 'Data, Data set operations'. This produces a window called 'Grace: Data set Operations' as shown in figure 2, left side. This window will list the various data sets but the list is shown empty as none exist yet.
2. **Create New:** Right-click and hold down the mouse button inside the data sets area of this window. Select 'Create new, In spreadsheet'. This produces the 'Spreadsheet data set editor' window. In the spreadsheet window, Type will be left as XY as we are dealing with just two columns of data.

3. **Data:** Enter the data shown in figure 2 . Use the tab key to move between x,y pairs of data in the spreadsheet. If you make a mistake, go back and edit the cell[3]. Then move the cursor out of the cell if entering or changing the value.[4]
4. **Set hint:** Change “Comment” to 'T and sqrt of (s+L)'[5]. Now click 'Accept'. This will close the dataset editor window and bring you back to the data set operations window.
5. **Accept/Apply?** The only difference between 'Apply' and 'Accept' is that Accept closes the window. Now you will see the data set operations window has a data set in it called G0.S0[2][6]. This is 'grace-speak' for 'graph 0, set 0 which contains 2 columns of values and 6 rows'. If you double-click on the set name G0.S0[2][6], Grace will load and display the data set in the spreadsheet editor again.
6. **View Set hint:** To see your comment right-click on the 'Data sets:' portion of the 'Data set operations' window. In this menu click on Selector operations, view set comments. Now your comment will be shown in the list of data sets. Labeling your data sets is helpful but not necessary. [6]
7. **Save:** Save your data to the hard-drive using the 'File, Save as' dialog. You have your own directory to store files in. For instance if your username is casey, your directory is /home/casey. This is the main directory you can use to store files in and make subdirectories.
 - (a) **Put .agr as the extension of your filename in the “Selection field” Eg. measure_g.agr or graph1.agr.** The 'Filter' field is for filtering out other files in the same directory so they are not displayed. Leave this alone, as the default extension for Grace files is .agr. Note that there are several useful areas of this window including the Directories list, the Files list and room for a description of the file. For more details see subsection .
 - (b) **Save your file often as you work. Control-s will execute a save file operation.**

B. Issue: xmgrace seems locked up

It very likely is not, but if a dialog window gets hidden behind another window, then xmgrace is waiting for user input and you have a different window focused. Alt-tab usually works through open windows, so check that[7].

C. Tuning a graph in Grace

Ideally, the axis should be scaled so that the data range covers 80 to 90 per cent of the graph's area. Press the button labeled A_S to auto-scale the graph. Now you will see each axes' range has been adjusted.

The line joining the data points is not desirable: it is not a fit to the data We want to see the data points represented by small circles and then have the “line of best fit” or regression line drawn in. This can be done by:

1. In the main window click on 'Plot, Set appearance'. Go to Symbol Properties and change 'None' to 'Circle'. Change the symbol properties size to between 50 and 70 from 100. Click Apply and you will now see your data points represented by small, open circles.
2. Now remove the line by using the 'Set Appearance' dialog box and change the Line properties from 'Straight' to 'None'. Now there should only be the circles representing the data. Click 'Accept' to close the Set Appearance window. Next we need the line of best fit.

D. Linear Fit: Regression analysis

With the data showing and the join-the-dots line removed, it is time to plot the best-fit line. Your graph requires the equation of the best-fit line with slope/intercept errors and units and the plotted variables (*not “x” and “y”*).

1. In the main window, click on 'Data, Transformations, Regression'. The set S0 should be highlighted[8], the 'Type of fit' set to 'Linear', load should be set to 'Fitted values', 'Restrictions' set to 'None'. These are the defaults.

2. Click Accept and a red or black line will appear on the graph. This line is the best fit for the data as the sum of the vertical separations from it to all the points is a minimum. A window called 'Grace: Console' will open. Do not close this window until you have copied the necessary values from it.

In fitting the observations (your data), Grace has created a second data set called G0.S1[2][6], which is set one of graph 0. A new window called "Grace: Console" contains messages, errors and information about the statistical analysis and the equation of your line of best fit. **Enlarge and scroll up and down in the console window to see what is there.**

The main points of interest are:

1. the slope, the intercept, and the standard error of the line's slope and intercept. The equation of the line is also shown as $y = 0.44812 + 0.40419x$. This equation is of form as $y = b + mx$ with the intercept b and the slope m .
2. Cut and paste this equation into the graph *as follows*:
 - (a) Double-click on the "Graph title" text in the main window to bring up the "Grace: Graph Appearance" window. Delete the subtitle text, we'll use it for the best-fit equation
 - (b) Back in the Console window, swipe or hi-lite the equation with the mouse. This automatically copies the hi-lited content into a buffer.
 - (c) paste the equation into the graph subtitle field by middle-clicking in the field or location you want to have the text appear. [9]
3. So to repeat, first, wipe across or hi-lite/select the line's equation in the console window using the mouse. Now bring the focus to the main window. Go to the field called 'Subtitle' and delete this text. Careful not to hi-lite this text with the mouse or you will have to go back and re-highlight the line's equation in the console window. Once this field is empty, perform a middle click as described above, then click Apply. You now have the equation of the line in the graph.
4. The default number of sig-figs is six for the values of the slope and intercept. This is too many. For now[10], we will use three sig-figs for the slope and intercept. Perform the necessary rounding to get three sig-figs showing in the line's equation. Graphs with six sig-figs showing will have marks deducted.
5. Back in the Graph Appearance window, change the title to 'T as a function of square root of (s+L)' by entering this text into the 'Title' field. Often a more descriptive title is possible but not in this case[11].
6. In the Graph Appearance window you will see six tabs below the 'Graph:' internal window. These tabs allow you to control many settings of the graph's appearance.
7. Click 'Accept' to close the Graph Appearance window.

E. Axis Labels

1. The axes do not have labels (with units) yet. Bring up the 'Grace: Axes' window by double-clicking on the x or y-axis of your graph. Double-clicking on the existing axis title will not produce the 'Axes' window, clicking must be done on the axis line itself.
2. Note that which axis is being modified is selected by clicking on the button beside 'Edit:'. Select 'X axis' if this is not the one showing.
3. Label the x-axis square root of (s+L) [$m^{1/2}$] by typing: square root of (s+L) [$m\backslash S1/2\backslash N$] into the 'Label string' field. To get the -1 superscript you have inserted font control escape characters which Grace interprets. Backslash tells Grace the next character is an escape character. S is for start super-scripting. All characters after a $\backslash S$ will display and print as superscripts. The $\backslash N$ tells Grace to go back to the default font so that the final square bracket is the correct size and location. Click Apply to have the changes take affect.
4. Change to the y-axis using the Edit: button and label the y-axis as T [s]. Click on the Accept button to close the Axes window.

F. Slope and intercept: Rounding and quoting \pm error

Question: How many sig-figs should be quoted? Answer: Use the errors from the best fit to determine this.

The slope and intercept values will have more figures quoted than are possible to know due to error. Grace provides the error in these constants in the console window. These errors are used to properly quote the values. The accepted practice is

1. round the error to one sig-fig but if that sig-fig is the digit “1”, then round that to two sig-figs, eg. error 0.013274 rounds to 0.013, not 0.01, error 0.003857 rounds to ± 0.004
2. Quote the value (intercept and slope) to the same precision.

G. Slope and intercept: units.

1. *The equation’s numbers has no units in it.* Both the slope and intercept have values with units. ***The y-intercept is simple: it’s units are those of the y-axis.*** So 0.448 should be 0.448[s]. Make this change by double-clicking on the subtitle to get the Graph Appearance window up.
2. ***The slope’s units are determined by the units of the y-axis divided by the units of the x-axis:***

$$\text{units of slope} = \frac{\text{units of } y - \text{axis}}{\text{units of } x - \text{axis}}$$

due to the fact that the slope = rise/run. Thus in this example we have $\frac{s}{m^{(1/2)}}$. A quick way of making a fraction is to use superscripts and subscripts with a normal sized ‘/’ between them.

3. In the Graph Appearance window, go to the subtitle field and behind the 0.404 enter: `[\Ss\N/\sm\S1/2\N]`. You are using the `\S` for superscript, `\s` for subscript and `\N` for normal text sizes. Fractions can also be achieved by using the `\z` (zoom) and `\v` (vertical shift) escape controls. Clicking on ‘Apply’ will allow you to check the results without closing the window. For example `\z{0.5}` will make a character 1/2 the size of normal text. `\v{0.5}` shifts text upward 1/2 a line, `\v{-0.5}` shifts the next characters downward 1/2 a line.
4. Finally change the y in the equation to T and the x in the equation to `'(s+L)\S1/2'`, because these are the names of the values you plotted, not x and y.
5. **NB: Remember that the numbers in your best fit equation have units, but the variable names should not have units.**

Now your graph should appear as shown in figure 3. **Please have your work checked by your lab instructor or demonstrator before proceeding.**

H. Adding Error Bars and Calculations in xmgrace

Error bars let the reader know visually the amount of uncertainty in a point, which may be a percentage of the measurement, based on equipment specs, etc. Grace uses columns in the spreadsheet called DX, DY, etc for this. The default set type is XY. Usually set type XYDXDY will be used. Since a graph has already been created, adding error bars can be the next step, but they could have been entered by hand previously in the above example.

The original set s0 will be used as a source to produce s2, as generally by now you have a set from the best fit and it is s1.

1. Bring up the “Data Set Operations” window and use “Create new” and use “By formula”.
2. Change the “Set type” to XYDXDY and additional fields will appear. The Y1 (aka DX) field is the error in the first column which is X. Y2 (aka DY) is the error in the second column which is Y.
3. Insert the following values: Start at: 0, Stop at: 5, Length: 6. This tells xmgrace to apply the operation over row zero to row 5 which is 6 values.

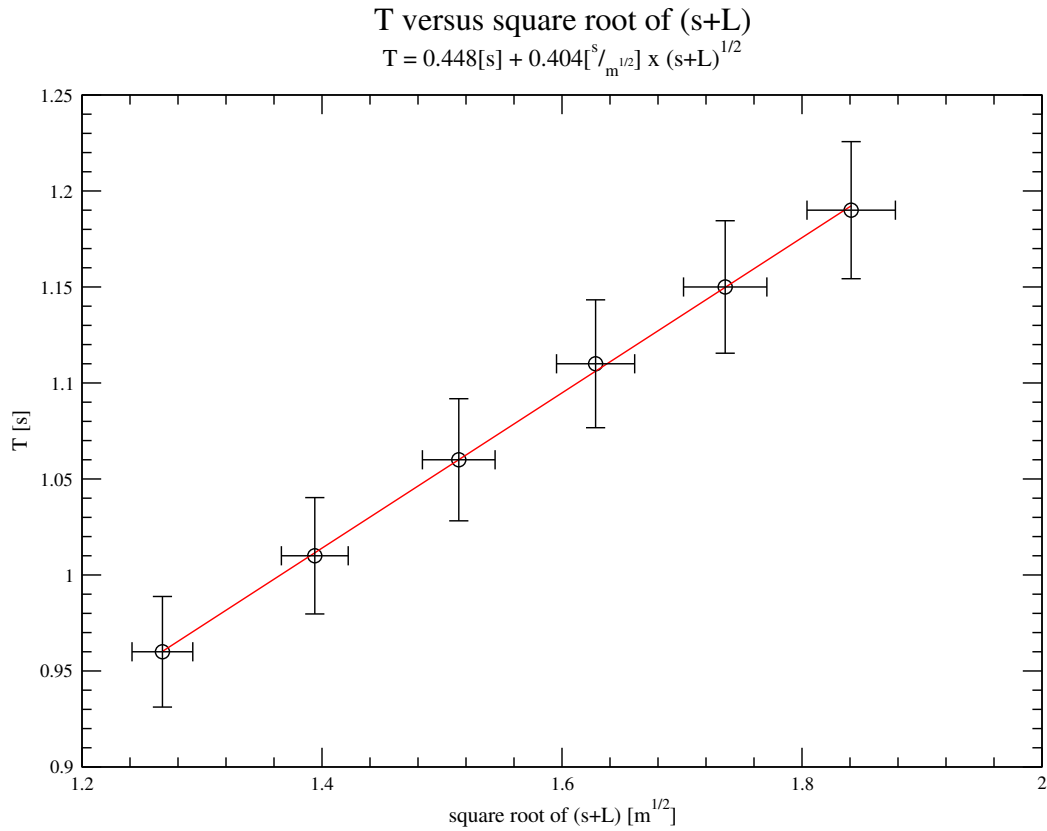


Figure 3: Appearance of completed graph number 1

Parameter mesh (\$t)

Start at: Stop at: Length:

Set type:

X =

Y =

Figure 4: Load & Evaluate for calculations, etc

4. We will simply copy s0.x and s0,y into the new set. We will put a 2% error on the x values and a 3% error on the y values. Use Figure 5 to see how this is done. Click Accept when this has been entered. Error bars will now appear.
5. If you make an error, kill the new set and use Create new, By formula to bring up the dialog again. You will see the previous calculation, etc.
6. Rescale the graph so that the y error bars are not truncated.

Parameter mesh (\$t)

Start at: 0.1 Stop at: 0.1 Length: 0.1

Set type: XYDXDY

X = s0.x

Y = s0.y

Y1 = s0.x*0.02

Y2 = s0.y*0.03

Apply Accept Close

Figure 5: values for calculating error bars

I. A Few Hints for xmgrace

1. Naming a file is done in the “Selection” field at the bottom of the Grace Save project dialog, not in the upper “Filter” field.
2. Control/formatting: Greek: δ returns to default font. $\underline{\quad}$ begins underline, $\overline{\quad}$ ends underline so \pm appears as \pm . \sup = superscript, \sub = subscript, \N returns to leave either.
3. $\text{\texttt{\{Courier\}\{Symbol\}}^\circ$ will produce a degree symbol, but you need to use the Font tool under menu item Window and cut/paste.
4. To remove a point in the dataset editor, you can either clear both cells or delete the row which contains the mistake. A row is selected by clicking on the row number on the left side of the data. Use 'Edit, delete selected rows' in the drop-down menu of the 'Spreadsheet data set editor' window to delete many rows.
5. To remove a line of best fit, delete the data set which was created for it. There is more than one location from which this can be achieved. One is to click 'Data, Set operations'. Then click on the appropriate set to select it, (not G0.S0; that may be your data) and then right-click on that data set to bring up a menu and click on 'Kill' or 'Kill data'.
6. When you close a file and reopen it, the console contents are gone. Refitting your data is useful in regenerating the analysis.
7. If you plotted the wrong variable on the x/y axes: A quick way swap columns to fix this is create a new set “By formula” and set the new x as the old y, the new y as the old x.
8. If you are not able to see the complete graph within the main window of Grace, you can change how many pixels Grace uses. Click on 'View', 'Page setup'. Confirm that X11 is the 'Device'. In the 'Page' section, change 'Size:' to Custom. Now you can modify the dimensions so that the complete graph is visible in the main window.
9. Calculations: operations on columns for a single graph do not need to reference the graph since there is only one graph. So one does not need to state g0.s0.x (graph 0, set 0, x column) but simply s0.x or s1.y for the y column of set 1. More on this later.
10. Compacting your sets can help keep sets in numerical order and is in the Data Set operations (right-click) menu.

Second Graph: More Calculations Using Grace's data set operations

Often data requires that mathematical operations be performed on it before plotting. Some examples are:

- Conversion of the measure units into the required units, eg. centimeters to meters.
- Removal of an offset of systematic error in the data.
- Calculation of uncertainties for the measured values so that each point in a plot has error bars.

Grace's data set operations provide easy manipulation of data. Unlike excel, the formula does not refer to an individual cell, but instead references the complete column in the data table. A new data set is created: G0.S0 could be the 'source' set and G0.S1 is the 'destination' set. Begin with entering the data shown in table I.

gauge pressure p_g [psi]	T [deg F]	P_A	T [deg C]
0.2	34		
0.7	44		
1.1	54		
1.3	64		
1.45	70		
1.65	74		

Table I: Data for second graph.

The data shown in Table I is such an example, and the steps below will be used to create the desired graph. This data set shows measured values of temperature in Fahrenheit and pressure in psi (pounds per square inch). It was collected by cooling and heating a small volume of air in a closed container. Pressure and temperature sensors were mounted inside to record the changes in the air.

This data set must be converted to metric units of Celsius (from the temperature T[F]) and absolute pressure in pascals (from the gauge pressure p_g) using the conversion equations below. After the conversion, the right hand columns' values for table I will be known, but inside Grace. The new values will then graphed, fitted, and the regression line extended to zero pressure. Absolute zero is the value of temperature when the pressure of gas goes to zero; we seek to find it's value.

The conversion equations are shown below:

$$T[C] = \frac{5}{9}(T[F] - 32)$$

$$\text{absolute pressure } P_A = p_0 - (p_r - p_g)k$$

where $p_0 = 98100[Pa]$ $p_r = 1.65[psi] = \text{pressure at room temperature}$ $k = 6894.6 \frac{Pa}{psi}$

1. Open a new file in Grace by clicking 'File, New'. Enter the data shown in table I. Put p_g in the X column and $t[F]$ in the Y column. Save this file to the hard-drive.
2. Click on 'Data, Data set operations' in the main window to open the 'Grace: Data set operations' window. Right click on the inner window listing the Data sets and the click on 'Create new, By formula'. This produces a window call 'Grace: Load & evaluate'.
3. We are going to create s1[12], the new set of data by operating on s0. Grace requires some information about which and how many points to operate on. We want to convert all the values in s0, so the 'Start at:' field should have 0 in it and the 'Stop at:' field should have 5 entered into it. Enter 6 into the 'Length:' field. This instructs Grace to take values from s0 starting at row 0, apply the formula to the data until reaching row 5, to create the new set. Grace begins numbering the spreadsheet rows at zero, not one.
4. In the field labeled 'X=' you must enter the conversion factor which will convert the readings of pressure from psi to pascals. Delete the "\$t" and enter (without the quotes) '98100 - (1.65- s0.x)*6894.6' into the X field. Note that s0.x represents the column of p_g (gauge pressure) values you enter in the data set s0.
5. In the 'Y=' field you can convert the temperature reading from their Fahrenheit values to Celsius. Type in '5/9*(s0.y - 32)'. Click Accept.

6. If you have any errors, then you will see the console window appear and a message will describe the problem. Often a typo results in a parse error, which means grace is expecting some type of value and not receiving it. Check your formula. When all goes well, you will see S1[2][6] has been created and your graph will now contain a plot of the new set.
7. The old set may still be visible and since we do not want to use it for fitting we will hide it. Bring up the 'Data set operations' window and hi-lite s0. Then right click on it and select Hide. Now you will see a minus sign in front of S0 instead of the plus sign. Note that Show is also in this drop-down menu. This allows you to select which data set(s) appears in the graph.
8. Next press A_S to auto-scale the graph. Double-click on the 'join-the-dots' line, to bring up the 'Set Appearance' window. Click on the new set (usually G0.S1) to hi-lite it. Change the symbol from none to a ~70-point circle, and change the Line properties to none. Make sure you make these changes to g0.s1.
9. Double-click on the y-axis. Scale the y-axis so that -300 C is the 'Start:' value. Click 'Apply'. If the x-axis does not start at 0, make that change as well and click 'Apply'.
10. Next add the linear regression line. Click on 'Data, transformations, regression. In the 'Regression' window, hi-lite set S1, type of fit is linear, load must be changed to Function, leave restrictions as none. The 'Start load at' the value of 0, 'Stop load at:' should be set to the same value as the end of the x-axis. A value of 1e5 is typical, although you should check your graph. ($1e5 = 1 \times 10^5$). '# of points:' can be set to 100. Click Accept. Grace will now produce g0.s2[2][100], which contains 100 xy pairs that fall on the linear regression line. The main window will now show this line, and the y-intercept has been plotted. Incidentally, the y-intercept coincides with the line's x=0 point.
11. The console window contains the line's equation and can be copied into the graph using the instructions from the first graph.
12. Complete the required changes so that this second graph is similar to the one shown in figure 6. *Some changes to the major spacing may be necessary as you may see an extremely crowded x and y set of axis labels.* Major spacing is the distance between points that are labeled with a value on each axis. Minor ticks are the marks between the major ticks. These are configured in the 'Tick properties of the 'Axes' window which appears when you double-click on either the x or y-axis.

Note that this data predicts a value of -205 degrees Celsius for absolute zero. The actual value is -273 Celsius. The standard error of the intercept is 17 degrees Celsius and is shown in the console window. Thus the data predicts a value of absolute zero of -205 ± 17 degrees Celsius. Since the range of this value (-222 to -188 degrees Celsius) does not include the true value, the experiment contained a systematic error which led to an unacceptably high value of absolute zero.

Have your work checked on screen before proceeding.

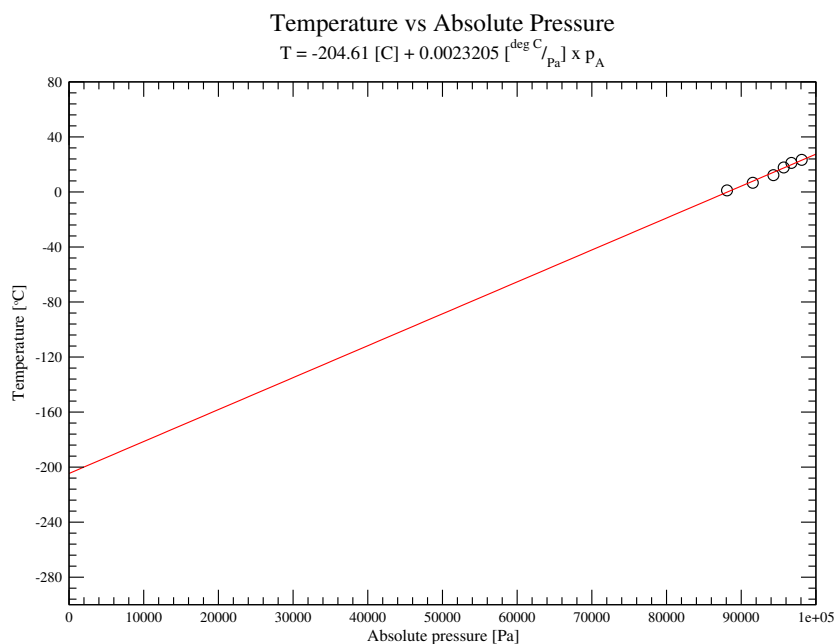


Figure 6: Graph of Temperature vs Absolute Pressure.

Additional Advice for Using xmgrace

J. Greek Letters

Greek letters such are available for use in titles and labels of your graphs. They are accessed by changing the font to Symbol. This is done using the `\f{Symbol}` or the `\x` escape control. Everything after will be displayed and printed in Greek characters. `\f{}` will return you the default or normal font. Use `l` (lower case L) for λ and `'D'` for Δ , `q` for θ , etc.

K. Extending the line of best fit.

The line of best fit can be extended in either direction by using and adapting the instructions of step 10 in Section I.

L. Importing Multicolumn Data From other Sources.

Xmgrace can import ascii or netcdf data files. If the source is multicolumn ascii data with columns separated by white-space it can be displayed in one graph using: 'Date, Import, ASCII' to display the 'Read Sets' dialog box. Here choose NXY as the 'Load as' setting. Then select your file from the Files list, adjusting the filter if required. Data sets can then be shown or hidden as necessary.

M. Plotting a function in xmgrace

To plot a theoretical function in xmgrace, use 'Dataset operations, Create new, By formula'. The 'start at' and 'stop at' are values of the x-axis which you will pick. For example to plot $y = x^2$ over the range of -1 to $+1$, set 'start at' to -1 and 'stop at' to $+1$. Length is the number of data-points grace will create in the new data set. Set it to 50. `$t` is the variable name to be used in the formula you wish to plot. If plotting $y = x^2$, then leave the 'X =' field as `$t` and put `X^2` in the 'Y=' field. Click accept and you will have a plot of $y = x^2$ generated in the plot window. To edit the equation you have entered, repeat the steps above: 'Dataset operations, Create new, By formula'. Section 4.1 of the tutorial within grace itself has some more examples. Click on 'Help, Tutorial'.

N. Removing or Selecting some data from a Set

Data can be removed both in the Spreadsheet dataset editor and by using a formula to select a range of data and place it into a new, smaller set.

1. In the Spreadsheet

In the spreadsheet, click on the index number on the left to select the complete row. Multiple rows can be selected by clicking on each row index to add them to the selection. Then click at the top on Edit, Delete selected rows.

2. By Formula

If a set has many points, for example, s0 has 650 points (index runs from 0 to 649) and only the points from index 50 to 230 are wanted, those can be copied into another new set. In the Data set operations window, right-click and use Create new, By formula. This will display the Load and evaluate window. For our example, put 0 in the Start at field, 180 in the Stop at field and 181 in the Length. (Use 1 more in the Length compared to the difference between Stop and Start values.) In the X= field put `g0.s0.x[50:230]` and in the Y= field put `g0.s0.y[50:230][13]`

If one makes an error in the indexing, the console window will indicate left and right vectors are on different lengths. Adjust your Start, Stop, Length values as needed. This error will also show in the values in the [] brackets don't match for length with the Start, Stop, Length values.

O. Placing Additional Text and Other Objects on a Graph

Additional text like the authors name or the date can be added as follows. Once the graph is plotted, click on 'Window' then 'Drawing objects'. In the 'Objects' dialog box, click on the Text button. Now click on the graph at the location you want the text to appear. A dialog box will appear which is used to enter the text in the 'String' field. The 'Objects' dialog box also contains tools for drawing lines, moving objects, etc.

Error Bars Again

Error bars are used to convey the uncertainty of each data point and can be on either or both the x and y directions, depending on the situation. Grace can put the error bars on each point using a set type of XYDXDY where DX and DY are the respective error values.

Other types of xmgrace sets can be used, for instance if the error of a measurement is not symmetric about the point.

The error values can be entered by hand in the spreadsheet using the DX and DY columns or calculated. The case of calculating the errors arises if the error depends on the value somehow, eg. is a percentage of the value. For example the steps below show how to calculate error bars for both a percentage error for the x variable and a constant error for the y variable.

Let's assume an error of 10% on the x measurements and a constant ± 0.5 mm on the y measurement:

1. Once the original data is typed into g0.s0, create a new set by formula
2. Change the new set's type to XYDXDY
3. Set the "start at" field to 0, and the "stop at" field to the last row number, "length" to the number of rows.
4. For the four formula:
 - (a) copy the x and y data to to the new set: X: `g0.s0.x`, and Y: `g0.s0.y`
 - (b) DX is labeled Y1 and would have Y1: `g0.s0.x*0.1`
 - (c) DY is labeled Y2 and would simply have Y2: 0.5
5. Apply the changes and g0.s1 will be created. Vertical and horizontal delimited lines will be drawn onto the graph points. Set s0 may be hidden if desired.

Graph 3: Nonlinear Curve Fitting

Xmgrace contains a number of preprogrammed, commonly used curve fitting functions. These are located in Regression window in the 'Type of fit' settings.

What if the list does not contain your desired function? In that case, xmgrace can be told what function you want it to attempt a fit: arbitrary curve fitting. Such a feature is not present on many graphing packages.

To proceed after entering a data set, click on Data, Transformations, Nonlinear Curve Fitting. Select the number of parameters (how many ways you want to use the x variable. In the 'Formula' field, enter your desired fit equation. For example $y=a_0+a_1*x+a_2*\cos(x)+a_3*x^{-1}$, which is not available in the 'Type of fit' list.

Xmgrace then needs to know the source set that it is to fit. Select your data set in the left side list of sets. Then click apply. The console window will have the values for the a_n coefficients.

An example of this capability is illustrated in figure 7. The comments in figure 7 diagram provide the details for creating that graph. The data points are shown in table II.

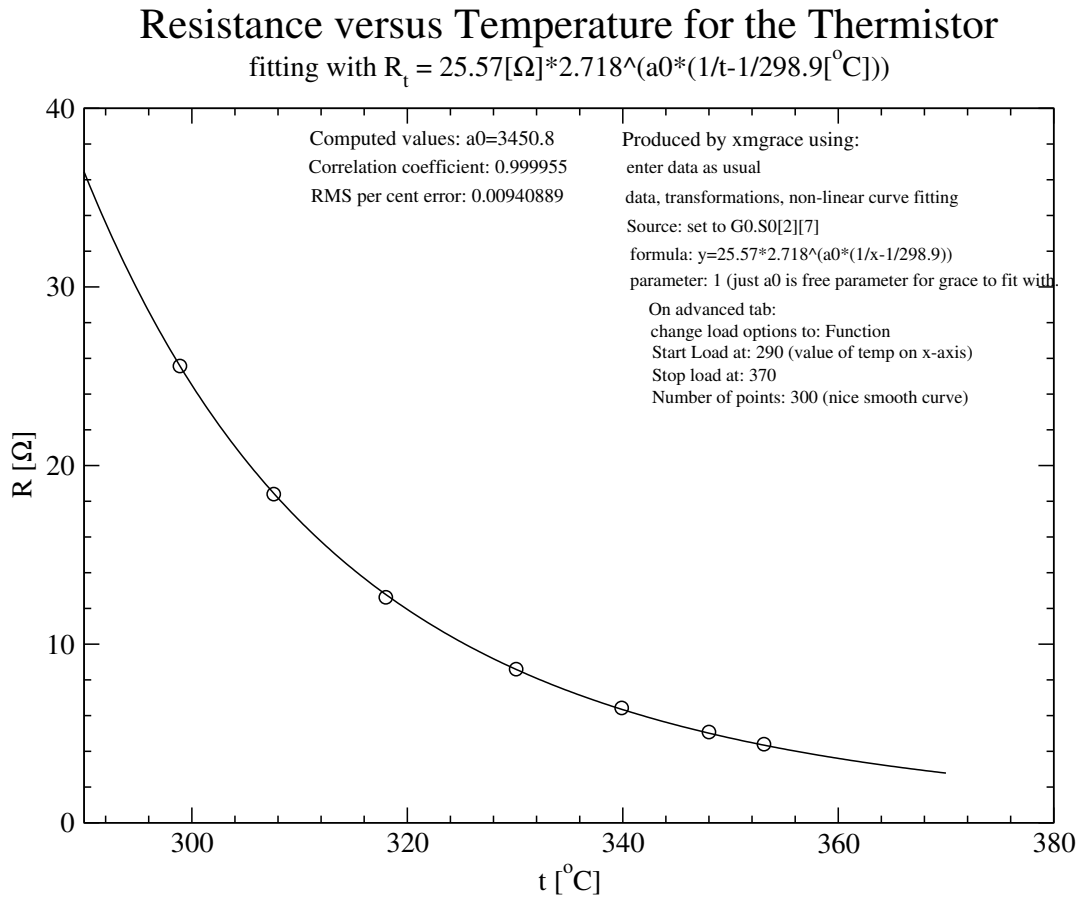


Figure 7: Fitting a curve with a user defined function.

Graph 4: Another Linear Plot

The last exercise mimics what you will see in the lab. A set of data is available which you have collected. Next you are asked to plot the data. The first decision you must make is what column of data on the paper goes into the appropriate column of xmgrace. Reread the bold text in section A to determine this. Entering the data in the wrong columns results in the incorrect value for the slope. Correcting this requires the data to be re-entered in the correct columns. This does not take long but is easily avoidable. Consider this your warning.

Table II: Data for Resistance vs Temperature graph

Temperature [K]	Resistance [Ω]
298.9	25.57
307.6	18.4
318.0	12.62
330.1	8.6
339.9	6.43
348.0	5.08
353.1	4.4

Instructions for Graph 4

Make a plot of temperature T as a function of motor speed MS (rpm stands for revolutions per minute) for an electric motor for the following data.

- Fit the data with linear regression to obtain the line's equation. Use the error values to properly round the values of slope and intercept.
- This time add error bars to both values. Consult section O. Create a new set by calculation of type XYDXDY. The uncertainty in the MS values will be $\pm 5\%$, and the temperature is $\pm 0.3^\circ C$.
- Print one copy with your name(s). Hand this in for marking.

motor speed MS [rpm]	Temperature T $^\circ C$
212	24.1
470	34.4
593	41.3
980	46.8
1427	53.1
1750	62.4
2230	74.4

Table III: Motor speed and temperature data.

Graphing with xmgrace: Quick Reference Guide

To create a graph with the required information:

1. Start grace, click on Data, Data Set Operations. Right click on the empty list area (no data sets listed yet), Create new, In spreadsheet, then enter the data. Exit the last cell, and click Accept. Set S0 is now created, and displayed in the graph. Click AS to scale the graph.
2. Double-click on one of the data line which will bring the Set Appearance window. Turn off the lines that are joining the data points using Line properties Type: None. Now display the data points using Symbol Properties Type: Circle.
3. Fit the data with a straight line. Click on Data, Transformations, Regression. Click accept if the correct set of data is highlighted in the Apply to set: list. (If S0 is the only set, it is already selected.) Click on Close to close the Regression window.
4. Double-click on the graphs title and make a title: 'your y-variable name' as a function of 'your x-variable name'.
5. Label each axis by double-clicking the existing label and modifying the label fields. Put the units in square brackets.

6. Delete all the text in the Subtitle field. Copy the equation of the regression line from the Console window by highlighting it and then middle-clicking in the Subtitle field.
7. Round the slope and intercept values using the errors for each number shown in the console window (scroll back in the console window to find them). State the error values rounded to one sig-fig.
8. Show error bars of: a 3% error on the motor speed values and a 4% error on the temperature values.
9. Put the correct units on the slope and intercept values (no square brackets).
10. Print as required.

Importing graphs to LyX

Grace can produce output suitable for importing into LyX or L^AT_EX software. *The grace file format can be directly imported into a LyX file as a graphic.* Alternatively an encapsulated postscript version (.eps) of the graph is used due to that format's vector graphics, and inclusion of size information. This format is also closely associated with T_EX and as such works well.

To produce the eps file, use the Print setup dialog under File. Select EPS as the Device. The Output section should change and show a red square beside "Print to file". Enter your choice of filename in the appropriate field. Close that dialog and print the graph using "File, Print". Other formats of file are also available such as portable network graphics (.png) and scale-able vector graphics (.svg).

Running Grace in Windows OS

The successful way to run Grace in MS Windows is to run it in a Linux virtual machine. Period, full stop.

The main advantage is that you will get software that will stay running and can be fixed more easily if there are problems. You can also run LyX inside the virtual machine, and learn some Linux tricks along the way.

This is done in general as follows:

1. Install VirtualBox from virtualbox.org
2. Install a Linux distribution that is widely used, IE. not a niche distro as not all distros have grace binaries. You will have to compile it if is not available in the package repository. Debian, Ubuntu, Linux Mint, Fedora, CentOS, openSUSE, Manjaro, ArchLinux are some distros that can be used and have binaries for Grace.
3. Use the distro's package manager to install grace
4. Nice but not necessary: Set up a shared folder between the host OS (in this case Windows) and the guest OS (Linux). This will let you see files such as graphs created as images for importing into the word processor of you choice on the windows host OS.

P. QtGrace for Windows

There is a project which is a port of the code to MS Windows for grace/xmgrace called QTGrace[14]. It has some new features and some new bugs too. At the time of this writing, it is not recommended for the following reasons:

1. It crashes often[15]. It may or may not run fine initially, only to start exhibiting more and more problems.
2. It does not understand some of the shortcuts, for instance using "deg" after an angle tells the Linux/OS X/Unix version that the angle is in degrees, not radians.
3. It has a smaller range of numbers that it can understand. For example when plotting data that is smaller than approximately 1e-17, it cannot scale the axis to the small of values. This is a problem when plotting energies of a few electron-volts which are represented in Joules.

There are probably more issues that have not been discovered.

- [1] This depends on what Linux distribution and desktop environment being used.
- [2] This data is from an experiment, the measurement of g .
- [3] A row can be deleted using Edit, Delete selected rows in the drop-down menu. A row is selected by clicking on the row number on the left side of the data.
- [4] **NB:** You must leave the last cell you have entered data into using the 'enter' or 'tab' key. Grace does not parse the data until you leave the cell. Failing to do so results in a zero being placed in the cell instead of your data. This will show up on the plot and throw the fit off considerably.
- [5] This becomes important when you have a lot of data sets!
- [6] Comments may also be made to appear in the graph as an alternative to a legend.
- [7] There will be many windows up on the desktop during the use of Grace. On a smaller monitor, this makes life difficult. Use <alt-tab> to cycle through the windows. Also pressing F11 will bring up a complete list of open/minimized windows to select from. Depending on window-manager settings, you might be able to shade the child windows (the main Grace window is considered the parent) by double-clicking on child window's title-bar. This will just leave the child's title-bar showing. To unshade it, double-click again.
- [8] It is the only set at this point, files with multiple sets would require a choice be made.
- [9] In an X-Window system, cut and paste is done using the middle mouse button if available. If your mouse does not have three buttons (which is the case for our lab) then 3-button emulation is used. To 'middle-click' using 3-button emulation, you simply press both buttons simultaneously.
- [10] More on this later when errors in the slope and intercept are considered.
- [11] Note the form: what_you_plotted_on_y-axis "as a function of" what_you_plotted_on_x-axis
- [12] Note that letter case does not matter when referring to graphs and sets.
- [13] If there is just one graph, the g0.s0 can be shortened to s0 as the software will assume graph zero. Click Accept and a new set with two columns and 181 points will be created. Double-click on the new set listed in the Data set operations window to view it.
- [14] It also has Linux and OS X versions
- [15] on at least 75% of the installs