

**User's Manual for**

# **Isoplot**

## **3.75**

**A Geochronological Toolkit for Microsoft *Excel***

**Berkeley Geochronology Center**

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**DISCLAIMER**

ISOPLOT is BGC's Visual Basic Add-in for Microsoft's Excel® for data analysis and graphical presentation of geochronology, earth science and other radiogenic isotope data only. BGC's ISOPLOT is not the Isoplot® for analysis of any measuring system as described at (<http://www.shainin.com/>). BGC is not affiliated with Red X Holdings, LC. Isoplot® is a registered trademark of Red X Holdings, and is licensed to Shainin LLC.

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## Introduction

*Isoplot* (an “Add-In” program than runs under Microsoft *Excel*) is a flexible tool for the interpretation of radiogenic-isotope data. In addition to the plotting and calculation of the usual (Rb/Sr, Sm/Nd...) isochrons, *Isoplot* can:

- Construct U-Pb concordia plots and calculate ages using conventional concordia intercepts, the “Concordia Age” algorithm, 3-D planar concordia intercepts, or 3-D linear (“Total U/Pb”) isochrons;
- Calculate uranium-series isochron ages using 3-D or 2-D isochrons and construct  $^{230}\text{Th}/^{238}\text{U}$ - $^{234}\text{U}/^{238}\text{U}$  evolution curves and isochrons;
- Construct single-stage growth-curves for plots of common-Pb data;
- Construct cumulative-probability+histogram plots and linearized-probability diagrams;
- Calculate and construct plots for either error-weighted or robust (nonparametric) averages of a single variable;
- Calculate both conventional (analytical-error weighted) and robust (nonparametric) x-y regressions for “classical” and Pb-Pb isochrons;
- Plot Ar-Ar step-heating diagrams and find the statistically-best plateau steps and age;
- Combine Ar-Ar isochron with Ar-Ar step-heating diagrams to obtain the logically optimum combination of both;
- Plot curves for almost any function;
- Use simple Bayesian constraints Improve the estimates and error-assignments for a package of stratigraphically-constrained radiometrically-dated units whose ages overlap within errors (with a special variant for  $^{230}\text{Th}/\text{U}$  ages);
- Deconvolute mixtures of components having Gaussian error-distributions using the Sambridge-Compston approach;
- Provide Monte Carlo errors as well as asymptotic (first-order) errors for most linear regressions, isochrons, and concordia-intercept solutions;
- Extract reliable ages and errors from complex suites of Phanerozoic single-zircon dates;
- Expand the number of *Excel* functions by more than 50, including many functions for radiogenic-isotopes (including 16 for U/Pb and 8 for  $^{230}\text{Th}$  -  $^{234}\text{U}$  -  $^{238}\text{U}$  alone).

*Isoplot* is available without charge – contact Ken Ludwig directly (kludwig@bgc.org).

### *Isoplot 3 Requirements*

For Windows computers, *Isoplot* requires an English-language version<sup>1</sup> of *Excel 97*, *Excel 2000*, *Excel 2002* or *Excel 2003*

*Isoplot 3 is not compatible with Excel 2007 or Excel 2010. If you must use Excel 2007 or Excel 2010, request a copy Isoplot 4, which is compatible with Excel 2007/2010 only. Isoplot 4 has no more functionality than Isoplot 3.7, and somewhat less flexibility. Expect a speed penalty of up to a factor of 10 when using Excel 2007/2010.*

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<sup>1</sup> For Windows systems, you must set the Control Panel's *Regional and Language Options* to *English*), and also check the *Use System Separators* box in the *International* tab of *Excel's Options* or *Preferences* sheet.

### Excel on Macintosh computers

To run *Isoplot* on the Macintosh, you will need to acquire a Windows-enabling program (*Fusion* will work, but not *Crossover* nor *Parallels*). Despite expectations on my part, *Excel 2011* is not *Isoplot*-compatible.

**When installing *Excel*, you must select a printer (say by printing anything from *Excel*) from within *Excel* before trying to run *Isoplot*.**

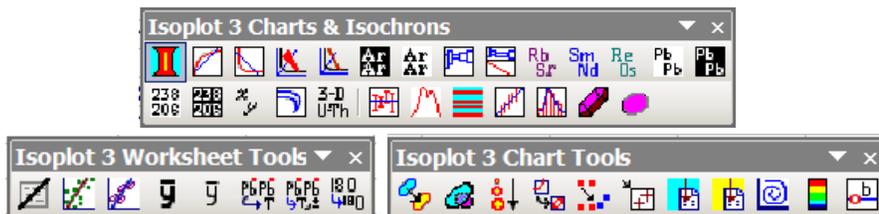
### Installing and Invoking *Isoplot* Under *Excel 2003* or Earlier

→If you have been running Version 1 of *Isoplot*, you must first find the old *Isoplot.xla* file and either delete it or (preferably) rename it (e.g. *IsoplotOld.xla*).

Start *Excel*, and from an open Worksheet, select Tools/Add-Ins. If *Isoplot.xla* is not in the list of available Add-Ins, select Browse to locate it. *Isoplot* will now be loaded every time you start *Excel* (if not wanted, uncheck *Isoplot/Ex 3.00* from the add-in list before exiting *Excel*).

To invoke *Isoplot*, first open the Worksheet that contains your data, and select (with the mouse or keyboard) the data-range that you want to work with (including any header-row). Then, either 1) press the *Isoplot* button  , on *Excel*'s Standard toolbar (the one at the top of the screen), 2) choose Run Isoplot from the Tools menu, or 3) Press **Ctrl-I**.

The items in the *Isoplot* drop-down menu can also be accessed from one of the *Isoplot* toolbars. To access the *Isoplot* toolbars, select View/Toolbars from the Standard (top) *Excel* toolbar and check the appropriate *Isoplot* item. One of the toolbars below will then appear on the screen:



To see the functionality of a toolbar button, pause the mouse-cursor briefly over the button, and a text summary of its use will appear. The first 11 buttons in the *Isoplot Charts & Isochrons* toolbar duplicate the items in the drop-down *Isoplot* menu; use of the last eight, whose functions are accessible only via the toolbar, are described in Appendix II (p. 66).

You can move any of *Isoplot* toolbar's buttons to any of *Excel*'s other toolbars, so that they will always appear when you run *Excel*, with the following:

- 1) Select Tools/Customize from the *Excel* Standard toolbar;
- 2) While holding down the *control* key, so that the button is copied rather than permanently moved, drag and drop any button you wish from the *Isoplot* toolbar to any other toolbar.

The changes will be permanent, until you either remove the button (by following the same procedure as above, except drag and drop the button to any area *outside* a toolbar) or *Excel* crashes. You can move the *Isoplot* toolbar anywhere on the worksheet, change its shape from horizontal to square or vertical (using the triangular-shaped handle at the lower right of the toolbar), or “dock” it at the top, bottom, or sides of the *Excel* workspace (drag and drop with the upper, stippled part of the toolbar).

Avoid invoking *Isoplot* by double-clicking on the *Isoplot.xla* file's icon, because 1) in some cases this can result in more than once copy of *Excel* running at the same time, and 2) the only way to unload a directly-invoked *Isoplot* from *Excel* is to quit the *Excel* program.

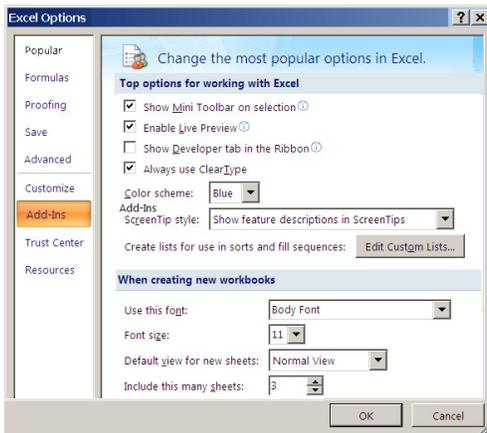
The speed of *Isoplot* can be greatly affected by the size of the active *Excel* workbook. If you have a lot of worksheets in the workbook, or a worksheet becomes very large and complex, *Isoplot* will slow down to a crawl, even when just displaying dialog boxes.

### Installing and Invoking *Isoplot* Under *Excel* 2007

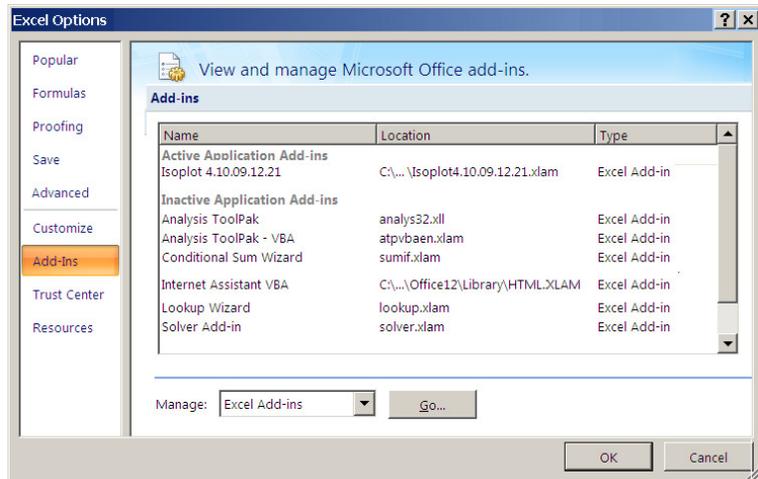
*Excel* 2007 is a much less-capable platform for VBA add-ins such as *Isoplot*, requiring many compromises in coding and user interface to run *Isoplot* at all, and, for many uses, exacts a significant penalty in speed. Thus even if you already have a copy of *Excel* 2007 installed on your computer, I urge you to find a copy of *Excel* 2003 and install that version on your computer as well. *There is no problem in having both versions of Excel operating on the same computer at the same time.*

If, however, you must use *Excel* 2007, you will need to use *Isoplot* 4, compatible only with *Excel* 2007. To install *Isoplot* 4,

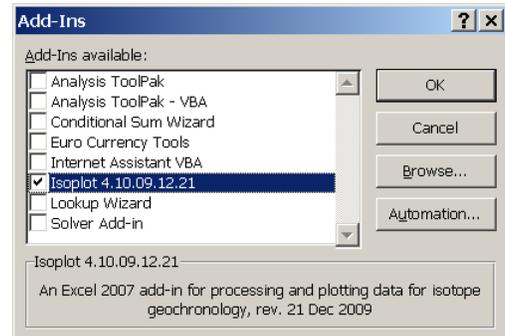
1. Click on the  icon at the upper left of the *Excel* window, then click on the *Excel Options* button at the bottom the the resulting drop-down.



2. Click *Add-Ins* on the next drop-down.

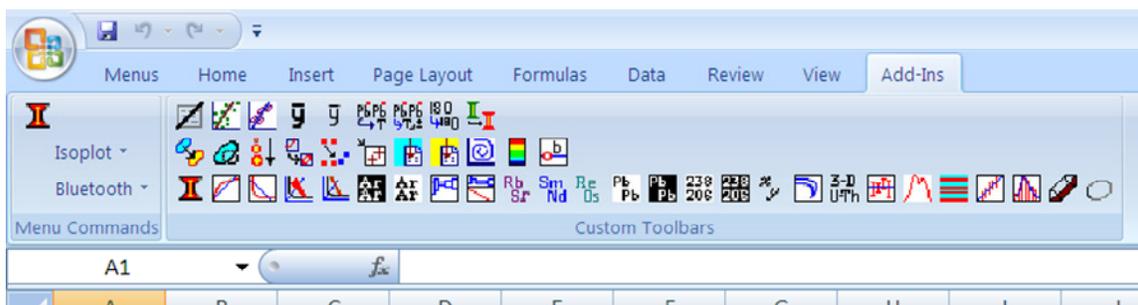


3. Click *Go*.



4. If the correct *Isoplot* 4 add-in appears in the resulting Add-Ins box, select it. Otherwise, click *Browse* and navigate to the folder containing the latest *Isoplot* 4. Click *OK*.

In *Excel 2007*, there are no drop-down menus for *Isoplot* – only *Isoplot*-specific toolbar buttons that appear in *Excel*'s *Add Ins* ribbon. To make the *Add Ins* ribbon appear, click the *Add Ins* in *Excel*'s main menu-bar. To see the function of any of the *Isoplot* buttons, hold the mouse-cursor briefly over the button.



## The Input Data-Range

### Header Rows

If the data-range has a header-row, regardless of whether the headers lie immediately above the selected data-range or several rows above, *Isoplot* will try to recognize the type of plot and type of errors from it (see TestData.XLS for examples). To determine the type of plot, *Isoplot* looks for isotope ratios in the X- Y- (Z-) columns that define a supported plot type – for example, X- and Y-column headers consisting of either 147/144 143/144 or of 147Sm/144Nd 143Nd/144Nd will convince *Isoplot* to select an Sm-Nd isochron plot as the default plot-type. *Isoplot* will also try to recognize the type and sigma-level of the errors from the header rows, and offer its best guess as the default error type.

### Data in a Single, Contiguous Range

If the cell-cursor is within a data range comprising a continuous set of cells bounded by blank rows/columns, the whole range will automatically be selected when you invoke *Isoplot*.

The simplest data range is a contiguous rectangular block of cells comprising a header-row at the top (optional), and 2 to 9 contiguous columns containing the data, errors (optional) and error correlations (optional). For isochron or 2-dimensional concordia data, the simplest way to arrange the columns is:

X      X-error      Y      Y-error      RhoXY

where RhoXY is the X-Y error correlation; or as

X      X-error      Y      Y-error

or as

X      Y.

If you don't supply columns for errors, *Isoplot* will ask you for values to apply to all of the data in the range. The errors can be either absolute or percent,  $1\sigma$  or  $2\sigma$ . Missing error correlations are assumed to be zero, except for conventional Concordia plots and "Normal" Pb-Pb plots, where you will be required to enter nonzero values.

For Argon-Argon Step-Heating data, 3 columns are required:

Cumulative <sup>39</sup>Ar-Fraction      Age      Age-error

where the <sup>39</sup>Ar gas-fraction can be expressed as percent if desired. For weighted averages or cumulative probability distributions, the columns must be:

X              X-error

For 3-dimensional regressions, use any of 9, 6, or 3 columns, in the order:

X X-error Y Y-error Z Z-error RhoXY RhoXZ RhoYZ

or

X X-error Y Y-error Z Z-error

or just

X              Y              Z

Blank rows will be ignored in all cases.

### Data in Discontinuous Rows

To use only the data in certain rows, select a range with two or more discontinuous areas; for example:

**A3:E3,A6:E9,A12:E22**

selects the 5 cells in row 3 from column A to E, then rows 6 through 9 of the same 5 columns, then rows 12 to 22. To do this with the mouse, hold down the Control key, select A3:E3, then A6:E9, then A12:E22.

### Data in Discontinuous Columns

If (and only if) your data are in contiguous *rows*, you can select a range with discontinuous *columns* to satisfy *Isoplot's* requirements. For example, if your data were arranged in rows 1 through 11, with columns:

<b>A</b>	<b>B</b>	<b>C</b>	<b>D</b>
<b><u>143Nd/144Nd</u></b>	<b><u>147Sm/<sup>144</sup>Nd</u></b>	<b><u>147/144 %err</u></b>	<b><u>143/144 %err</u></b>

your range selection would be:

**B1:C11,A1:A11,D1:D11**

so that as interpreted by *Isoplot* the data would be arranged as:

**147Sm/143Nd    147/144 %err    143Nd/144Nd    143/144 %err**

### Excluding Data with Fonts in Strikethrough

If you don't want to use a discontinuous-row selection to exclude certain data-rows (perhaps because you want to use discontinuous columns, or just to simplify the range-selection), you can exclude any data-row by using a font in Strikethrough mode (**Format Cells Font Strikethrough**) for the excluded data-cells.

### Using Bolded Fonts to Specify Added Emphasis to Plot-Symbols

If the font for a data-row is bolded, *Isoplot* will emphasize the plot-symbol by making it solid instead of open (circle, square, diamond, and triangle symbols), or by constructing the symbol with thicker lines (un-

filled [outline] error ellipses and error boxes). However, no symbol-by-symbol emphasis is possible for filled error-symbols, or for the error-cross, +, or X symbols.

### Specifying Symbol Colors with Font Colors

Normally, a single color is specified for the symbols of all of the data points in a plot. You can use different colors for each data-point, though, by using the desired colors as the font color for each data-row, and specifying **Font Color** as the symbol color from the *Isoplot* dialog-box.

### Early versus late data selection

Usually, you will find it easiest to select the desired data-range before invoking *Isoplot*. On a Windows platform, you can also select the data range with the mouse after *Isoplot* is invoked (provided the *Range* edit-box is active).

### Numeric Output from Isoplot

The results of a calculation are always shown first in a popup-box such as the one at right, with or without buttons/checkboxes to select additional information or calculations. These popups are ephemeral, but all contain a checkbox labeled Show Results with Data,

If Show Results with Data is checked, the information in the results-box will be transferred in a text-box to the worksheet containing the source-data (at the upper-right of the source-data range), and look something the box at right. These text-box results aren't very easy to use for further spreadsheet calculations. However, in many cases, *Isoplot* also supplies a user-available array-function (see p. 54) that will place the results as numbers directly in worksheet cells.

3-D Planar Concordia-Intercept Ages

3-D Planar regression

Upper intercept: 2697 ± 48 Ma

Lower intercept: 66 ± 51 Ma

Isochron age in Common-Pb Plane = 2721 ± 55 Ma

# points	6
MSWD	0.41
Probability of fit	0.75

Pb growth-curve intercepts at -3032 and 3364 Ma

Show decay-const. errs in Concordia curve

Behind data-symbols       In Front of data-symbols

Show results with data       Insert wtd-residuals column

OK Cancel Details

### Isoplot Charts

If the Plot checkbox of the main *Isoplot* dialog-box is checked, *Isoplot* will construct an X-Y plot (or “Chart” in *Excel* nomenclature) of the data on a separate sheet in the same workbook as the source-data.

### Hidden Worksheets Created by Isoplot

The data-symbols plotted in an *Isoplot* chart are coupled to a hidden worksheet entitled *PlotDat3* (or some other number), rather than to the worksheet containing the data that you selected for plotting. If you delete one of *Isoplot*'s chart-sheets, the associated hidden worksheet is no longer needed, and *Isoplot* will automatically remove the hidden sheet the next time it's invoked.

### Adding New Data to an Existing Chart

You can add a second series of data points, complete with regression lines and age-results, to most *Isoplot* charts. To do this,

- 1) select the range of the new data (the new data must be in the same worksheet as the chart's primary data);
- 2) switch to the *Isoplot*-created chart-sheet to which you want to add data;
- 3) select Add Data -Points from the *Isoplot* menu;

- 4) specify what you want done with the new data, how to plot it, and click **OK**.

You can also plot data along a secondary axis whose label and axis-ticks are at the right-hand side of the plot box, so that, for example, the first data-series for  $^{207}\text{Pb}/^{204}\text{Pb}$  values, with  $y = 15.4$  to  $15.8$  are plotted as usual, and a second data-series consisting of  $^{208}\text{Pb}/^{204}\text{Pb}$  values, with  $y = 36$  to  $39$ , are plotted according to the range and axis-ticks of the right-hand axis. To do this,

- 1) select the range of the new data (the new data must be in the same worksheet as the chart's primary data);
- 2) switch to the *Isoplot*-created chart-sheet to which you want to add data;
- 3) select **Add Data -Points** from the *Isoplot* menu;
- 4) select any plot symbol but an error ellipse or error box (these will not work with a secondary axis);
- 5) select the new data-series on the plot (you may have to scroll through the plot-elements with the up or down arrows to do this, if the data are not visible on the plot);
- 6) select **Format/Selected data series**, and click on the **Axis** tab;
- 7) specify **Secondary axis**;
- 8) double-click on the new axis to adjust its formatting and scale.

## Modifying Charts

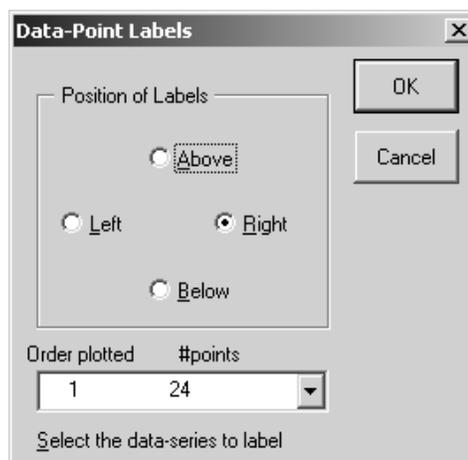
You can modify any graphical element of a chart by simply clicking on the element (say the Y-axis, or a regression line), pulling down the **Format** menu, and selecting the desired graphical element (usually the first one in the list, if you pre-selected an item). You can then change the foreground/background colors of the object, line colors, line styles, line widths, numeric format, font, font size, and so on. You can also add a limited range of graphical objects to the plot (arrows, textboxes, circles, polygons, curves, lines...) with the Drawing button on one of the *Excel* toolbars.

### *Selecting and modifying simple data-point symbols and outline error-symbols*

For data plotted as a symbol without error information – that is, a circle, square, diamond, triangle, **+**, or **X** – clicking on any member of the data-series will select the whole data series, so that any formatting changes will affect the symbols for all of the members of the data series. To select an individual member of such a data series, first click on any plot-symbol within the data series, then repeatedly press the right-arrow key to step through the individual data-points. For error ellipses and boxes plotted as outlines (unfilled symbols), you can only select one data-point at a time; to step through the different data points, use the up- and down-arrow keys.

### *Adding Data-Point Labels*

If you're not sure which symbol on the chart belongs to which data-row on the source-data sheet, *Isoplot* can attach a label to each plotted point. To do this you'll need a column of data-point labels somewhere on the source-data sheet (just to the left or right of the data itself would be fine). From the Chart sheet, select **Label Data Points** from the *Isoplot* menu. Select where you want the labels to appear (relative to the corresponding data points) and, if you have more than one data-series plotted, which series to label. Finally, enter the range containing the labels (must match the data-point range in both number and or-



der). After plotting, the labels can be reformatted or moved as desired.

*Selecting individual labels:* Plots with U-Pb concordia curves, U-series evolution curves, or Pb-isotope growth curves all contain labeled age-ticks on those curves. The labels will often be positioned inconveniently, so that you will want to move or delete some or all of them. To select an individual label for moving, deleting, or formatting first select all of the labels by clicking on one of them. Wait a second, click on the particular label you want to change *and hold down the mouse button*. After about another second, the individual label will be selected.

#### *Embedding charts into the data-worksheet*

If you would like the chart to be part of the worksheet containing its source-data, switch to the chart-sheet and select **M**ove **C**hart to data **W**orksheet from the **I**soplot menu. The chart will be shrunk about 4 times and moved to the source-data worksheet, just to the right of the source-data range. You can further re-size the chart from the worksheet by first selecting the chart itself, then the various chart elements. Once you have done this, you can also cut/paste the chart to a blank worksheet and assemble a page of nothing but reduced-size charts (and any related commentary, such as figure legends (you may want to turn off the worksheet gridlines to improve appearance, using **T**ools/**O**ptions/**V**iew/**G**ridlines). Or, you can copy/paste the moved/shrunk chart to within an existing chart-sheet, so as to create an inset (as in the cover figure). *An Embedded Chart can be edited and manipulated just like a full-sheet chart, but is less transportable to other applications.*

#### *Embedding images of charts into the data-worksheet*

If you don't need to edit the chart once it has been embedded into the source-data worksheet, it is probably better to select **C**opy **C**hart-image to **D**ata **W**orksheet. The chart will then be transferred as a picture object which can be easily pasted into other applications if desired. On Windows platforms, this object will be created at very high resolution and quality.

#### *Superimposing charts*

You can also superimpose charts – for example, if you need an inset showing a magnified view of a part of a chart. To do this, first have *Isoplot* create the master chart, in the usual way (as a separate chart-sheet), then create the chart to be inset, also in the usual way. Move/shrink the inset chart as described above, then cut/paste (or copy/paste) the resulting reduced-scale chart onto the master-chart sheet. Reformat the superimposed inset-chart as desired. Alternatively, just select one or more charts and copy/paste them to a worksheet in the usual way (note that the size of the pasted chart depends on the zoom-ratio of the destination worksheet). Shrink and superimpose the charts as required.

### **Using filled error-ellipses and error-boxes**

Error ellipses and boxes will be plotted as either a simple outline or as a filled shape, depending on the status of the filled **S**ymbols checkbox in the main *Isoplot* dialog-box. *There are important differences in the way outline and filled error-symbols can be used, as listed below:*

Outline symbols are always accurately plotted, no matter how or when the plot is re-scaled or re-sized;

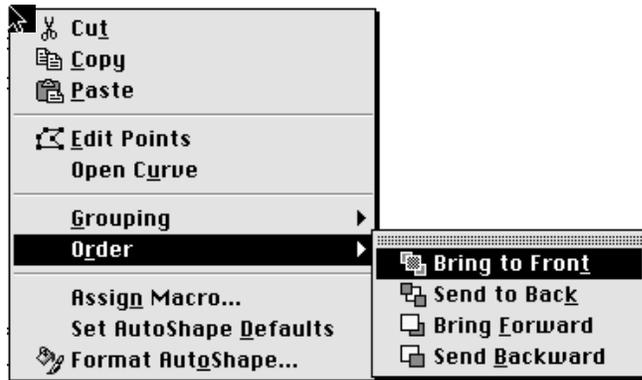
Filled symbols will become slightly but noticeably mislocated whenever the magnification (zoom) of the chart is changed;

Filled symbols do not respond to re-scaling or re-sizing of the chart, and so will become significantly mislocated when you change either the physical dimensions of the plot or the logical scale of either axis;

The only changes that can be made to the visual appearance of outline symbols are to modify the outline color and thickness;

Filled symbols can be modified in many ways, including not only their outline color/thickness and fill-color, but also the pattern, color gradient, and transparency of the fill.

- *Outline symbols cannot be moved, even temporarily (though they can be deleted);*
- *Filled symbols can be temporarily or permanently moved using the usual click-and-drag (for example, to see what lies underneath a filled symbol).*



right-click a filled symbol to bring up the menu at left, select the **O**rder item, then the desired placement with the resulting sub-menu (above left).

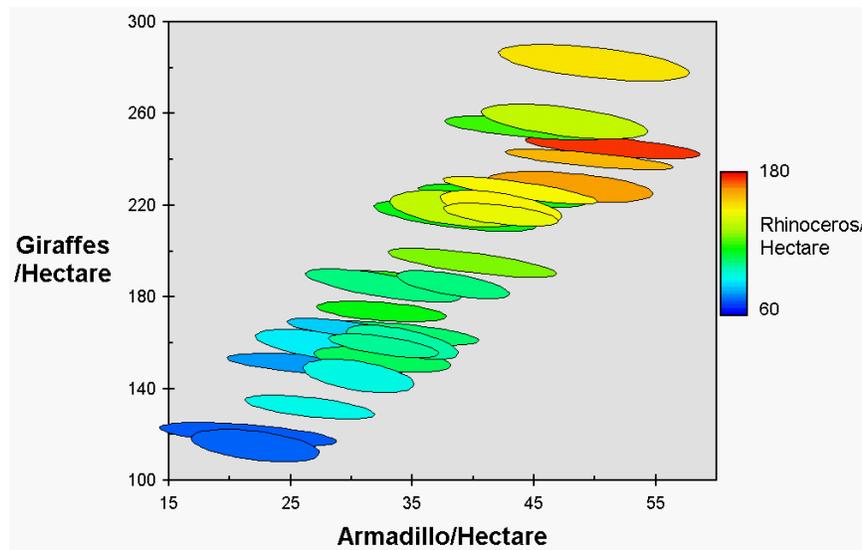
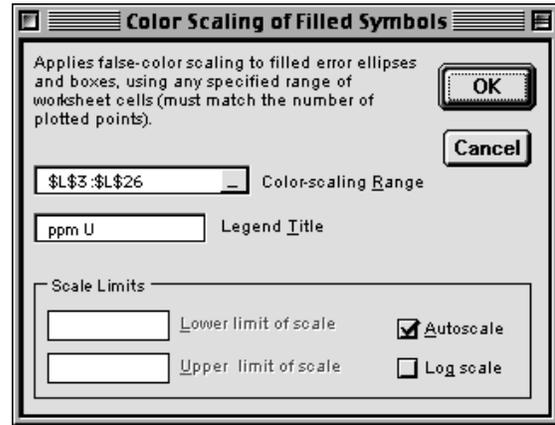
*You should always re-scale filled symbols before printing to make sure that they are accurately placed. In some cases, you may need to first zoom in to the maximum (400%) to eliminate any residual offset.*

To rectify the location of filled symbols after any re-scaling or re-sizing action, or after any zoom-in or zoom-out, select **R**escale Filled Symbols from the *Isoplot* menu on the Chart or Worksheet menu-bar. Any filled error-boxes or error-ellipses will then be accurately relocate and resized. You can also stack these symbols according to their size (actually, the length of their diagonal), so that smaller ellipses or boxes will lie on top of progressively larger ones, using the **S**ort Filled Symbols by Size menu-item. To change the order yourself,

### Color-scaling of filled symbols

If your data are plotted as filled error-ellipses or error boxes, you can use color scaling (or gray-scaling, if not a color plot) to represent the value of a third, z-parameter. To use color scaling:

- Plot your data in the usual way;
- Select a columnar range of cells to use for the color scaling—for example, a *ppm Uranium* column. Make sure that the number of valid cells in this range matches exactly the number of data symbols in your plot;
- Select the plot again, and select **Color Scale Filled Symbols** from the drop-down **Isoplot** menu;
- Re-select the scaling range if necessary;
- Select how you want the colors scaled. Use **Autoscale** to use the lowest- and highest-values of the color-scaling range define the “lowest” (pure blue) and “highest” (pure red) colors.



**Figure 1:** Example of color scaling to show a third, z-parameter on an x-y plot.

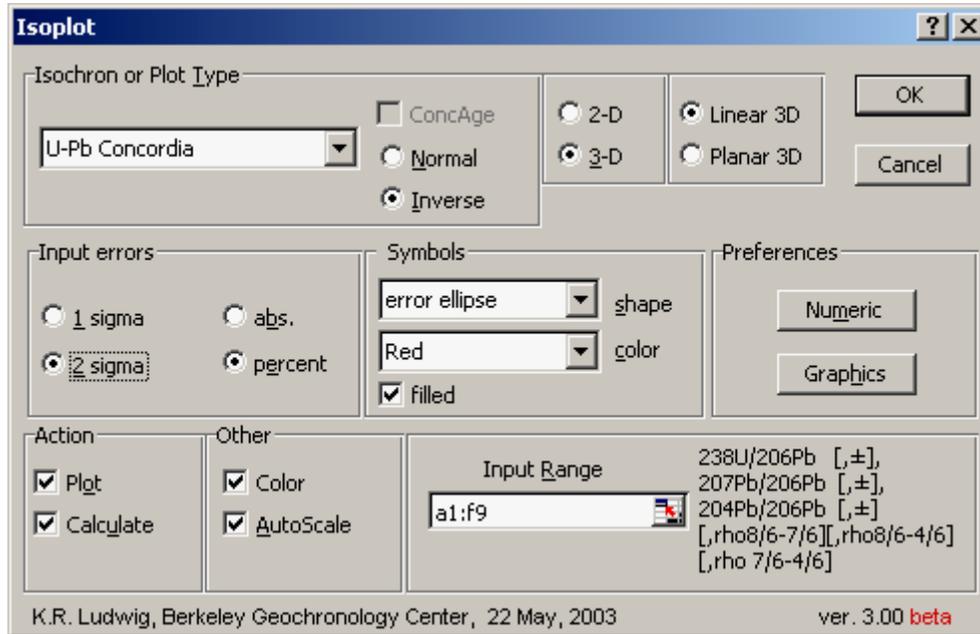
### Exporting charts to other programs

Simply using **Copy/Paste** to export *Excel* charts to another application generally results in unacceptable quality, because of the default Windows Clipboard resolution of 1/72". As mentioned earlier, for Windows users, *Excel*'s **Copy Picture** method (invoke the **E**dit menu from the chart sheet with **Shift** depressed) will yield excellent resolution in the exported graphic.

Another method (used for the preceding figure, for example) is to import *Isoplot*'s charts as a bitmap using a screen-capture utility. Before capturing the screen select **V**iew/**F**ull Screen from the chart sheet, then enlarge the plot-box as much as possible. After pasting the image into your document and shrinking it 4x or more, you should have acceptable (though not really publication quality) resolution.

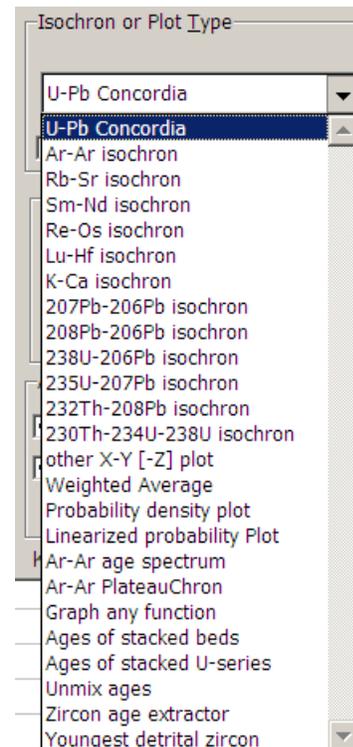
## The Main Isoplot Dialog Box

When *Isoplot* is invoked, the main *Isoplot* dialog-box will appear:



If you included a header-row with the data-range that was selected when you invoked *Isoplot*, some of the choices will already have been correctly made; others require some thought. Your choices will include some or all of:

**Input Range:** The range, if any, that was selected when *Isoplot* was invoked. You can type in any other range as well, e.g. “A10:E22”, “MyData”, “B3:F6,B8:F8, B14:F22”. On Windows platforms, you can also use the mouse to select a range *after* invoking *Isoplot*. The ranges can include discontinuous rows (so as to exclude unwanted data in a contiguous sequence), or discontinuous columns (so as to rearrange the column-order to meet *Isoplot*’s requirements), but not both. Rows without numeric data are ignored, as are rows whose data are shown with the Strikethrough attribute. The prompt to the right of the Input Range edit-box indicates what sort of data is assumed to be in columns (in left-to-right order) of the input range.



**Isochron or Plot Type:** Select from the drop-down list (right):

For isochrons (including U/Pb concordia), “Normal” plots yield the age from the slope of the linear regression, and initial ratios from one of the intercepts, whereas the opposite is true of “Inverse” plots. The plot-types offered by *Isoplot* are:

*U-Pb Concordia* Data for a “Normal” ( $^{207}\text{Pb}/^{235}\text{U} - ^{206}\text{Pb}/^{238}\text{U}$ , or “conventional”, or “Wetherill”) Concordia plot, or for an “Inverse” ( $^{238}\text{U}/^{206}\text{Pb} - ^{207}\text{Pb}/^{206}\text{Pb}$ , or “Tera-Wasserburg”) Concordia plot. The data points can be regressed using a modified York two-error regression algorithm (York, 1969), and the resulting concordia-intercept age-errors can be calculated using either a first-derivative expansion approach or (if there is no excess scatter) a more-reliable Monte Carlo approach. If an “Inverse” Concordia plot, you can also include Z-axis ( $^{204}\text{Pb}/^{206}\text{Pb}$ ) data for either *planar* 3-D or *linear* 3-D (“Total Pb/U Isochron”) regressions. Finally, you can select the “Concordia Age” method to calculate ages and X-Y means for 2-D data that are both concordant and X-Y equivalent. If desired, a conventional Concordia plot can be constructed directly from Tera-Wasserburg data, or *vice-versa* (p. 27)

*Ar-Ar isochron* Argon-Argon isochron data, where “Normal” is  $^{40}\text{Ar}/^{36}\text{Ar}$  versus  $^{39}\text{Ar}/^{36}\text{Ar}$ , and “Inverse” is  $^{36}\text{Ar}/^{40}\text{Ar}$  versus  $^{39}\text{Ar}/^{40}\text{Ar}$ .

*Rb-Sr isochron* Classical  $^{87}\text{Rb}/^{86}\text{Sr} - ^{87}\text{Sr}/^{86}\text{Sr}$  isochron (“Normal” only).

*Sm-Nd isochron* Classical  $^{147}\text{Sm}/^{144}\text{Nd} - ^{143}\text{Nd}/^{144}\text{Nd}$  isochron (“Normal” only).

*Re-Os isochron*  $^{187}\text{Os}/^{188}\text{Os} - ^{187}\text{Re}/^{188}\text{Os}$  isochron (“Normal” only).

*Lu-Hf isochron*  $^{176}\text{Hf}/^{177}\text{Hf} - ^{176}\text{Lu}/^{177}\text{Hf}$  isochron (“Normal” only).

*K-Ca isochron*  $^{40}\text{Ca}/^{42}\text{Ca} - ^{40}\text{K}/^{42}\text{Ca}$  isochron (“Normal” only).

*207Pb-206Pb isochron*  $^{206}\text{Pb}/^{204}\text{Pb} - ^{207}\text{Pb}/^{204}\text{Pb}$  (“Normal”) or  $^{204}\text{Pb}/^{206}\text{Pb} - ^{207}\text{Pb}/^{206}\text{Pb}$  (“Inverse”) isochron.

*208Pb-206Pb isochron*  $^{206}\text{Pb}/^{204}\text{Pb} - ^{208}\text{Pb}/^{204}\text{Pb}$  (“Normal”) or  $^{208}\text{Pb}/^{206}\text{Pb} - ^{204}\text{Pb}/^{206}\text{Pb}$  (“Inverse”) regression.

*238U-206Pb isochron*  $^{238}\text{U}/^{204}\text{Pb} - ^{206}\text{Pb}/^{204}\text{Pb}$  (Normal) or  $^{204}\text{Pb}/^{206}\text{Pb} - ^{238}\text{U}/^{206}\text{Pb}$  (Inverse) isochron.

*235U-207Pb isochron*  $^{235}\text{U}/^{204}\text{Pb} - ^{207}\text{Pb}/^{204}\text{Pb}$  (Normal) or  $^{204}\text{Pb}/^{207}\text{Pb} - ^{235}\text{U}/^{207}\text{Pb}$  (Inverse) isochron.

*232Th-208Pb isochron*  $^{232}\text{Th}/^{204}\text{Pb} - ^{208}\text{Pb}/^{204}\text{Pb}$  (Normal) or  $^{204}\text{Pb}/^{208}\text{Pb} - ^{232}\text{Th}/^{208}\text{Pb}$  (Inverse) isochron.

*230Th-234U-238U isochron* For 3-D  $^{230}\text{Th}/\text{U}$  isochrons (required if  $^{234}\text{U}/^{238}\text{U}$  cannot be assumed to be in secular equilibrium!), any combination of  $^{232}\text{Th}/^{238}\text{U} - ^{230}\text{Th}/^{238}\text{U} - ^{234}\text{U}/^{238}\text{U}$  as the X-Y-Z axes. For 2-D  $^{230}\text{Th}/\text{U}$  isochrons (requires all  $^{234}\text{U}/^{238}\text{U}=1$ ), either  $X=^{238}\text{U}/^{232}\text{Th}$ ,  $Y=^{230}\text{Th}/^{232}\text{Th}$  or  $X=^{232}\text{Th}/^{238}\text{U}$ ,  $Y=^{230}\text{Th}/^{238}\text{U}$ . Also permitted is  $X=^{230}\text{Th}/^{238}\text{U}$ ,  $Y=^{234}\text{U}/^{238}\text{U}$  to calculate the  $^{230}\text{Th}/\text{U}$  age of a single point, or to plot data for several points (in which case one or more  $^{230}\text{Th}/\text{U}$  evolution curves for different initial  $^{234}\text{U}/^{238}\text{U}$  can be requested).

*Other X-Y [-Z] plot* Any other X-Y or X-Y-Z plot, X-Y isochron, or X-Y-Z regression.

*Weighted Average* Classical inverse variance-weighted average, with two approaches for dealing with excess scatter, plus the Tukey’s Biweight robust estimator.

*Probability density plot* Constructs the cumulative Gaussian probability curve for an assemblage of single-valued data and errors, with or without a histogram for the data.

*Linearized probability plot* Constructs a probability plot for a normal distribution using the selected data.

*Ar-Ar age spectrum* Constructs the classical Ar-Ar step-heating diagram (age versus  $^{39}\text{Ar}$  gas-fraction), and identifies the best plateau defined by the data.

*Ar-Ar Plateau Chron* Determines the isochron age of the contiguous heating steps with the largest amount of gas, which corresponds to a classical step-heating plateau age without the assumption that the trapped component  $^{40}\text{Ar}/^{36}\text{Ar}$  is that of air.

***Graph an arbitrary function*** Must be invoked from an existing *Isoplot* chart; allows the user to algebraically define any simple or parametric  $x$ - $y$  curve and place a graph of the curve on the plot.

***Ages of stacked beds*** Uses Bayesian statistics with a Monte Carlo approach to get the most precision out of a stratigraphically-constrained sequence of units whose dates overlap within their assigned errors.

***Ages of stacked U-series*** Similar to *Age of stacked beds*, but uses the radiogenic  $^{230}\text{Th}$ - $^{234}\text{U}$ - $^{238}\text{U}$  ratios, errors, and error correlations as input instead of the  $^{230}\text{Th}/\text{U}$  age directly, and includes the additional constraint of a closed system for the Th-U isotopes.

***Unmix ages*** Deconvolutes an assemblage of dates that overlap within their assigned errors but have more than one age-component, using the Sambridge and Compston approach.

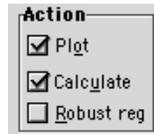
***Zircon age extractor*** Implements the *TuffZirc* algorithm of Ludwig and Mundil (Ludwig and Mundil, 2002) for extracting reliable ages and age-errors from suites of  $^{206}\text{Pb}/^{238}\text{U}$  dates on complex single-zircon populations.

***Youngest Detrital Zircon*** Determines the age and age-uncertainty of the youngest zircon in a suite of dated (single-crystal) detrital zircons, assuming only that 1) the errors assigned to the individual zircon dates are accurate and normally distributed, 2) none of the dated zircons are contaminants.

**Action/Plot:** Check the Plot box in the Action group to obtain a plot as a separate *Excel* Chart-sheet.

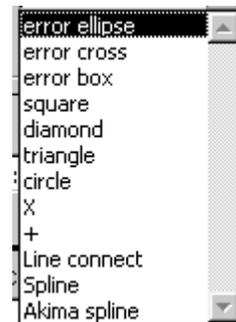
**Action/Calculate:** Check the Calculate box in the Action group to have *Isoplot* perform a regression or other calculation on the selected data. Results will be included in the plot, if one is specified.

**Action/Robust Regr:** Instead of calculating the best-fit line, isochron, or chord using the usual 2-error regression (Yorkfit), use a robust (nonparametric) regression which makes no assumptions about the nature or distribution of the scatter about a straight line. Not available for U-Pb Concordia or  $^{230}\text{Th}$ - $^{234}\text{U}$ - $^{238}\text{U}$  isochrons (see p. 25).



**Input Errors:** Specify the type and sigma-level of the errors you have assigned to your data here (if you will be regressing the data, or plotting with error-symbols). Be especially careful to correctly specify the errors as absolute or percent. The sigma-level is important for (nonrobust) regressions, as the resulting MSWD will be affected by a factor of 4. Also, if you have specified (from the Preferences/Graphics/Error Symbols dialog box) that error symbols are to be plotted at the sigma-level of the input-data, the sizes of error ellipses, error crosses, and error boxes will reflect the sigma-level you specify (see p. 20).

**Plotting Symbols:** The available plotting symbols are shown in the Symbols drop-down:



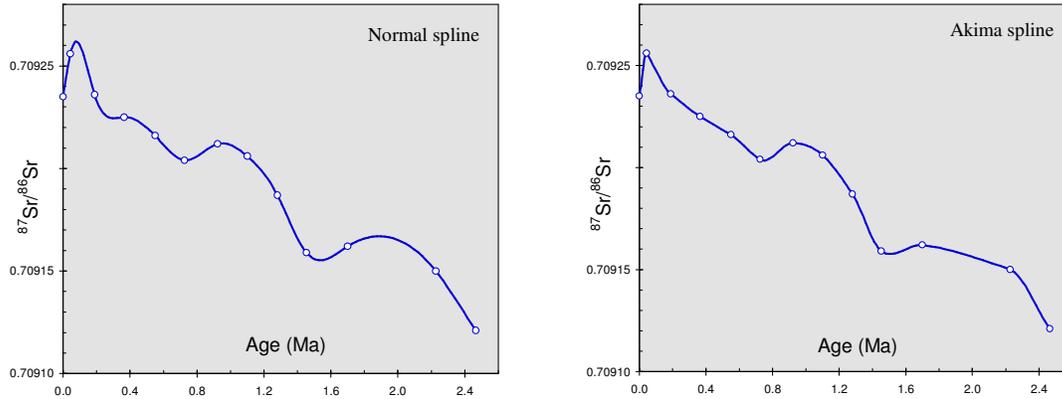
Note that error cross and error box symbols will not be enabled for plot types whose  $X$ - $Y$  data-errors are always significantly correlated—that is, for conventional concordia Pb-Pb isochron plots.

The “line connect” option constructs a line connecting the data points, in the same order that they appear in the worksheet, but without any data-point symbols. By default, the line is smoothed. Double-click on it to cancel smoothing. The “line connect” option is useful for plotting custom curves, such as non-single stage Pb-isotope growth curves<sup>2</sup>.

The “Spline” option constructs a classical spline curve – that is, a smoothly-joined assemblage of third-order polynomials forced through the data-points.

<sup>2</sup> The age ticks could be added by plotting a data range corresponding to the age ticks as circles, then invoking *Isoplot*'s Label Data-Points menu-item to label the ticks.

The “Akima spline” option constructs a somewhat different sort of spline curve – one that eliminates the “overshoots” that can occur with classical splines, at the expense of allowing much sharper “bends” in the curve (Akima, 1970), as shown below.



**Figure 2:** Examples of spline curves. The “Normal” spline (left) is constructed of connected segments of cubic polynomials whose slopes are matched at each data-point. The “Akima” spline uses a different algorithm which eliminates the “overshoot” typical of Normal splines.

**Plot-Symbol Colors:** Select the outline-color of the plot-symbols from the **Symbol/Colors** drop-down. You can have the symbol-outline colors vary for each data-point by selecting **Font Color**, in which case the symbol color will match the color of the font used for each data-point. For non-filled symbols, the default interior color of polygonal, non-error plot-symbols is white; to use filled symbols of this type, use a bold font for the data.

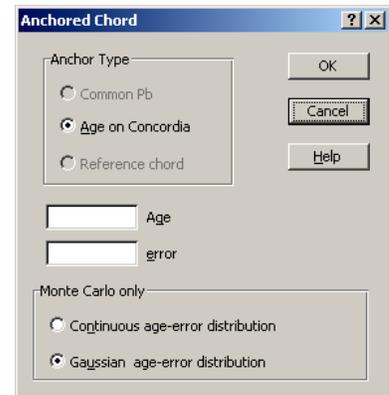
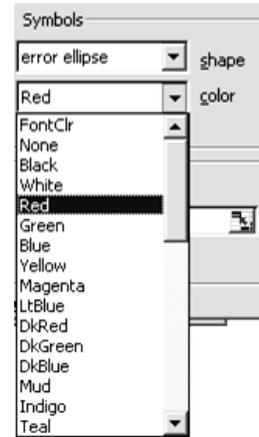
**Other/Color:** Check this box if you want the plot to use the colors specified in **Options/Colors**; leave unchecked for a black-and-white plot.

**Other/Autoscale:** Check this box to have *Isoplot* select the X- and Y-limits of the plot-box, based on the range of the selected data. Leave unchecked to specify these limits yourself.

**Other/Anchored** (Two-dimensional Concordia plots only): Check this box to (1) force one of the Concordia intercepts to be a specified age; (2) force the regression line to intersect the  $^{207}\text{Pb}/^{206}\text{Pb}$  axis at some specified common-Pb ratio (Inverse Concordia plots only); or (3) construct a reference chord between two specified ages, using the dialog-box at right:

**Other/PbGrowth** ( $^{207}\text{Pb} - ^{206}\text{Pb}$  or  $^{208}\text{Pb} - ^{206}\text{Pb}$  isochrons only): Check this box to specify construction of a single-stage Pb-isotope growth curve. From the dialog-box (p. 37) that appears later, you can specify Stacey-Kramers parameters, or any other initial age, Pb-isotope ratios, and Mu for the growth curve.

**Other/Reject OK** (Weighted-averages only): Check this box to permit outlier-rejection using a modified  $2\sigma$  criterion.



### Isoplot Preferences

Preferences are grouped into two types: Numeric and Graphics, indicated by buttons in the main *Isoplot* dialog box.

#### Numeric Preferences

The Decay constants/Half lives sheet contains the relevant values for all of Isoplot's age calculations. When editing, values can be entered as either decay constants or half lives (see example at right). The Model age parameters sheet contains the source-region isotope ratios for Sm-Nd, Rb-Sr, Lu-Hf and Re-Os model ages.

The U-Th, Ar-Ar, & statistical sheet permits editing of the U and Th decay-constant uncertainties (used in calculated U-Pb and  $^{230}\text{Th}/\text{U}$  age errors), as well as parameters used in the calculation of age plateaus for Ar-Ar step-heating spectra. An additional, very important parameter defined in this sheet is the "Probability of fit below which errors are expanded by Students- $t \times \sqrt{\text{MSWD}}$ ". Errors of weighted averages or regressions whose probability-of-fit exceeds the specified value (acceptable range = 0.05 to 0.30) will be reported with the "internal 2-sigma" error – the error propagated only from the assigned data-point errors. Errors of weighted averages or regressions having a lower probability of fit will be reported with the "95%-confidence errors" calculated by multiplying the 1-sigma internal error by the Student's- $t$  value for the appropriate degrees of freedom, and again by the square root of the MSWD parameter for the calculation (The MSWD is the sums of squares of weighted residuals divided by the degrees of freedom of the calculation). The default value for this "minimum probability of fit" parameter is 0.15.

Decay Constant / Half Life	Isotope
1.55125E-10	238U
9.8485E-10	235U
4.94752E-11	232Th
1.42E-11	87Rb
6.53999E-12	147Sm
1.666E-11	187Re
2.82629E-6	234U
9.15771E-6	230Th
1.94E-11	176Lu
5.543E-10	40K tot
2.13276E-5	231Pa

**Show/enter as**

Decay constants

Half Lives

**U-Th decay constant uncertainties**

enter as percent, 2-sigma

0.107	238U	0.2	234U
0.136	235U	0.3	230Th
137.88	Natural (present-day) 238U/235U		

**Ar-Ar Plateau**

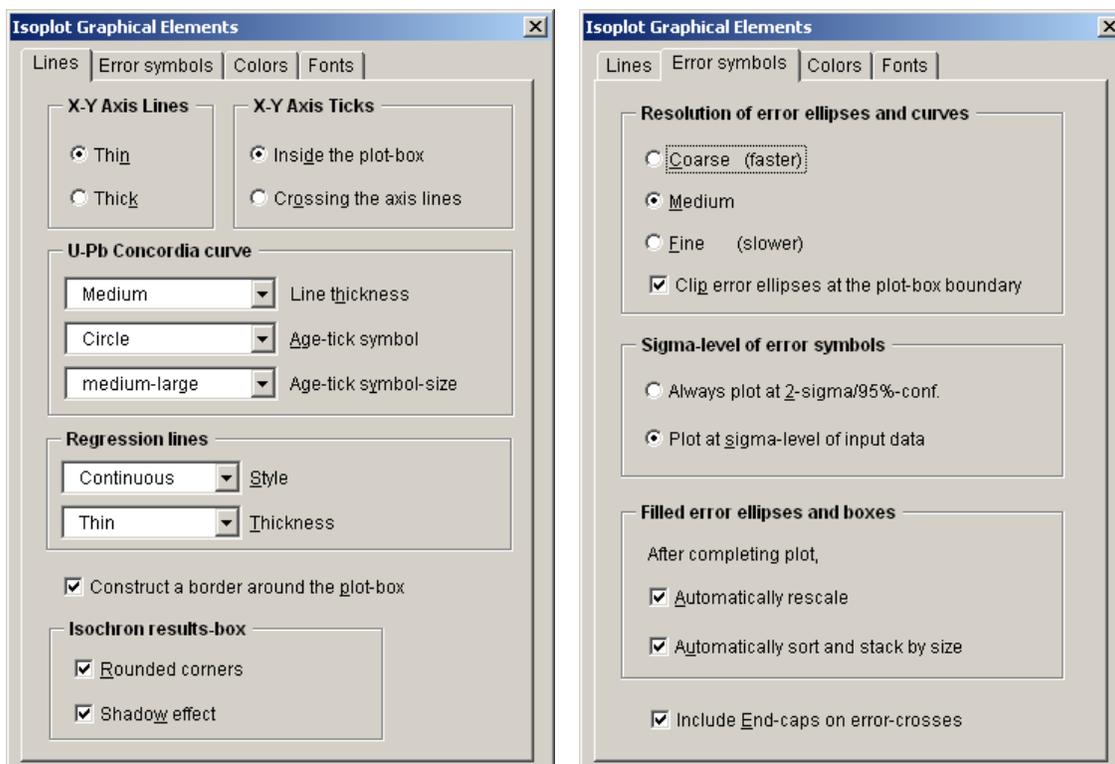
60 Minimum amount of 39Ar (as percent of total 39Ar released) to define an acceptable Ar-Ar plateau

295.5 Value assumed for atmospheric or trapped 40Ar/36Ar

**Weighted Averages and Linear Regressions**

0.15 Probability-of-fit below which regression errors are expanded by Students-t \* Sqrt(MSWD)

## Graphics Preferences



**Lines:** Specify attributes of various lines in the *Isoplot* charts:

**Error symbols:** Specify attributes of error symbols when used as data-point symbols:

*Resolution of error ellipses & curves:* **F**ine yields in a large number of line-segments defining the curves and ellipses, but takes slightly more time; **C**oarse is the fastest, with a slight compromise on line-smoothness. Don't judge the quality of the outline curves/ellipses at low magnification, though – to evaluate, zoom to 400% and temporarily change the line-thickness of the curve/ellipse to the thinnest available.

If **C**lip ellipses at the plot-box boundary is checked, error ellipses will be clipped at the plotbox borders; if unchecked, they will continue beyond. Don't use clipped ellipses if you might re-scale the plot-limits later—if you do so, the clipped ellipses will be revealed as arcs (outline ellipses) or abruptly terminated shapes (filled ellipses).

*Sigma-level of error symbols:* You can specify that error symbols (error ellipses, error boxes, and error crosses) be plotted at 2-sigma, (regardless of the sigma-level of the input-data), or at the sigma-level of the input-data. Thus the only way of plotting 1-sigma error symbols is to have the input-data errors at 1-sigma and also to specify “at sigma-level of input data” in the Error Symbols group of Options/Lines.

*Filled error ellipses & boxes:* Check **A**utomatically rescale to have the position of the error symbols fine-tuned before quitting plot-construction. Usually unnecessary, but may improve symbol-positioning in some cases. Check **A**utomatically sort & stack by size to arrange the relative position of the filled symbols by size, with smaller symbols are superimposed on larger ones so that the smaller symbols are not hidden by the larger.

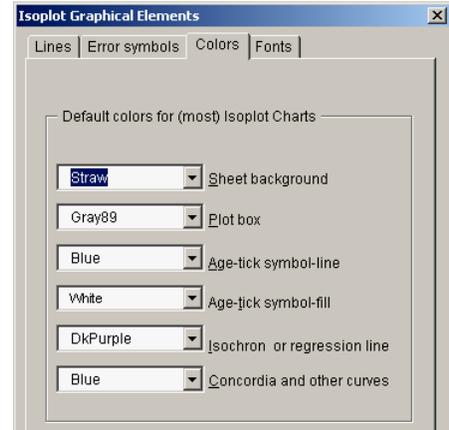
The **E**nd-caps on error crosses box specifies whether or not error crosses will be terminated by a



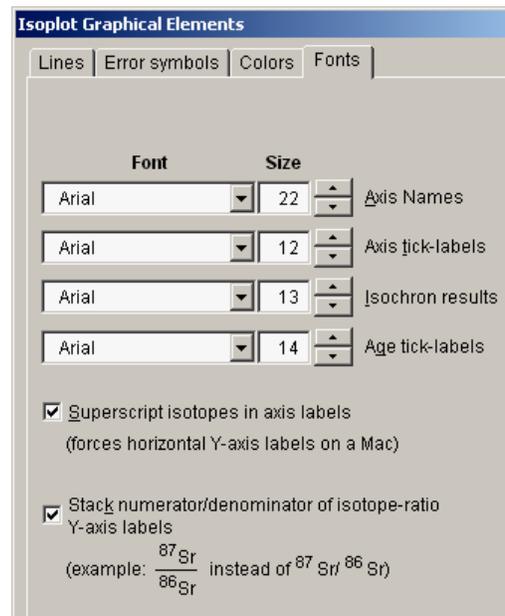
short, horizontal line in both the X- and Y-error directions ( versus )

*Rescale shapes when done:* Check this box to have the filled symbols in the plot automatically rescaled and ordered by size just before the plot is finished. Because this takes extra time, if your plots take more than a few seconds to construct you may want to leave this box unchecked (make sure to rescale the plot from the *Isoplot* drop-down menu before printing).

**Colors:** Specify the default colors for the various elements of the *Isoplot* charts (you can always change the colors after the plot is completed).



**Fonts:** Specify the default fonts and font-sizes for different elements of the *Isoplot* charts. If **Superscript isotopes in axis labels** is checked, number-prefixes of common geochronologic isotopes will be superscripted in the usual way (e.g.  $^{87}\text{Sr}/^{86}\text{Sr}$ ).



## Classical Error-Weighted X-Y Regressions and Isochrons

### Regression Models

Unless Robust Regr. were checked (p. 25), two-dimensional ( $x$ - $y$ ) data are initially regressed using the algorithm of York (1969), with errors propagated using the (maximum-likelihood estimation) algorithm of Titterton and Halliday (1979). If the probability of fit of the regression is low, other approaches (“Models”) for weighting the data-points may be used. The 3 “Models” used by *Isoplot* are:

#### *Model 1*

The Model 1 fit is York’s original algorithm, and assumes that the assigned errors are the *only* reason the data-points scatter from a straight line. The points are therefore weighted proportional to the inverse square of these errors (taking into account the error correlations). A test of the Model 1 assumption is provided by the *Probability of Fit* calculated by the program. If this probability is reasonably high (more than 15%), then the Model 1 assumptions are considered justified, and the regression is complete. If the probability is low (usually less than 15%, but user-definable in the range of 5% to 30%), you may choose another model. The *Probability of Fit* is actually the probability that, if the only reason for scatter from a straight line is the analytical errors assigned to the data points, the scatter of the data points will exceed the amount observed for your data.

If you accept the Model 1 fit even though the *Probability of Fit* is less than 15%, *Isoplot* then calculates the 95%-confidence errors from the *observed* scatter (thus invoking the use of the Student’s- $t$  multiplier to convert from estimated errors — equivalent to the *a priori* errors multiplied by the square root of the MSWD<sup>3</sup> — to 95%-confidence errors). Note that in this case, weighting of the data points remains inversely proportional to the square of their analytical errors.

*Isoplot* will always attempt a Model 1 fit first. In the results-box, the *a priori* errors are the errors in the slope and intercept calculated by propagating only your assigned errors for the points; therefore, no matter how much the points scatter, the *a priori* errors will not increase. The *including scatter* errors, however, are calculated from the actual scatter of the points from a line, and are independent of the assigned errors. These errors, given at the  $1\sigma$  level, are provided mainly for comparison purposes with the output of other implementations of York’s algorithm. The only geologically useful errors for data sets with few points are the ones given as 95% *Confidence-Limit* errors.

How the 95% confidence-limit errors are calculated depends on the probability that the assigned data-point errors can account for the observed scatter. If the probability is greater than 15%, the 95% confidence-limit errors are given as simply 1.96 (Student’s- $t$  for an infinite number of points) times the *a priori* errors (the reason for this is discussed by Brooks and others, 1972).

#### *Model 2*

A Model 2 fit (not supported for classical isochrons such as Rb-Sr or Sm-Nd) assigns equal weights and zero error-correlations to each point. This is seldom justified by any real mechanism, but at least avoids the mistake of weighting the points according to analytical errors (see above discussion of Model 1 regressions) when it is clear that, in fact, some other cause of scatter is involved. The 95% confidence-limit errors are

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<sup>3</sup>MSWD = Mean Square of Weighted Deviates. This does not refer to porcine pervers; it is, roughly, a measure of the ratio of the *observed* scatter of the points (from the best-fit line) to the *expected* scatter (from the assigned errors and error correlations). *The MSWD parameter cannot be compared to the classical  $R^2$  parameter, and is not a measure of how highly correlated the X- and Y-values are.* If the assigned errors are the only cause of scatter, the MSWD will tend to be near unity. MSWD values much greater than unity generally indicate either underestimated analytical errors, or the presence of non-analytical scatter. MSWD values much less than unity generally indicate either overestimated analytical errors or unrecognized error-correlations. See Wendt and Carl (1991) for a detailed discussion.

calculated from  $t_{n-2}$  times the *including scatter* errors. Because this relatively know-nothing approach still makes the assumption of a normal distribution of residuals, it is arguably more realistic in most cases to choose a robust regression instead.

### Model 3

A Model 3 fit (for classical isochrons such as Rb-Sr or Sm-Nd) assumes that the scatter is due to a combination of the assigned errors plus an unknown but normally distributed variation in the Y-values. This model (similar to the Model 3 algorithm of McIntyre and others, 1966) may be realistic in the case of Rb-Sr or other isochron data for rocks whose initial ratios were variable. For this model, the program will solve for the unknown Y-variation (= initial-ratio variation) as well as for the best-fit line, so you can judge whether or not the solution is realistic.

Remember, though, that it is physically quite possible (even likely) that the initial ratios of the samples were significantly correlated with their Rb/Sr (or other parent/daughter ratio), in which case the Model 3 assumptions are not valid. For an extended discussion of the problem, see Zheng (1989a), or Juteau and others (1984) for an excellent example.

### A Word About 3-Point Isochrons

You should be aware that the reliability of isochron ages for regression lines with only 3 or 4 data points and no resolvable “geological” scatter can be significantly less than suggested by the uncertainties calculated by most regression algorithms, including that of *Isoplot*. The reason is that with only 1 or 2 degrees of freedom (3 or 4 data points), the probability of getting an MSWD close to 1 even though some “geological” scatter exists in the population is significant. For such data sets, the lack of statistical resolution of this “geological” scatter can be expected to occur in a significant number of cases, and, because the use or non-use of a very large (12.7 for  $N=3$ ) Student’s-*t* multiplier is involved, can lead to a large underestimate of the true isochron uncertainties.

### Comments on Regressions with Low Probabilities-of-Fit

Exactly how to quantitatively and qualitatively interpret a regression with a low probability-of-fit (sometimes referred to as an “excess scatter” regression) is a thorny issue, with no real consensus among the geochronological community. The problem centers around two points:

- 1) If the only reasons for scatter about a regression line are truly the errors assigned to the data points, then the only relevant regression-line uncertainties (of slope and intercept) are those propagated solely from the assigned data-point errors—in other words, the *a priori* regression-line errors;
- 2) If the probability-of-fit (that the assigned data-point errors account for the observed scatter of the data-points about the regression line) is very low, one must abandon the presumption of (1), and use the actual scatter of the data-points to estimate the regression-line uncertainty.

The first point was emphasized by Williamson (1968), who unfortunately did not address the complications of the second point, which are:

- 1) How low should the probability-of-fit be before *a priori* regression-errors are abandoned? 0.01? 0.05? 0.15?
- 2) If the assigned errors are not the reason for (most of) the observed scatter, how should the data-points be weighted?
- 3) Should one maintain the assumption of a normal error-distribution once analytical errors are shown to be inadequate to explain the scatter?
- 4) What is the significance of an “isochron” whose scatter arises from geologic/geochemical complications rather than analytical error?

The answer to (1) above is necessarily arbitrary—*Isoplot's* default is 0.15, but can be specified by the user at from 0.05 to 0.30 from the Numeric/U-Th, Ar-Ar, & statistical dialog-box. In some cases, an objective weighting algorithm (for scatter clearly in excess of analytical errors) can be applied to deal with (2) above (e.g. Model 3 below), though often not. Fortunately, use of an invalid weighting algorithm should not *bias* the regression, but merely fail to make the most *efficient* use of the data, in the sense that one could have obtained a more precise regression if the true errors (and distribution) of each data-point were known. This is why (in a Gaussian world, at any rate) if the probability-of-fit of a regression is low, expansion of the *a priori* regression errors by the square root of the MSWD (which takes into account the actual scatter of the points) and a Student's-*t* factor (which takes into account the fact that the true scatter of the data-point population is only *estimated* from a finite number of actual points) can be justified.

The question of weighting and of intuitively-offensive probability break-points for regression-errors can be avoided by using a robust regression (*sensu lato* – a linear relationship between *x* and *y* is still assumed), in which no assumptions are made about why the data-points scatter from the regression line. The drawbacks of robust regressions, however, are that a) they are inefficient for the typically small data-sets of geochronology in those cases when data-point errors are adequate to explain the regression-line scatter; and b) the geological-significance question raised by point (4) above.

The *significance* of a low probability-of-fit regression is perhaps the most difficult question of all to address, since there are no mathematical or algorithmic approaches that are really relevant. One should perhaps start with the simple statistical meaning of a correctly calculated error of such a regression – say 8 points whose regression gives an isochron age of 320 ± 8 Ma at 95% confidence – which can be stated as something like:

“If one were to repeat the sampling and regression procedure an infinite number of times, the probability that the grand mean of the resulting isochron ages would fall between 312 and 328 Ma is 95%.”

Notice that this statement does not say that the *true* age of the samples has a 95% probability of falling between 312 - 328 Ma, only that the mean of the infinitely-replicated regressions would yield an isochron age within this interval. Thus even the most robust, assumption-free regression algorithm will yield a biased isochron age if the samples comprising the isochron do not meet the basic isochron assumption of a closed system (except for the special, unlikely case of random redistribution of parent and daughter elements among the samples). The validity of the invariant initial isotope-ratio assumption is not a requirement for the isochron age to be unbiased, however, so long as the variation is not correlated with the parent-daughter ratio. For U-Pb concordia intercepts or Pb-Pb isochrons, however, it is difficult to conceive of geochemically reasonable mechanisms that would yield a very low-probability regression yet still be unbiased.

In sum, I recommend treating the errors assigned by *Isoplot* to ages derived from a low probability-of-fit regression as a *lower bound* on the true errors, rather than a reliable, mathematically firmly-constrained uncertainty. I also recommend treating age uncertainties in the literature that were derived from low (say <5%) probability-of-fit regressions as geochronologic disinformation if either 1) the *a priori* regression errors were used, or 2) the regression comprises only a small (say <5) numbers of points and “1-sigma” regression errors were used.

### Examining Residuals of Regressions

You can look at the weighted residuals<sup>4</sup> of any of *Isoplot's* regressions by checking the Insert **Wtd-Residuals Column** box when it appears in one of the dialog boxes. After regressing, the cells to the left of the input-data's *X*-values (a new, blank column will be inserted any of these are already occupied) will then contain the weighted residuals for each of the data-points selected for the regression. In addition, *Isoplot* will place a small Linearized Probability Plot of the weighted residuals to the right of the input-data (see p. 48). By definition, the MSWD of an error-weighted regression will equal the sum of the squares of the weighted residuals, divided by the degrees of freedom of the regression. For York (*x*-*y*) regressions, this

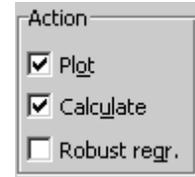
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<sup>4</sup> Defined as  $(y_i - \hat{y})/\sigma_{y_i}$ , where  $\sigma_{y_i}$  is the value of  $y_i$  predicted by the regression.

will be true only for Model-1 fits; for Model-2 fits the MSWD calculated from the values in the Wtd Resids column will be meaningless, and for Model-3 fits are forced to ~unity.

### Robust Regressions

Classical isochrons and  $x$ - $y$  regressions assume that the residuals (observed scatter) of the data-points from a straight line have a normal (Gaussian) distribution, either because of the assigned analytical errors (Model-1 fits) or other causes. If this assumption is invalid, or even if a true, Gaussian form of the expected scatter of each data point cannot be modeled, the analyst is traditionally expected to take responsibility for whatever data-trimming is required to restore the legitimacy of the initial assumptions.



When such data-trimming becomes uncomfortably arbitrary or extreme, yet the data-set is still believed to contain age-information worth extracting, the analyst may prefer instead to use a robust, nonparametric regression that makes no assumptions about the cause(s) of the observed scatter of the data from a straight line, and that requires no arbitrary<sup>5</sup> decisions about what data should or should not be included in the regression. In such cases, *Isoplot* offers a robust regression option<sup>6</sup> via the Action/Robust Repr checkbox. The robust regression algorithm used by *Isoplot* is either

- 1) The median of all pairwise slopes (Theil, 1950), with errors calculated according to Rock and Duffy (1986) after Vugrinovoch (1981); or
- 2) The median of the medians of all pairwise slopes taken through each successive point (Siegel, 1982), with errors generated via a bootstrap.

Because of *Excel* constraints, the first method is used for data sets smaller than  $N=363$ , and the second for larger data-sets.

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<sup>5</sup> *a priori* criteria such as chemical or mineralogical characteristics are fair enough, so long as applied consistently and not specially constructed for each data-set.

<sup>6</sup> Not offered for U-Pb Concordia data.

### U-Pb Concordia Plots

There are three possible U-Pb concordia plots: Conventional (Wetherill, 1956), with

$$x = {}^{207}\text{Pb}/{}^{235}\text{U} \quad y = {}^{206}\text{Pb}/{}^{238}\text{U} \quad z = {}^{204}\text{Pb}/{}^{238}\text{U} ,$$

Tera-Wasserburg (Tera and Wasserburg, 1972), with

$$x = {}^{238}\text{U}/{}^{206}\text{Pb} \quad y = {}^{207}\text{Pb}/{}^{206}\text{Pb} \quad z = {}^{204}\text{Pb}/{}^{206}\text{Pb} ,$$

and its variant (Tatsumoto and others, 1972), with

$$x = {}^{235}\text{U}/{}^{207}\text{Pb} \quad y = {}^{206}\text{Pb}/{}^{207}\text{Pb} \quad z = {}^{204}\text{Pb}/{}^{207}\text{Pb}$$

(the  $z$  coordinate is relevant to the discussion of 3-dimensional concordia, pages 32-34). *Isoplot* supports both Conventional and Tera-Wasserburg concordia in their 2-dimensional forms, and just Tera-Wasserburg for 3-dimensional concordia. If you intend to calculate concordia-intercept ages by regressing a suite of discordant analyses (as opposed to calculating a “Concordia Age” for a suite of *concordant* analyses), make sure that the **ConcAge** box in the main *Isoplot* dialog-box is unchecked.

### Conventional versus Tera-Wasserburg Concordia Representations

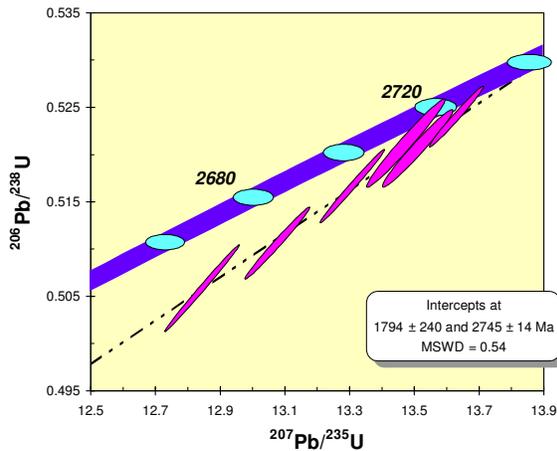


Figure 1: Conventional concordia plot.

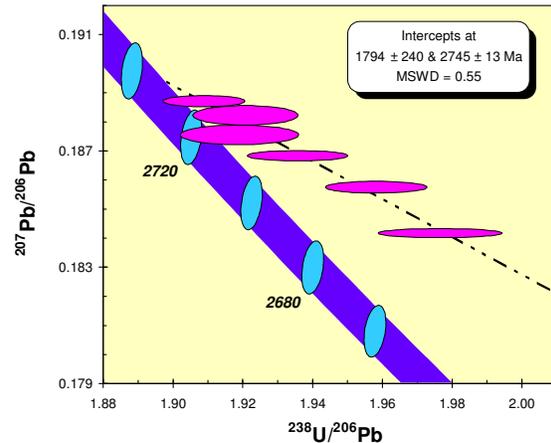


Figure 2: Tera-Wasserburg concordia plot (same data as Fig. 2).

Tera-Wasserburg concordia diagrams are mathematically equivalent to Conventional concordia diagrams. Tera-Wasserburg plots can have advantages in visualization, however, because the errors in their X- and Y-values are generally much-less correlated than those of the Conventional concordia diagram, so that the relative scatter of their error ellipses is more (visually) apparent. Moreover, as long as the magnitude of the common-Pb correction is small, and the error in the  ${}^{206}\text{Pb}/{}^{238}\text{U}$  ratio is significantly greater than for the  ${}^{207}\text{Pb}/{}^{206}\text{Pb}$  ratio, error correlations for Tera-Wasserburg concordia data can be satisfactorily approximated by zero, whereas a precise and accurate value for error correlations is always essential for conventional concordia-data. A disadvantage of Tera-Wasserburg concordia is that it is difficult to show data with a large range of U/Pb ages (say from 100 Ma to 2700 Ma), and impossible to show a zero-age point.

Quantitative comparison of Yorkfit calculations for the two types of concordia diagrams is logical only for Model 1 fits. If you do so (being careful to use the correct errors and error-correlations in both cases), you will find that the ages and age-errors are not *exactly* the same for the two types of (mathematically equivalent) data. This is not due to roundoff errors in the calculations, but rather to the assumption of a normal distribution for the isotope-ratio errors (only approximately true) and the first-derivative expansion formulae used to obtain the regression-line and concordia-intercept errors.

The formulae for transforming errors for conventional Concordia plots to Tera-Wasserburg Concordia plots are:

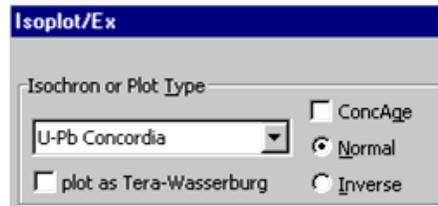
$$S_{x'}^2 = S_y^2 S_{y'}^2 = \sqrt{S_x^2 + S_y^2 - 2S_x S_y \rho_{xy}} \quad S_{z'} = \sqrt{S_y^2 + S_z^2 - 2S_y S_z \rho_{yz}}$$

$$\rho_{x'y'} = \left( S_y^2 - S_x^2 \rho_{xy} \right) / S_{y'} \quad \rho_{x'z'} = \left( S_{x'}^2 + S_{z'}^2 - S_z^2 \right) / \left( 2S_{x'} S_{z'} \right)$$

$$\rho_{y'z'} = \left( S_x S_z \rho_{xz} - S_{x'}^2 + S_{x'} S_{y'} \rho_{x'y'} + S_{x'} S_{z'} \rho_{x'z'} \right) / \left( 2S_{y'} S_{z'} \right)$$

where  $S_x = \sigma_x/x$  and  $\rho_{xy}$  is the x-y error correlation, et cetera. Note that the corresponding equation for  $\rho_{xy}$  in Ludwig (1980) is incorrect (sorry).

You can create Tera-Wasserburg concordia plots directly from conventional concordia data by checking the box labeled “plot as Tera-Wasserburg” (“Normal” specified next to the Plot-Type drop-down); or you can create conventional concordia plots directly from Tera-Wasserburg data by checking the box labeled “plot as conv. concordia” (“Inverse” specified next to the Plot-Type drop-down). *Isoplot* will do the necessary data, error, and error-correlation transformations for you, with the assumption that the measured Pb was highly radiogenic ( $^{206}\text{Pb}/^{204}\text{Pb}$  more than ~ 500-1000). If this assumption is invalid, you should do the data-transformation yourself with the exact equations for error propagation (e.g. Ludwig, 1980).



### Errors of Concordia-Intercept Ages

#### Symmetric

The simplest form of concordia-intercept age errors is obtained by propagating the variance/covariance of the regression-line slope and intercept via the usual first-derivative approximations. These age-errors are the first ones given in the results-box (above), and are of necessity symmetric — that is, the upper age-error and the lower age-error are identical, and so are given as a simple ± value. For reasonably precisely-determined ages where the uranium decay-constant errors are ignored, these symmetric age-errors are generally quite satisfactory.

Model 1 Solution without [with] decay-const. errs	
Upper intercept:	256.4 ± 2.4 [±4.9] Ma
Lower intercept:	-2 ± 42 Ma

Age errors are shown both with [in brackets] and without incorporation of the uranium decay-constant errors (see Ludwig, *in press*, for method and discussion), unless the two types of age errors are almost equivalent. When decay-constant errors are acknowledged, the best possible precision for an upper concordia-intercept age is about 5 Myr ( $2\sigma$ ), or worse if the angle of intersection of the discordia line with the concordia curve is shallow. To view or change the errors assigned to the  $^{235}\text{U}$  and  $^{238}\text{U}$  decay constants, invoke Options/Consts/Decay-Constant Errors from *Isoplot*.

#### Asymmetric

For imprecise concordia-intercept ages (because the regression line is either imprecise or intersects the concordia curve at a shallow angle), the true age-errors

Lower Intercept	Upper Intercept
1849 (-120 +110) Ma	2755 (-20 +27) Ma

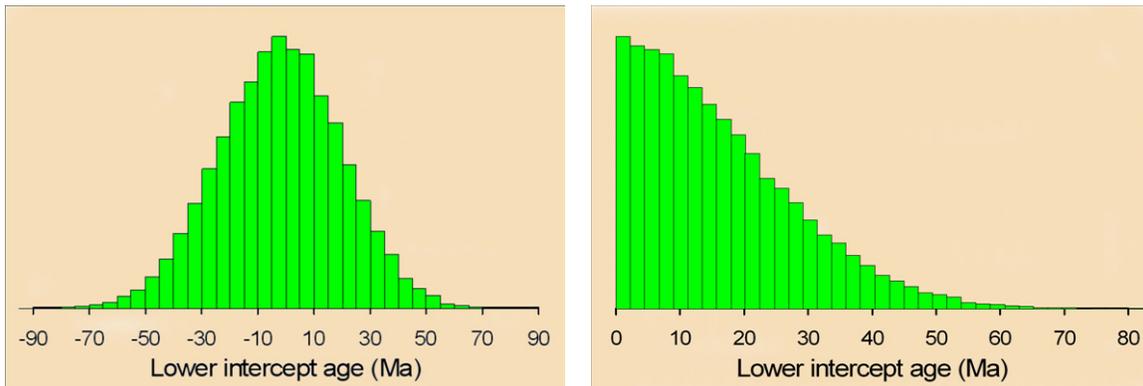
Age errors do not include decay-constant errors

will be significantly asymmetric — that is, with different plus and minus errors (e.g. +32/-17 Ma). Asymmetric age-errors *that ignore decay-constant uncertainties* are given in the lower part of the Details box (above) that can be invoked from the Concordia-Intercept Ages results-box.

### Monte Carlo

*The most reliable errors for concordia-intercept ages are obtained with a Monte Carlo simulation that involves the regression procedure itself (not just the intercepts of a regression line with pre-calculated slope-intercept errors), and so does not rely on the usual first-derivative expansion approximations at any stage.*

Such Monte-Carlo age-errors are offered only if the regression-line probability-of-fit is greater than 0.05 (so that the assigned data-point errors have a reasonable likelihood of accounting for the observed scatter about the regression line). When the probability-of-fit drops below about 0.3, you will notice that the Monte Carlo errors deviate increasingly from the conventional (first-derivative expansion) errors. This discrepancy evidently arises when the assumption of dispersion from analytical errors alone is tenuous.



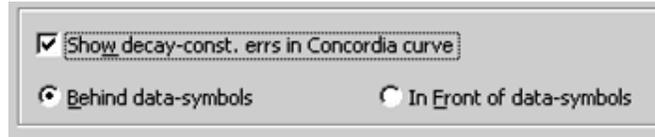
**Figure 3:** Graphics for Monte Carlo solutions of concordia-intercept ages. Both are the results of 30,000 trials for the same data-set: the unconstrained distribution is shown at left, the distribution constrained to positive, finite ages at right.

To take into account the uncertainties in the  $^{235}\text{U}$  and  $^{238}\text{U}$  decay constants, check Include decay-constant errors. Also, if you are convinced that the lower intercept of the discordia line with the concordia curve reflects a real geologic event, you can constrain the Monte Carlo solutions of the regression to those which have a positive lower concordia-intercept age: check the box labeled Accept Only Positive Lower-Intercept Ages (equivalent to the Bayesian constraint of Davis, 1982).

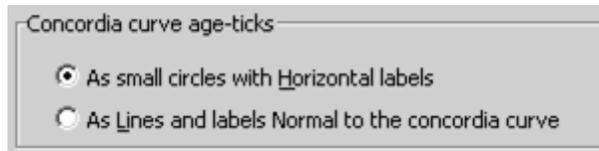
To visualize the distribution of the Monte Carlo solutions (which can be very non-Gaussian), you can ask *Isoplot* to construct a small plot (Fig. 3) next to the input data that shows a histogram of the Monte Carlo age solutions

### Showing Decay-Constant Errors in the Concordia Curve

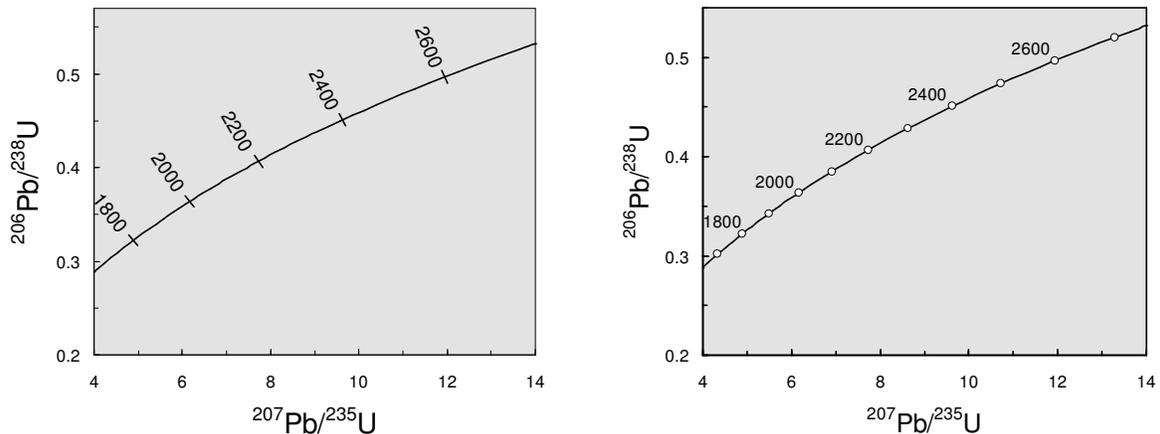
The concordia curve can be constructed to show the effect of decay-constant errors on the position of the concordia curve. Check the **Show with decay-const. errors** box when it appears, and the concordia curve will be plotted as a band that reflects the  $^{238}\text{U}$  and  $^{235}\text{U}$  decay-constant errors, with error ellipses for age-ticks. *Note that the concordia band and ticks are always plotted at  $2\sigma$ , even if the data-point error-symbols have been specified to be  $2\sigma$ .*



### Specifying the Style of the Concordia-Curve Age Ticks



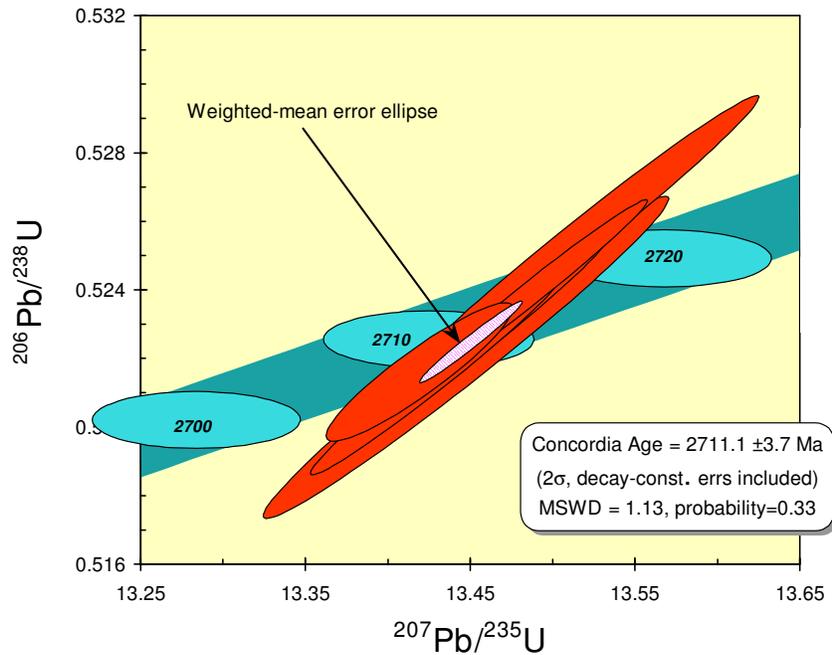
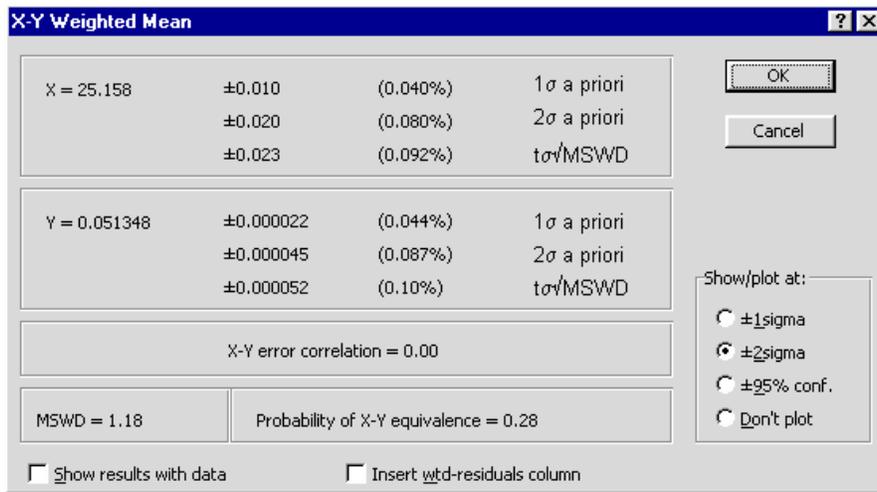
Unless you request that the concordia curve be constructed as a band reflecting the decay-constant errors, you can specify that the age ticks be constructed as either small, open circles with horizontal labels, or as short lines normal to the concordia curve (Fig. 4).



**Figure 4:** Concordia-plot age-tick styles: short lines normal to the concordia curve with coaxial labels (left), or small open circles with horizontal labels (right).

### The “Concordia” Age

In addition to the usual  $^{206}\text{Pb}/^{238}\text{U}$ ,  $^{207}\text{Pb}/^{235}\text{U}$   $^{207}\text{Pb}/^{206}\text{Pb}$  ages, you can use any pair of  $^{206}\text{Pb}/^{238}\text{U}$  -  $^{207}\text{Pb}/^{235}\text{U}$  or  $^{238}\text{U}/^{206}\text{Pb}$  -  $^{207}\text{Pb}/^{206}\text{Pb}$  ratios to calculate a single “Concordia Age” (Ludwig, 1998). A Concordia Age is the most-probable age for a data-point (or weighted-mean data-point) on a concordia-diagram, where the true location of the data point is assumed to fall precisely on the concordia curve (Fig. 5). Because a Concordia Age makes optimal use of all of the radiogenic Pb/U and Pb/Pb ratios at the same time, it will be slightly to significantly more precise than any single U/Pb or Pb/Pb age. Though *the precision advantage for Concordia Ages younger than Late Paleozoic (where most of the chronometric power resides in the  $^{206}\text{Pb}/^{238}\text{U}$  ratio) is negligible*, the technique still can be worth using even for analyses of geologically young material, because it yields an objective and quantitative measure of concordance.



**Figure 5:** Concordia Age plot with concordia curve (oblique band) and age ticks (labeled horizontal ellipses) constructed with decay-constant errors.

### Calculating a Concordia Age

To calculate a Concordia Age, select a range comprising one or more data-points for either a Conventional or a Tera-Wasserburg Concordia diagram. If the range contains several data-points, they must be assumed (at least provisionally) to be equivalent, except for scatter induced by their assigned analytical errors. From the main *Isoplot* dialog-box, check the **ConcAge** box (above the **Normal/Inverse** buttons), select **U-Pb Concordia** as the **Isochron or Plot Type**, and specify **Normal** or **Inverse** for  $^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$  or  $^{238}\text{U}/^{206}\text{Pb}$ - $^{207}\text{Pb}/^{206}\text{Pb}$  data, respectively. If your data-range contained more than one point, the first popup will be the results of the *X-Y* weighted-mean calculation. This is the 2-dimensional weighted mean of the data — that is, with their *X-Y* error correlations as well as their *X*- and *Y*-errors taken into account. The MSWD shown in this box refers to the goodness-of-fit of just the *X-Y* weighted mean — that is, how well the data fit the assumptions that the data points are repeated measurements of the same point, and that these data-points scatter only because of the assigned *X-Y* errors. This MSWD is for *X-Y* equivalence (likewise the weighted residuals, if requested). To have *Isoplot* plot the error ellipse of the *X-Y* weighted mean, check the appropriate **Show/Plot At** button (**1 $\sigma$**  - **2 $\sigma$**  - **95% conf.**).

**Concordia Age**

<b>With <math>\lambda</math> errors</b> Age = 251.45 Ma $\pm 0.15$ $\pm 0.29$ $\pm 0.36$	<b>Without <math>\lambda</math> errors</b> Age = DISCORDANT	<input type="checkbox"/> 1 $\sigma$ a priori <input type="checkbox"/> 2 $\sigma$ a priori <input type="checkbox"/> $t\sigma\sqrt{\text{MSWD}}$
<b>Concordance only</b> MSWD = 4.5 Probability = 0.034	<b>Concordance only</b> MSWD = 27 Probability = 0.000	<b>Show Age</b> <input checked="" type="radio"/> with decay-const errs <input type="radio"/> w/o decay-const errs
<b>Concord. + Equiv.</b> MSWD = 1.4 Probability = 0.14	<b>Concord. + Equiv.</b> MSWD = 2.7 Probability = 0.000	<input type="radio"/> at 1-sigma <input checked="" type="radio"/> at 2-sigma <input type="radio"/> at 95%-conf.
<input type="checkbox"/> Show results with data	<b>Concordia band</b> <input checked="" type="radio"/> Behind data-symbols <input type="radio"/> In Front of data-symbol	<input type="button" value="OK"/> <input type="button" value="Cancel"/>

### Concordia Age MSWD's

There are three MSWD statistics (and associated probabilities) that are relevant to the Concordia Age calculation: the MSWD for *X-Y* equivalence, the MSWD for concordance, and the MSWD for combined equivalence and concordance. The Concordia Age is meaningful only if the data are both equivalent and concordant, so *Isoplot* considers the last MSWD to be the most significant. Another way of looking at the statistics is to first require a probability of equivalence of, say, greater than 5%, then to look at the probability of concordance as a final arbiter, without further consideration of the probability of equivalence. Note that because there is only a single degree of freedom involved, the MSWD for concordance can be as high as 3.8 before the probability of concordance becomes less than 5%.

### Concordia Age Errors

Errors for both the *X-Y* weighted mean and the Concordia Age are given at 3 levels. The  $1\sigma$  and  $2\sigma$  errors are *a priori* errors — that is, calculated by propagating only the assigned data-point errors, without consideration of the actual scatter of the data points from one another or from the Concordia curve. As long as the probability for *X-Y* equivalence and Concordance are not too low (say  $>.05$ ), these errors are appropriate. The  $t\sigma\sqrt{\text{MSWD}}$  errors are the  $1\sigma$  *a priori* errors multiplied by the square root of the MSWD (to take into account the actual scatter of the data, which for low probabilities must be the result of “geologic” error

rather than analytical error) and again by a Student's-*t* factor (to take into account the fact that the true  $\sigma$  of the data is estimated from only a few points). The  $t\sigma/\text{MSWD}$  errors are 95%-confidence errors, provided that the true data-point errors are Gaussian and for some reason are reasonably proportional to the assigned errors. In practical use, however, very high MSWD values must reflect a failure of the assumptions of either data-point equivalence or of concordance, in which case the concordia age has no physical significance. *Thus if the probability of data-point equivalence is less than 0.001, no further calculations will be attempted. Similarly, if the probability of concordance is less than 0.001, only the word DISCORDANT will be displayed.*

Note for users of the SQUID add-in (for SHRIMP ion-microprobe analyses): To avoid double-counting of the Standard Calibration error, you must use SQUID's built-in Concordia-Age utility rather than Isoplot's.

#### *Effect of Decay-Constant Errors on Concordia Ages and Errors*

Ages calculated from  $^{206}\text{Pb}/^{238}\text{U}$ ,  $^{207}\text{Pb}/^{235}\text{U}$ , and  $^{207}\text{Pb}/^{206}\text{Pb}$  ratios are independent of errors in the uranium decay-constants, and the effects of these errors on the age errors are usually ignored. However, because the position of the Concordia curve is affected by the decay-constant errors (and so the location of the most-probable concordant age), not only is the age error affected by consideration of decay-constant errors, but also the Concordia Age itself. Equally important, the evaluation of concordance (on which the validity of a Concordia Age depends) should only be made with the decay-constant errors taken into account. *Isoplot* therefore offers two columns of Concordia Ages and errors — one ignoring the decay-constant errors, the other acknowledging them. As one would expect, the uncertainty in the difference between two Concordia Ages is best estimated without decay-constant errors.

### **Three-dimensional Regressions for U-Pb Concordia**

#### *Planar Regressions*

Three-dimensional planar regressions of U-Pb concordia data (pioneered by Levchenkov and Shukolyukov, 1970) can be extremely useful for suites of samples whose  $^{206}\text{Pb}/^{204}\text{Pb}$  ratios are relatively low (say <1000), and whose Pb/U systematics conform to either:

	<b><i>Radiogenic Pb/U Component</i></b> <i>(properly corrected for common Pb)</i>	<b><i>Common Pb Component</i></b>
<b>Type I</b>	Defines a linear discordia	Isotopically equivalent for all samples
<b>Type II</b>	Only one, which is concordant	Defines a line on the $^{206}\text{Pb}/^{204}\text{Pb}$ - $^{207}\text{Pb}/^{204}\text{Pb}$ plane (i.e. a secondary Pb-Pb isochron)

The crucial advantage of the planar regression is that one need not know the isotopic composition of the common Pb, and in fact a crucial parameter of the common Pb — the  $^{207}\text{Pb}/^{204}\text{Pb}$  at a given  $^{206}\text{Pb}/^{238}\text{U}$  — is part of the regression solution itself (for detailed discussions, see Levchenkov and Shukolyukov, 1970; Neymark and Levchenkov, 1979; Wendt, 1984; and Zheng, 1989b). Another use of planar regressions is for the case when the isotopic composition of the common Pb can be assumed to be invariant, but whose ratios are only approximately known. In this case, the estimated common-Pb isotope ratios should be included as a data-point for the regression, together with its estimated errors and error correlations.

*Isoplot* offers planar concordia-intercept solutions only for Tera-Wasserburg (= "Inverse") concordia data, where the third, Z axis is  $^{204}\text{Pb}/^{206}\text{Pb}$ . The data range for *Isoplot* must consist of 3 columns (X-Y-Z), 6 columns (X, X-error, Y, Y-error, Z, Z-error), or 9 columns (X, X-error, Y, Y-error, Z, Z-error,  $\rho_{x,y}$ ,  $\rho_{x,z}$ ,  $\rho_{y,z}$ ). And, of course, both the 3-D and Planar option buttons must be on. In many cases, it is reasonable to ap-

proximate the  $X$ - $Y$  ( $= {}^{238}\text{U}/{}^{206}\text{Pb} - {}^{207}\text{Pb}/{}^{206}\text{Pb}$ ) and  $X$ - $Z$  ( $= {}^{238}\text{U}/{}^{206}\text{Pb} - {}^{204}\text{Pb}/{}^{206}\text{Pb}$ ) error correlations as zero; however, if the  ${}^{204}\text{Pb}/{}^{206}\text{Pb}$  errors are not much greater than the  ${}^{207}\text{Pb}/{}^{206}\text{Pb}$  errors (e.g. for relatively low  ${}^{206}\text{Pb}/{}^{204}\text{Pb}$  measured on a thermal-ionization mass spectrometer), the  $Y$ - $Z$  error correlation can be significantly nonzero and negative.

The plot (if specified) will be of simply the  $X$ - $Y$  plane of the 3-D concordia – in other words, just the usual Tera-Wasserburg concordia plot. If you request plotting of the  $X$ - $Y$  projection of the data-points, you must also specify whether the points are to be projected parallel to the  ${}^{204}\text{Pb}/{}^{206}\text{Pb}$  axis (that is, down the best-fit plane with no change in the  $X$ -values), or through some specified  ${}^{204}\text{Pb}/{}^{206}\text{Pb}$ . The latter is useful if you have a pretty good idea of the  ${}^{204}\text{Pb}/{}^{206}\text{Pb}$  of the common Pb, and will show you where the points would have plotted if their common Pb had each been correctly subtracted.

As for a conventional 2-D discordia regression, the popup-box for the concordia-intercept ages of the planar regression will contain the upper and lower concordia-intercept ages. For 3-D planar discordia, however, two other age results are also given: the Pb-Pb isochron age defined by the intersection of the regression plane with the  ${}^{204}\text{Pb}/{}^{206}\text{Pb} - {}^{207}\text{Pb}/{}^{206}\text{Pb}$  plane, and the intercepts of this isochron with the Stacey-Kramers single-stage Pb-isotope growth curve (Stacey and Kramers, 1975). The latter two types of ages are relevant only for Type II data (concordant radiogenic Pb/U plus common Pb dispersed along a secondary isochron), in which case only one of the concordia-intercept ages will have a geologic meaning.

As usual, the errors given in the popups will be the  $2\sigma$  *a priori* errors if the probability of obtaining more than the observed amount of scatter of the points (from the best-fit plane) with the assigned errors is greater than 15%. For lower probabilities-of-fit, the age errors will be the  $1\sigma$  *a priori* errors expanded by both Student's- $t$  for  $N-3$  degrees of freedom and by the square root of the MSWD. In other words, the age errors for low probabilities-of-fit are calculated by expanding the analytical errors until they predict precisely the actual amount of scatter, then converting these  $1\sigma$  errors to 95% confidence with the appropriate Student's- $t$ .

Note that If the planar regression fails, it may be because the data actually define a *line* rather than a *plane* in  $XYZ$  space, so try a 3-dimensional *linear* regression (Total Pb/U Isochron) before giving up (see below).

One interesting advantage of planar 3-D regressions of U-Pb data is that such regressions will correctly propagate the errors arising from a large common-Pb correction. For example, consider the case of a suite of, say, sphene analyses that appear to fall along a (common-Pb corrected) discordia line, where there is a reasonable, but not extremely precise idea of the common-Pb's isotopic composition. If one simply propagates the errors assigned to the common-Pb  ${}^{206}\text{Pb}/{}^{204}\text{Pb}$  and  ${}^{207}\text{Pb}/{}^{204}\text{Pb}$  into the  ${}^{206}\text{Pb}^*/{}^{238}\text{U}$  and  ${}^{207}\text{Pb}^*/{}^{235}\text{U}$  ratios required for a conventional, 2-D concordia diagram, the errors for each data-point will be correct, but all of the data-points will tend to be shifted in the same direction on the concordia diagram. The result will be an artificially low MSWD for the regression (because the errors from point-to-point will be correlated, not just the  $X$ - $Y$  errors of each point), and the concordia-intercept errors will be correspondingly elevated (this is assuming a constant common-Pb from sample to sample). The correct way to deal with this situation is to use your estimate of the common-Pb's isotopic composition (whether from growth-curve estimates or a feldspar analysis) and errors, and include these ratios as an additional point on a 3-D planar regression. The MSWD of the regression will then correctly reflect the common-Pb uncertainty, yielding not only a more precise age, but also a more accurate one.

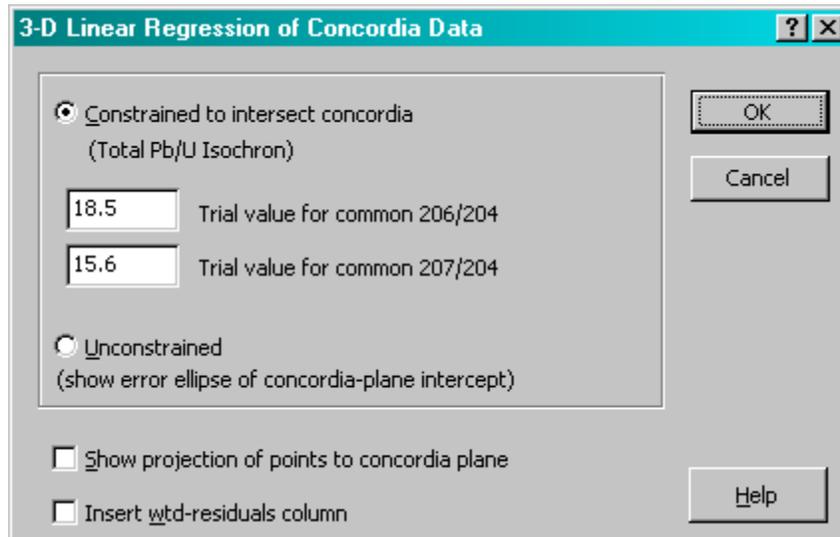
#### *Linear, Concordia-Constrained 3-D Regressions (The Total Pb/U Isochron)*

Cogenetic samples with an undisturbed U-Pb system that shares the same common-Pb isotopic composition must define a line in  ${}^{238}\text{U}/{}^{206}\text{Pb} - {}^{207}\text{Pb}/{}^{206}\text{Pb} - {}^{204}\text{Pb}/{}^{206}\text{Pb}$  space, whose intersection with the  ${}^{238}\text{U}/{}^{206}\text{Pb} - {}^{207}\text{Pb}/{}^{206}\text{Pb}$  plane must fall precisely on the U-Pb concordia curve, and whose intersection with the  ${}^{204}\text{Pb}/{}^{206}\text{Pb} -$  plane is the isotopic composition of the common Pb. The 3-D linear regression that constrains the  $X$ - $Y$  plane intercept to the concordia curve is called the Total Pb/U Isochron (Ludwig, 1998). This isochron has some unique attributes and advantages, including:

- 1) The regression MSWD tests for both closed-system behavior (=concordance) and the assumption of an invariant common Pb;

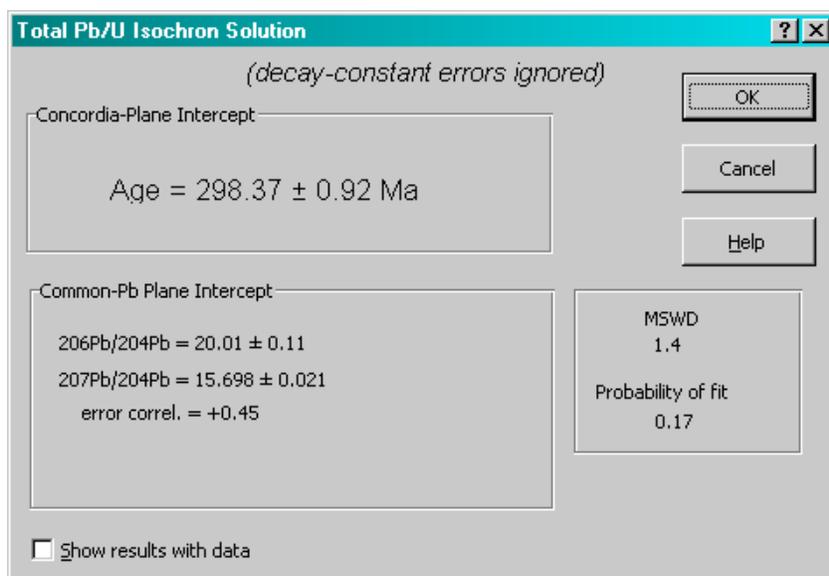
- 2) All of the relevant isotope ratios are used at the same time, yielding the smallest justifiable age-error of any possible U/Pb or Pb/Pb isochron.

To invoke the Total Pb/U isochron, specify U-Pb Concordia, Inverse, 3-D, Linear. When the dialog box shown below appears, specify Constrained to intersect concordia (use Unconstrained when you don't need quantitative age information, but just want to see where a 3-D linear regression would intersect the Concordia diagram were it not constrained to do so). If you have some idea of the isotopic composition of the common-Pb, enter its  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$ . If not, the default values will probably be close enough to allow convergence of the solution, and yield identical results to any other nearby estimate).



The Total Pb/U Isochron is the 3-D equivalent of the Concordia Age, in the same way that a planar solution (p. 32) is the 3-D equivalent of the conventional concordia-intercept age, and the data-range requirements are exactly the same as for a planar 3-D regression. The Total Pb/U isochron should be the first step in evaluating a suite of high- $^{204}\text{Pb}$  data. If the regression fails, or if its probability of fit is low, the next step should be a Planar regression, followed as a last resort by the classical  $^{206}\text{Pb}/^{204}\text{Pb}$  -  $^{207}\text{Pb}/^{204}\text{Pb}$ ,  $^{238}\text{U}/^{204}\text{Pb}$  -  $^{206}\text{Pb}/^{204}\text{Pb}$ , or  $^{235}\text{U}/^{204}\text{Pb}$  -  $^{207}\text{Pb}/^{204}\text{Pb}$  isochrons.

The results of the Total Pb/U Isochron are shown in two boxes — one for the Concordia-plane intercept, the other for the common-Pb plane intercept. The upper consists simply of the Total Pb/U Isochron age and error. As usual, the error is the  $2\sigma$  *a priori* error if the probability-of-fit calculated from the MSWD is more than 15%; if less, the  $1\sigma$  *a priori* error is expanded by the square root of the MSWD and Student's *t* for  $2N-3$  degrees of freedom. The lower box consists of the results of the intersection of the isochron with the common-Pb plane, including the  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$  ratios and errors, and the single-stage Stacey-Kramers growth-curve age and Mu (Stacey and Kramers, 1975) for those ratios.

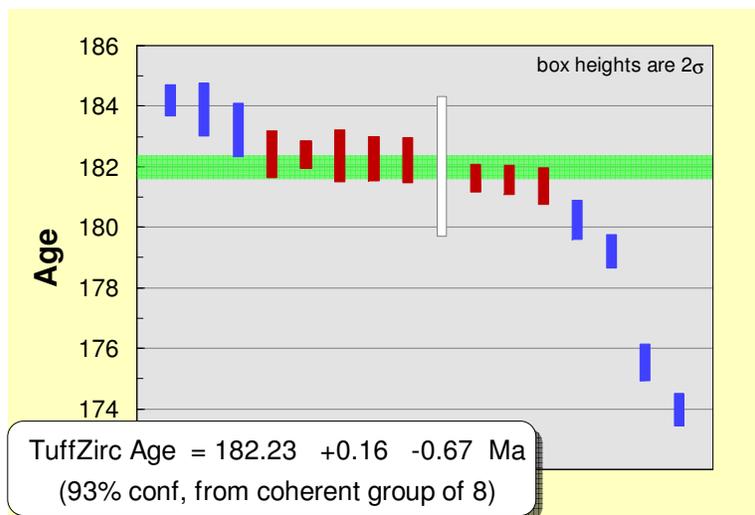


Note that, like planar regressions compared to 2-D discordia (and for the same reasons), the Total Pb/U Isochron can have a distinct advantage over a Concordia Age if the common-Pb correction required by the latter is significant. For data-sets on Phanerozoic samples, however, the main utility of the Total Pb/U Isochron is to evaluate the concordance of the U-Pb system and provide a complete estimate for the ratios and errors of the common-Pb component, *not* to improve the age precision, which is almost entirely provided by the  $^{206}\text{Pb}/^{238}\text{U}$  system alone.

### Extracting Reliable Ages from Suites of Single-Zircon $^{238}\text{U}/^{206}\text{Pb}$ Dates

U-Pb ages of zircons from Phanerozoic tuffs are invaluable for studies requiring timescale geochronology. However, modern studies show that zircon populations from such rocks are often vulnerable to both positive (from xenocrysts or cores) and negative (from Pb loss) age biases. Though biases from significantly older zircon cores and large degrees of Pb loss are easily avoided, problems arising from slightly older xenocrysts and from subtle degrees of Pb loss can be difficult to resolve, and often force the analyst into uncomfortably subjective decisions. In particular, strong trimming of data sets to obtain clusters with MSWD values close to 1 is likely to yield a biased age, with assigned errors that are erroneously small. To improve this unsatisfactory situation, *Isoplot* offers the *TuffZirc* algorithm (Ludwig and Mundil, 2002), a conceptually and mathematically simple approach that is largely insensitive to both Pb loss and inheritance, without entirely ignoring the valuable information provided by analytical errors.

The  $^{206}\text{Pb}/^{238}\text{U}$  ages (and errors) submitted to *TuffZirc* should consist of at least 10 (preferably more) analyses of internally-concordant  $^{206}\text{Pb}/^{238}\text{U}$  dates on single crystal or smaller samples. If desired, these analyses can also be trimmed using any other *a priori*, objective criteria (e.g. anomalously high uranium or  $^{204}\text{Pb}$ , anomalous crystal morphology or appearance ...) – though note that such pre-trimming must have been done *before* numerical evaluation of the data. The *TuffZirc* algorithm then proceeds as follows: 1) the data-set is pre-cleaned for analyses with anomalously high errors, then ranked according to  $^{206}\text{Pb}/^{238}\text{U}$  age; 2) the largest cluster of the ranked analyses is found that yields a "probability-of-fit" (in the conventional geochronological sense) of  $>0.05$ ; 3) the median age of the largest cluster, without regard to analytical errors (except for the initial pre-cleaning of anomalously imprecise data), is taken as the true age, with the (asymmetric) 95%-confidence errors of the median age as its uncertainty. Monte Carlo testing indicates that, as long as a reasonable fraction (say  $>40\%$ ) of the analyzed crystals are both cogenetic with the main eruption that produced the tuff and also free of Pb loss, both the *TuffZirc* age and its error are reliable – even in the presence of xenocrysts only few Myr older than the syn-eruptive tuff zircons, regardless of when the xenocrysts themselves have suffered Pb loss, and for a variety of distributions and magnitudes of Pb loss.



**Figure 6:** Example of *TuffZirc* graphics. Horizontal green band shows the inferred age and uncertainty of the syngenetic zircons; red boxes are the error bars for the arguably syngenetic zircons, blue boxes are the error bars for zircons likely to be xenocrystic or to have experienced Pb loss, white boxes indicate analyses ignored because of anomalously high errors.

To invoke *TuffZirc*, select a range of zircon  $^{206}\text{Pb}/^{238}\text{U}$  dates and errors (remember, these dates *must* be on either single crystals or domains within single crystals), then either click on the *TuffZirc* toolbar button, or invoke *Isoplot* and choose Zircon Age Extractor from the Isochron or Plot Type dropdown menu.



If *TuffZirc* can find a coherent (that is, statistically within analytical error) group of at least 5 analyses (or  $0.3 \times \text{\#analyses}$ , whichever is larger), the age and uncertainty of the median of the coherent group is reported and, if specified, shown graphically (above).

Use of *TuffZirc* requires that at least 30-40% of the input dates

(larger sets of dates being more robust) are from crystals or crystal-domains that are:

1. Cogenetic with eruption age -- that is, neither xenocrysts, inherited from source-rocks, nor with an unusually long magma-residence time, and
2. Unaffected by Pb loss.

In most cases, failure of one or the other of these assumptions will prohibit *TuffZirc* from calculating an age. For *TuffZirc* to fail (that is, report an incorrect age) requires either that xenocrystic zircons with a common age are more abundant than syn-eruptive zircons, or that a "plateau" level of Pb loss at some nonzero value exists. Though neither of these scenarios should be common, they will occur in some cases, and their likelihood should be evaluated by the geochronologist.

Three appealing attributes of *TuffZirc* are that

1. The asymmetric uncertainties of the ages tend to expand in the direction of most complexity,
2. the degree of expansion is more or less proportional to the subtlety of the complexity (for example, while severe amounts of Pb loss result in little increase in age-uncertainty, small amounts that approach analytical error cause significant increase in age uncertainty, reflecting the difficulty of recognizing which analyses are completely uncorrupted by Pb loss), and
3. Even in the best cases, the reported age uncertainty will not be much better than the analytical error of the most-precise analyses.

The third attribute accords with the concept that the real limit on accuracy for U/Pb dates is only a factor of two or so better than the analytical error of the individual analyses, rather than amenable to arbitrary improvement by increasing the number of analyses alone. This concept follows from statistical limitations on the ability to resolve complexity in the true age-structure of a suite of analyses arising from open-system behavior, presence of xenocrysts, or a variable and nonzero magma-residence-time.

The *Tuffzirc* algorithm is not intended to be a substitute for obtaining a suite of analyses that are unaffected by Pb loss, and should never be used unless the anneal/leach method of Mattinson fails to remove all evidence of Pb loss.

## Pb-Pb Isochrons and Growth Curves

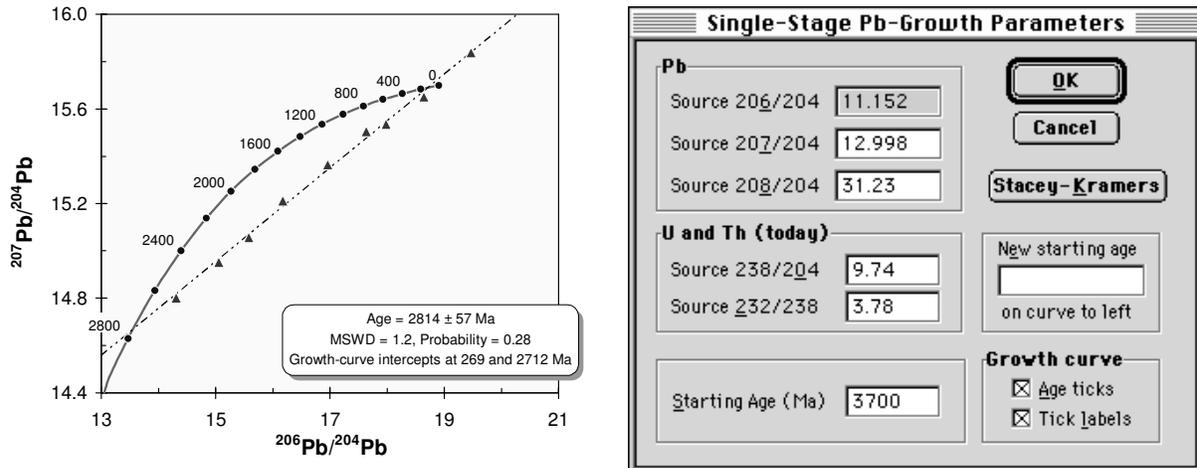


Figure 6: Pb-Pb isochron with growth curve.

*Isoplot* will determine the Pb-Pb isochron age for  $^{207}\text{Pb} - ^{206}\text{Pb}$  plots, which include both  $^{206}\text{Pb}/^{204}\text{Pb} - ^{207}\text{Pb}/^{204}\text{Pb}$  (“Normal”) and  $^{204}\text{Pb}/^{206}\text{Pb} - ^{207}\text{Pb}/^{206}\text{Pb}$  (“Inverse”) types. In addition to the isochron age and age error<sup>7</sup>, the age of the intercepts (if any) of the isochron with the Stacey-Kramers growth curve will be given, as well as the  $^{207}\text{Pb}/^{204}\text{Pb}$  of the isochron at the Stacey-Kramers  $^{206}\text{Pb}/^{204}\text{Pb}$  for the isochron age.

For plots of both  $^{206}\text{Pb}/^{204}\text{Pb} - ^{207}\text{Pb}/^{204}\text{Pb}$  and  $^{208}\text{Pb}/^{204}\text{Pb} - ^{207}\text{Pb}/^{204}\text{Pb}$  data, you can request construction of a single-stage Pb-isotope growth-curve by checking the **PbGrowth** box. The default parameters of the growth curve will be the Stacey-Kramers (1975) values, but you can specify any curve when the Growth-Curve dialog box (below) appears.

<sup>7</sup> *Isoplot* will calculate the  $^{207}\text{Pb}/^{206}\text{Pb}$  age-error both with and without decay-constant errors. If there is a significant difference between the “with” and “without” age-errors, both errors will be given.

## The $^{230}\text{Th}$ - $^{234}\text{U}$ - $^{238}\text{U}$ System

### $^{230}\text{Th}/\text{U}$ Isochrons with Variable $^{234}\text{U}/^{238}\text{U}$

A variety of isochrons have been used to obtain  $^{230}\text{Th}/\text{U}$  ages. For systems with variable  $^{234}\text{U}/^{238}\text{U}$ , perhaps the most common (Rosholt, 1976) are a coupled pair of isochrons, the first being  $^{230}\text{Th}/^{232}\text{Th}$  versus  $^{234}\text{U}/^{232}\text{Th}$ , and the second being  $^{234}\text{U}/^{232}\text{Th}$  versus  $^{238}\text{U}/^{232}\text{Th}$ . The slopes of the isochrons are then used to infer the  $^{232}\text{Th}$ -free  $^{230}\text{Th}/^{234}\text{U}$  and  $^{234}\text{U}/^{238}\text{U}$ , from which a  $^{230}\text{Th}/\text{U}$  age can be calculated. But this representation is one of the worst possible, because:

- 1) The most desirable samples will have relatively little  $^{232}\text{Th}$ , yielding large errors for both  $X$  and  $Y$  parameters (at least when measured alpha-spectrometrically), and high  $X$ - $Y$  error correlations for both isochrons;
- 2) Any spread in  $^{238}\text{U}/^{232}\text{Th}$  will disperse the points along the  $X$ -axis, yielding a visually rather well-defined trend (and  $r^2$  statistic) *even in the absence of geochronologically meaningful systematics*;
- 3) Because  $^{232}\text{Th}$  and  $^{234}\text{U}$  each appear in both of the isochrons, the results of the regressions are necessarily correlated in a complex way – but these correlations are never taken into account when calculating the ages or age-errors.

**Uranium-series evolution curves** [X]

Initial  $^{234}\text{U}/^{238}\text{U}$  AR (first curve)

Age at end of curve (ka)

Multiple evolution curves

Label the evolution curves at the  ka isochron

Age indicators

Isochrons

Age ticks

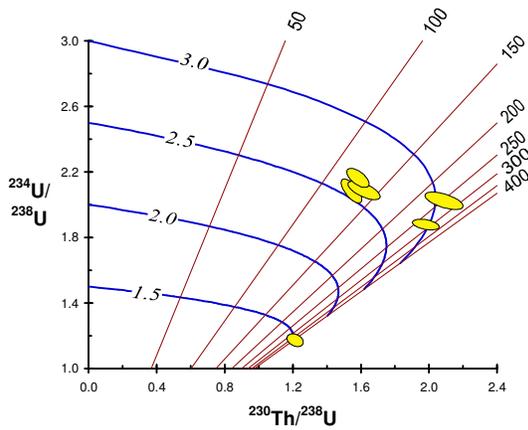
Neither

Tick/isochron interval (ka)

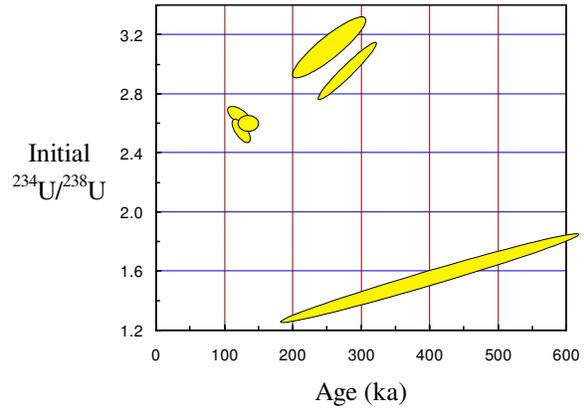
Label the age-ticks/isochrons?

Inside plot-box

Outside plot-box



**Figure 7:** U-series evolution diagram with labeled evolution curves and isochrons.



**Figure 8:** The data of Fig. 7 transformed to coordinates of Initial  $^{234}\text{U}/^{238}\text{U}$  versus age.

The first and second problems are addressed by using  $^{230}\text{Th}/^{238}\text{U}$  versus  $^{232}\text{Th}/^{238}\text{U}$  and  $^{234}\text{U}/^{238}\text{U}$  versus  $^{232}\text{Th}/^{238}\text{U}$  isochrons (Osmond *et al.*, 1970, modified by Ludwig and Titterton, 1994), where the intercepts of the isochrons are used to calculate the age; however, the third problem requires a simultaneous solution using all three of the ratios for the modified Osmond ratios, resulting in a regression for an isochron line in three dimensions. Using  $X = ^{230}\text{Th}/^{238}\text{U}$ ,  $Y = ^{234}\text{U}/^{238}\text{U}$ ,  $Z = ^{232}\text{Th}/^{238}\text{U}$ , the X-Y plane intercepts of this linear 3-D isochron define the ratios used to calculate a  $^{230}\text{Th}/\text{U}$  age and initial  $^{234}\text{U}/^{238}\text{U}$  (Ludwig and Titterton, 1994).

You can assign any combination of the  $^{232}\text{Th}/^{238}\text{U}$  -  $^{230}\text{Th}/^{238}\text{U}$  -  $^{234}\text{U}/^{238}\text{U}$  to be X, Y, Z for plotting purposes so any of the three possible X-Y projections of the isochron can be viewed.

If you specify  $X = ^{230}\text{Th}/^{238}\text{U}$ ,  $Y = ^{234}\text{U}/^{238}\text{U}$ , you can also request that one or more  $^{230}\text{Th}$ - $^{234}\text{U}$  evolution curves be placed on the plot, with ages indicated either by isochron lines or age-ticks (see below, and resulting plot in Fig. 7). Isochron age-indicators will be labeled by age, parallel to the isochron line and along the top or right, inside or outside (you specify – see dialog box below) of the plot-box. Figure 7 shows the results of the above dialog-box settings, with multiple evolution curves later specified for initial  $^{234}\text{U}/^{238}\text{U}$  of 3.0, 2.5, 2.0, and 1.5.

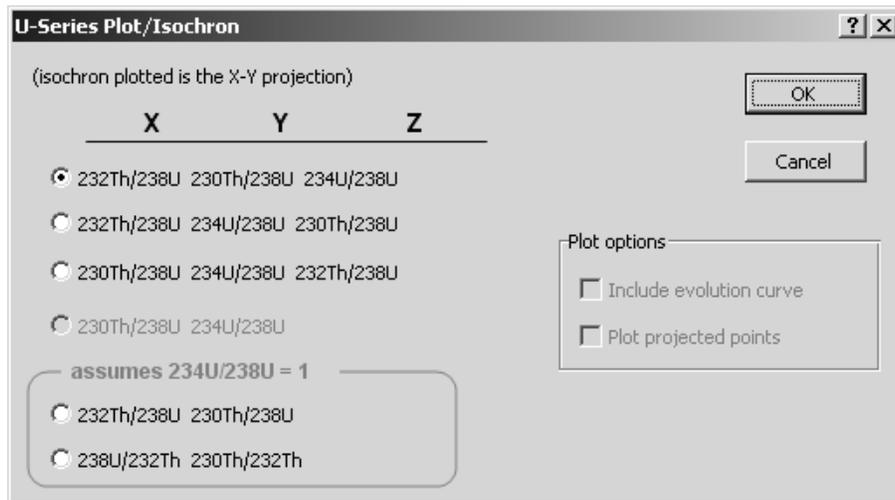


Figure 8 is the mathematically equivalent plot of the same data, transformed to Age - Initial  $^{234}\text{U}/^{238}\text{U}$  coordinates. This diagram, which can only be accurately created using error-propagation equations that include the error correlations (without which the tilted error ellipses of Fig. 8 would turn into rectilinear ellipses with much larger areas), is much more accessible to the non-specialist than the evolution diagram of Fig. 7.

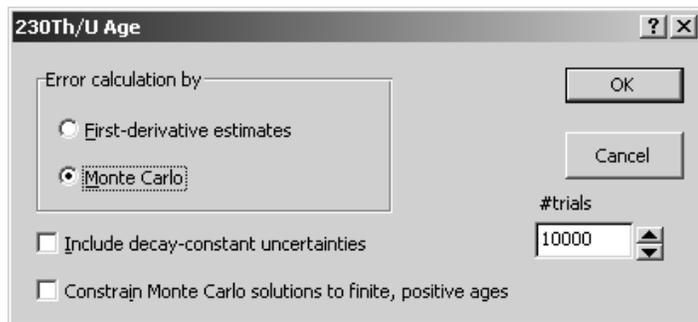
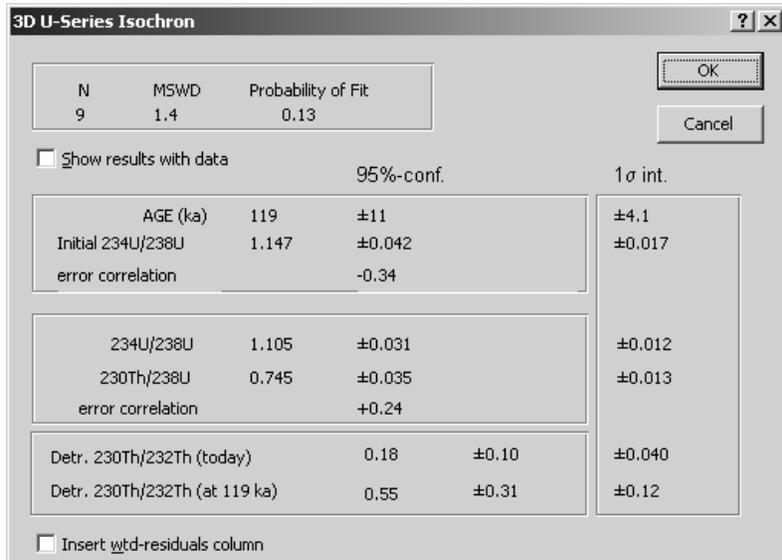
If you've already corrected your  $^{230}\text{Th}/^{238}\text{U} - ^{234}\text{U}/^{238}\text{U}$  data for detrital Th and U (or if the correction is negligible), you can specify a range of 2-dimensional data, with  $X = ^{230}\text{Th}/^{238}\text{U}$ ,  $Y = ^{234}\text{U}/^{238}\text{U}$ , and simply plot these data on the resulting  $^{230}\text{Th} - ^{234}\text{U}$  evolution diagram. If your data range contains only one row of data for a 2D  $^{230}\text{Th}/^{238}\text{U} - ^{234}\text{U}/^{238}\text{U}$  plot, the  $^{230}\text{Th}/\text{U}$  age and initial  $^{234}\text{U}/^{238}\text{U}$  will be calculated and displayed for that data-point. If the probability-of-fit of the isochron is greater than 0.05, you will have the option (see below) of calculating the  $^{230}\text{Th}/\text{U}$  age error from either the usual first-derivative expansion (e.g. Ludwig and Titterton, 1994, p. 5033, eqn. 6-8) or by a Monte Carlo simulation. The choice is offered because age errors by usual first-derivative expansion are significantly inaccurate in cases where the age is close to the limit of the technique (say >250 ka for alpha-spectrometric analyses, >350 ka for TIMS) or the isotope-ratio errors are large.

You can include the  $^{230}\text{Th}$  and  $^{234}\text{U}$  decay-constant errors in the age-error calculation. To do this correctly, you must know how the activity ratios of  $^{230}\text{Th}/^{238}\text{U}$  and  $^{234}\text{U}/^{238}\text{U}$  were calculated: by normalizing the measured ratios (whether alpha-spectrometric activity or mass-spectrometric atomic) to a secular-equilibrium standard, or by multiplying measured atomic ratios by the ratio of the relevant decay constants.

You can also constrain the Monte Carlo solutions to those with finite ages – that is, without excess  $^{230}\text{Th}$  (P. Marianelli, oral comm. 2000). This Bayesian constraint requires merely that the system being analyzed have been a closed system for U-Th isotopes, which of course is the assumption built into the age equations themselves, and thus adds no assumptions that effectively have not already been made.

As usual, for isochron ages the  $1\sigma$  internal error is the  $1\sigma$  error propagated from the assigned data-point errors and error-correlations only (the scatter from the regression line is ignored), so this error is only relevant if the *probability of fit* value shown is reasonably high, in which case the *95%-confidence* errors shown are simply 1.96 times the  $1\sigma$  internal errors. If the *probability of fit* is low, the *95%-confidence* errors are the “ $1\sigma$  internal” errors multiplied by the square root of the MSWD (to take into account the fact that the data points scatter by more than can be expected from the analytical errors alone) and by Student's-*t* for  $2N-4$  degrees of freedom (to take into account that the true scatter of the points from the isochron line is estimated from a small number of data-points).

It is important that the data-point error correlations greater than about 0.5 be reasonably accurate. Entering arbitrary error-correlations can result in ages and, especially, age-errors that are significantly invalid. This



point, and methods for the calculation of the error correlations, are discussed in detail in Ludwig and Titterton (1994).

### **$^{230}\text{Th}/\text{U}$ Isochrons with Secular Equilibrium $^{234}\text{U}/^{238}\text{U}$**

For volcanic rocks and minerals, one can generally assume that the  $^{234}\text{U}/^{238}\text{U}$  is now, and has always been, in secular equilibrium. The 3D isochron approach is then not required, and one can simply regress either  $^{230}\text{Th}/^{238}\text{U}$  against  $^{232}\text{Th}/^{238}\text{U}$  or  $^{230}\text{Th}/^{232}\text{Th}$  against  $^{238}\text{U}/^{232}\text{Th}$  to obtain the  $^{232}\text{Th}$ -free  $^{230}\text{Th}/^{238}\text{U}$  from which a  $^{230}\text{Th}/\text{U}$  age can be calculated. The regression algorithm is the usual  $X$ - $Y$  error-weighted algorithm of York (1969), with errors calculated from the maximum-likelihood approach of Titterton and Halliday (1979). As always, unless the regression has a reasonably high probability-of-fit (say  $>0.05$ ), the 1-sigma *a priori* errors have no geologic significance.

$X$ - $Y$  error correlations for mass-spectrometric input-data of  $^{230}\text{Th}/^{238}\text{U}$  -  $^{232}\text{Th}/^{238}\text{U}$  or  $^{230}\text{Th}/^{232}\text{Th}$  -  $^{238}\text{U}/^{232}\text{Th}$  isochrons will generally be negligible (because the  $^{230}\text{Th}$  measurement error is typically much larger than for  $^{238}\text{U}$  or  $^{232}\text{Th}$ ). For alpha-spectrometric input-data, however, these error correlations will typically be in the range of +0.2 to +0.4, which will have a noticeable (but not large) effect on the isochron's MSWD and errors.

### **Single-Analysis $^{230}\text{Th}/\text{U}$ Ages**

If the range passed to *Isoplot* is a single row containing only  $^{230}\text{Th}/^{238}\text{U}$  [error]  $^{234}\text{U}/^{238}\text{U}$  [error] [err-correl], *Isoplot* will calculate a single age without correction for detrital Th and U. Generally, though, it's probably more convenient to do this directly in the worksheet with the `Th230Age` or `Th230AgeAnd Initial` functions (p. 59), using the `CorrThU` function as necessary (p. 59), unless the Monte Carlo age-error option is required.

### Weighted Averages of a Single Variable

To plot and calculate a classical error-weighted average, select a 2-column range (values and errors) and the **Weighted Average** plot-type. The results-popup (below) will show first the error-weighted (actually, inverse-variance weighted) mean and  $2\sigma$  error propagated from the assigned errors only (=“ $2\sigma$  internal error”), then the “95% conf.” error. The “95% conf.” error will be 1.96 times the  $1\sigma$  internal error if the probability-of-fit is more than 15%, or Student’s-*t* times the square root of the MSWD if the probability is less.

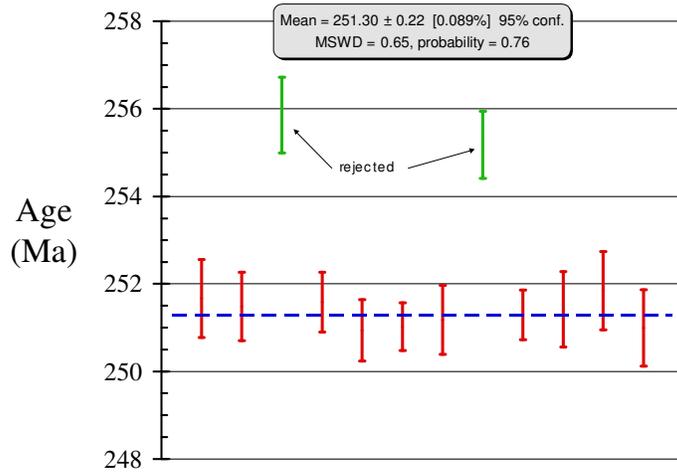


Figure 8: Weighted average plot.

If the probability of fit (of the simple error-weighted average) is low,

*Isoplot* will also calculate a somewhat more complicated error-weighted average using the assumption that data-point scatter arises from two sources: the assigned (Gaussian) errors, plus a constant but unknown "external" (also Gaussian) error. For this calculation, the constant external error must also be solved for, in this case using a Maximum-Likelihood approach and calculating the 95%-confidence uncertainty of the weighted average using a Student's-*t* multiplier for  $2N-2$  degrees of freedom. This calculation in *Isoplot 3* is slightly different than in previous versions of *Isoplot*, and should be more accurate for small *N*.

If the probability of fit is more than 5%, you can choose either the “ $2\sigma$  internal”, or “95% conf.” error to be shown on the plot. Outlier rejection (via a modified 2-sigma set of criteria) can be enabled or disabled from a checkbox in the **Other** section of the main *Isoplot* dialog-box.

The screenshot shows the 'Weighted Average' dialog box with the following options and values:

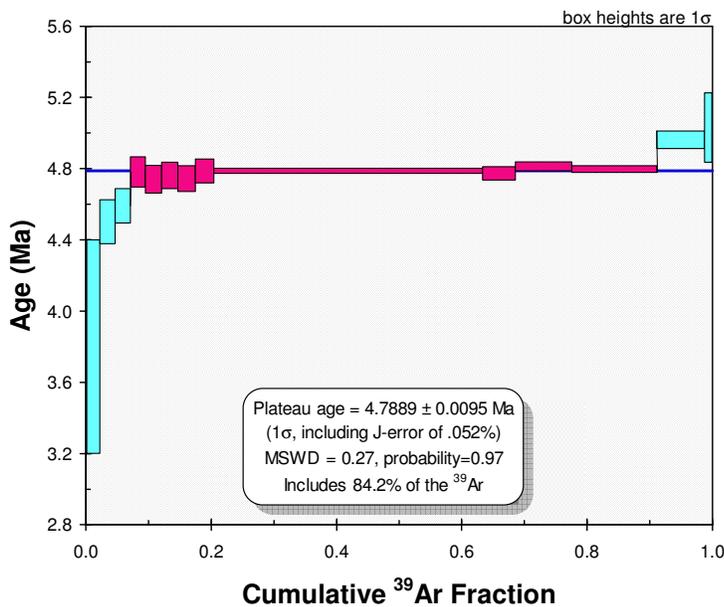
- Wtd by assigned/internal errors only:**
  - 25.158 ± 0.020 [0.080%] **2σ internal**
  - 25.158 ± 0.032 [0.13%] **95% conf. (=t\*MSWD)**
  - MSWD = 1.9
  - Probability of fit = 0.059
- Wtd by assigned errors + constant external error:**
  - 25.159 ± 0.029 [0.12%] **(95% conf.)**
  - External 2-sigma err req'd (each pt) = 0.053 [±0.21%]
- Robust (Tukey's Biweight):**
  - 25.162 ± 0.030 [0.12%] **(95% conf.)**
- Robust (Median):**
  - 25.157 +0.051/-0.063 [0.23%] **(97.9% conf.)**

Additional controls include a 'Show As' section with radio buttons, a '#rejected' field showing '1 of 10', and checkboxes for 'Show with data', 'Show with plot', and 'Insert wtd-residuals column'.

As an alternative to explicit, error-weighting plus outlier rejection, *Isoplot* also offers two robust methods: the Tukey's Biweight" mean (Hoaglin, Mosteller, and Tukey, 1983), and the simple median. The former is best-suited to a normal distribution that is slightly "contaminated" with points not belonging to that distribution, while the latter makes no assumptions whatsoever about the distribution of the input-data (any assigned data-point errors are ignored with both methods). See Rock and Duffy (1986) for a discussion of the error-algorithm for the median.

You can also place the formula and results for the Weighted Average calculation directly under a range of values and errors with *Isoplot's*  toolbar-button (p. 66). If an even more-robust "average" is desired, use the median function and binomial-distribution errors (Rock and others, 1987, p. 167), using *Isoplot's*  toolbar-button (p. 67; if you missed it, the difference between the button-images in this sentence is that the latter is in a bolded font).

### Argon-Argon Age Spectra and Plateau Ages



To create an Argon-Argon Age Spectrum (age versus %<sup>39</sup>Ar or gas-fraction <sup>39</sup>Ar), select Ar-Ar age spectrum as the plot type. The data range must comprise 3 columns, the first being <sup>39</sup>Ar, either as absolute amounts (say moles <sup>39</sup>Ar), as fraction of <sup>39</sup>Ar in the experiment, or as percent <sup>39</sup>Ar in the experiment. The second column must contain the calculated Ar-Ar age for that fraction, and the third the error in the Ar-Ar age. As usual, the age error can be 1σ or 2σ, percent or absolute — but must not include the propagated uncertainty in *J*. *Isoplot* will also try to pick the best statistically-justifiable plateau and plateau-age from the data, using an algorithm that selects the plateau with the largest amount of gas that meets the following criteria:

- 1) Has three or more contiguous steps comprising more than 60% of the <sup>39</sup>Ar (default – can be set to anywhere between 30% and 99% by the user from Options/Consts).
- 2) The probability-of-fit of the weighted-mean age of the steps is greater than 5%;
- 3) The slope of the error-weighted line through the plateau ages is not different from zero at 5% confidence;
- 4) The ages of the outermost 2 steps for either side of the plateau must not be significantly different (at 1.8σ) than the weighted-mean plateau age (6 or more steps only);
- 5) The outermost 2 steps for either side of the plateau must not have nonzero slopes (at 1.8σ) with the same sign (9 or more steps only).

Criteria 2 and 3 are justified by simple statistical considerations, while criteria 1, 4 and 5 are arbitrary, and intended to reproduce one's "visual" sense of a plateau. The plateau selection of *Isoplot*, while arguably at least as valid and justifiable as any of the existing ones (e.g. Dalrymple and Lanphere, 1974; Lanphere and Dalrymple, 1978; Fleck *et al.*, 1977; McDougall and Harrison, 1999, p. 111; Berger and York, 1970; Foland *et al.*, 1986; Heizler and Harrison, 1988; Singer and Pringle, 1996; Snee *et al.*, 1988; Dallmeyer and

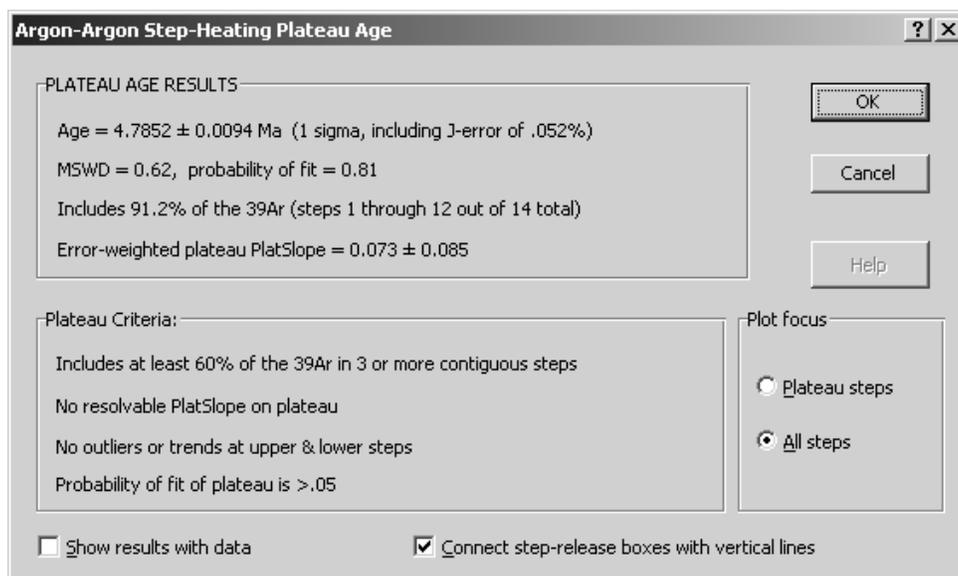
Lecorche, 1990; Berger and York, 1981) is intended primarily as a tool for data evaluation, and should not be used without contemplation.

### User-Specified Plateau Steps

You can override *Isoplot's* concept of the best plateau-steps by putting any other sequence of contiguous steps in a bolded font. *Isoplot* will calculate the weighted-mean age of your selection, and indicate that the plateau criteria are user-defined. If the probability-of-fit of the weighted mean is less than 5%, *Isoplot* will expand the *a priori*  $1\sigma$  error by  $t\sqrt{\text{MSWD}}$  to obtain the 95%-confidence age-error.

### Connecting Lines for Error Boxes

You can specify that the boxes showing adjacent heating-steps be connected by vertical lines, according to the usual practice. Note, however, that because of an *Excel* limitation, if filled symbols are selected the connecting lines are vulnerable to slight mis-positions. These can be minimized by re-scaling before printing, and look worse on the screen than when printed, but are unavoidable except by canceling the filled symbols option.

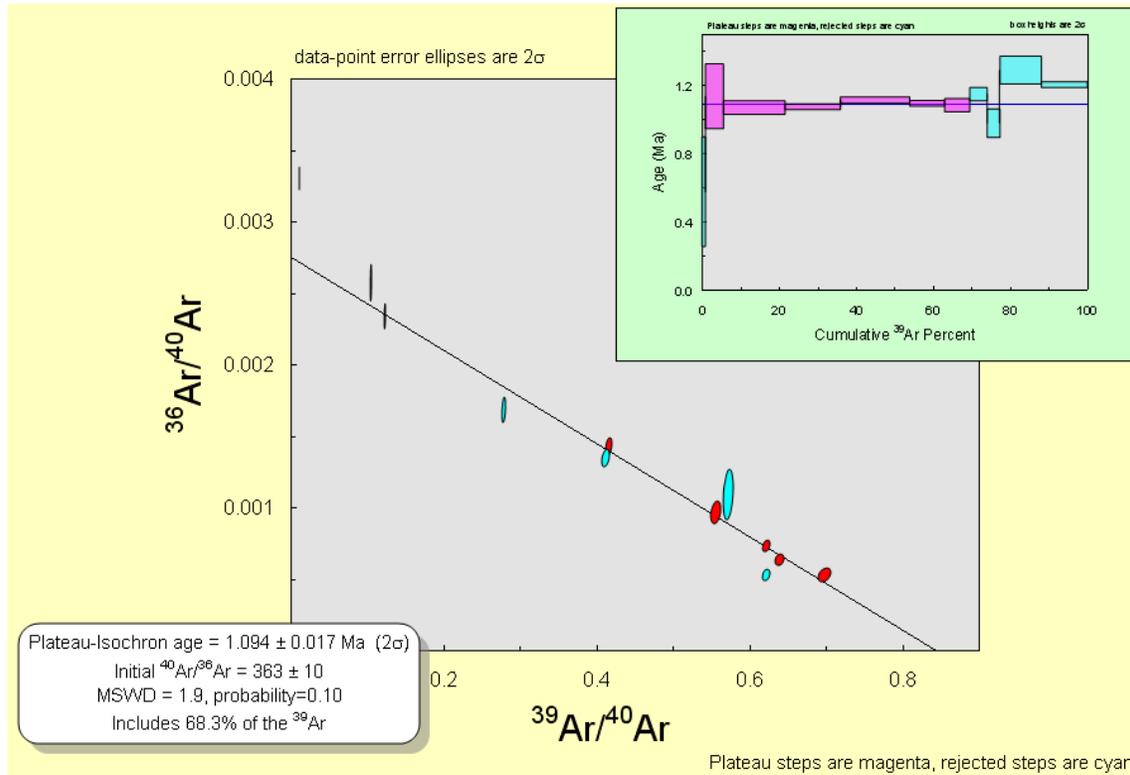


### The Argon-Argon Plateau-Isochron

If one has obtained an assemblage of isotopic analyses on argon obtained by thermally-initiated step-wise-release, the usual choice is to interpret the data via either a plateau on an Ar-Ar age spectrum, or via an argon-argon isochron constructed from the same analyses. Some workers prefer to first validate the assumption of an atmospheric composition of the trapped argon with an isochron, moving on to the plateau age only if the isochron indicates that the trapped argon cannot be statistically resolved from an atmospheric composition.

However, such a procedure is fundamentally flawed in that the resulting age is both biased (because the isochron-derived estimate of the trapped  $^{40}\text{Ar}/^{36}\text{Ar}$ , though ignored in the age plateau calculation, is never exactly atmospheric) and less precise than claimed (because the plateau calculation ignores the uncertainty in the trapped  $^{40}\text{Ar}/^{36}\text{Ar}$ ). The analyst in this case cannot argue that it is obvious (from geologic, geochemical, mineralogical considerations) that the trapped Ar is precisely atmospheric, since if that were actually the case, the analyst would not have gone to the trouble of regressing the

data on an isochron plot. In other words, a statistical penalty must be paid for even asking the question (via an isochron calculation) of whether or not the trapped  $^{40}\text{Ar}/^{36}\text{Ar}$  is atmospheric.



**Figure 9:** Graphics for the Argon-Argon Plateau-Isochron. The Isochron diagram shows the steps accepted for the isochron on the basis of their goodness-of-fit for both the isochron regression. The inset shows the stepwise-release age pattern of the same data, with ages calculated using the  $y$ -intercept of the isochron to define the trapped argon  $^{40}\text{Ar}/^{36}\text{Ar}$ .

One solution is for the analyst to iterate from age spectrum/age plateau information (to identify likely plateau-steps) to an isochron (to determine the trapped  $^{40}\text{Ar}/^{36}\text{Ar}$  and uncertainty for these steps) back to the age spectrum/age plateau and so on. However, in addition to being clumsy, the procedure is sensitive to the order in which possible plateaux are tested, as their apparent validity must change according to the assumed  $^{40}\text{Ar}/^{36}\text{Ar}$  of the trapped component. A more reliable and more straightforward approach is a hybrid "Plateau-Isochron" procedure, whose algorithm is as follows:

1. Isochron regressions for all possible combinations of sequential gas steps (e.g. 4-5-6-7 or 6-7-8-9, but not 5-7-8-9-11) which comprise at least  $N$  steps and more than  $F$  fraction of the gas, are calculated.
2. For each of these isochrons and associated suites of steps, if the probability-of-fit is greater than  $P$ , the isochron steps are taken as defining a "provisionally acceptable" age plateau.
3. The suite of "provisionally acceptable" steps comprising the most gas is selected as "best".
4. Ages and age-errors are then calculated for all of the gas-release steps, using the measured Ar isotopic ratios and assuming the trapped  $^{40}\text{Ar}/^{36}\text{Ar}$  indicated by the isochron of the "best" steps, without propagating the error in  $J$  (the neutron-flux parameter). The resulting ages and errors are then plotted on a conventional age-spectrum diagram.

5. The Plateau-Isochron age and age-error is calculated from the isochron for the "best" suite of steps, this time propagating the uncertainty in  $J$ .

In short, an Argon-Argon Plateau-Isochron age is the isochron age defined by the set of contiguous steps with the greatest amount of argon that defines a true isochron. Appropriate values for  $N$ ,  $F$ , and  $P$  are inevitably somewhat subjective. *Isoplot* uses  $N=3$ ,  $F=0.60$  (default; can be modified from the Preferences / Numeric / U-Th, Ar-Ar, Statistical dialog box) and  $P=0.05$ .

#### When is the Ar-Ar Plateau-Isochron Useful?

The Plateau-Isochron approach will be most useful for age spectra wherein most or all of the steps have relatively low  $^{40}\text{Ar}/^{36}\text{Ar}$  (say less than  $\sim 1000$ ) – most commonly for samples that are very young, very small, or low in K (or any combination of these). For many or even most types of age spectra, however, the Plateau-Isochron is not a useful tool – for example, age spectra for which:

1. All or most of the steps are extremely radiogenic (say with  $^{40}\text{Ar}/^{36}\text{Ar} > 5000$ );
2. The analytical errors are relatively small for only 2 of the steps, so that the isochron parameters are controlled by these steps and yield essentially a 2-point isochron;
3. There is reason to believe that there are multiple trapped components (though in this case, the Plateau-Isochron should still be more useful than a conventional age plateau approach assuming an atmospheric trapped component);
4. There is very little spread amongst the steps when plotted on the isochron diagram;
5. Because of any combination of (1) or (4), the  $^{40}\text{Ar}/^{36}\text{Ar}$  or  $^{36}\text{Ar}/^{40}\text{Ar}$  intercept of the isochron is poorly defined.

### Cumulative Probability Plots and Histograms

This plot-type shows the cumulative probability distribution obtained by summing the probability distributions of a suite of data with normally-distributed errors. The input range must comprise 2 columns — the values and their errors. You can also have a histogram of the data included in the plot by checking the **Include Histogram** box. You can then define the bin-width for the histogram either by checking the **Auto bins** box and specifying the number of bins to use (typically 20-50), or by specifying the bin width and the **Bin start**, which is interpreted as the lower-limit of any particular bin. In the example at left, specifying the **Bin start** as any number evenly divisible by 0.2 would give the same plot.

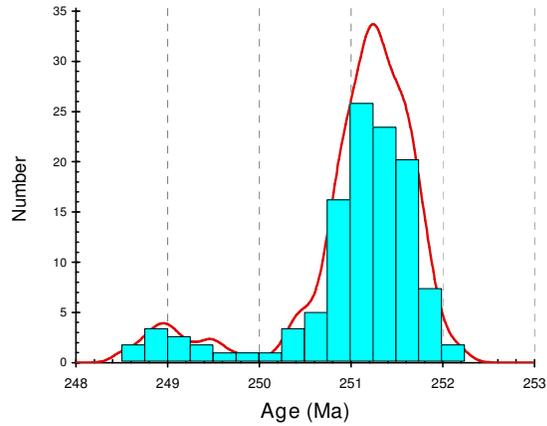
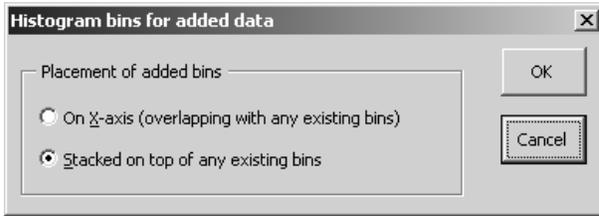


Figure 9: Cumulative Gaussian plus histogram plot



You can add data-series to an existing Cumulative Gaussian + Histogram plot, in which case *Isoplot* will automatically change the colors for each new data-series. You can also choose whether to have each new set of histogram bins start at the *x*-axis, or to be stacked on top of existing bins as in the charts below.

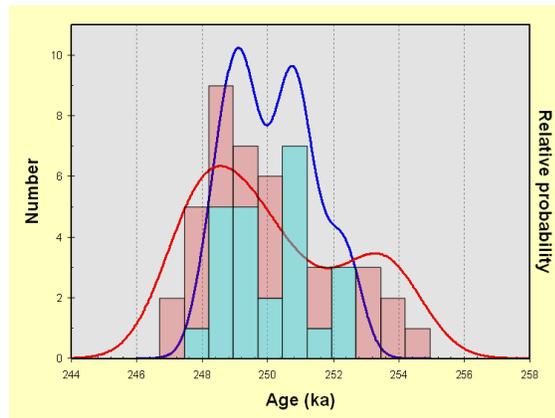
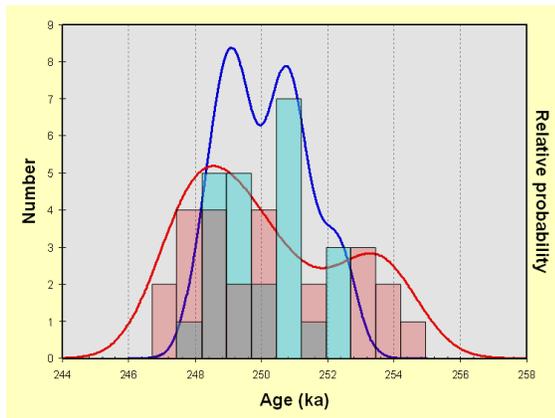


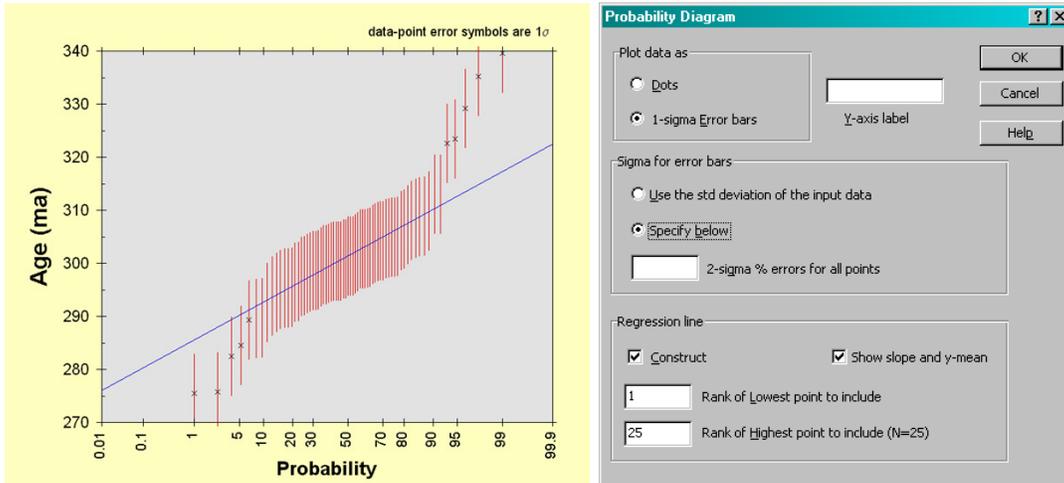
Figure 10: Cumulative Gaussian plus histogram plots for two data sets. In plot at left, histogram bins for the second data-set were placed on the *x*-axis; in plot at right, stacked on top of the bins of the first data-set.

### Probability Plots

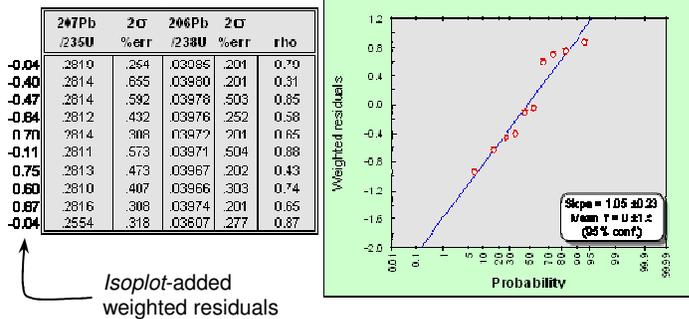
A useful visual way to evaluate whether or not a suite of data conforms to a normal distribution is to plot the data on a (linearized) Probability plot. On such a diagram, all of the data points from the same, normal distribution will be dispersed more or less along the same linear trend with a slope of 1 (Figure 10), whereas data from some different distribution (that is, outliers) will deviate distinctly above or below that linear trend at its lower or upper probability limits.

You can plot the points as dots or as 1-sigma error bars. In the latter case, you can specify the same error for all of the points (select a 1-column input range; Figure 10), or use individual data-point errors (select a 2-column input range, the second column containing the errors). A regression line through the data is optional, and if selected can be constructed from any order-contiguous subset of the data. Data excluded from the regression will be plotted with an X, as shown above. If a regression line is included and the data are to be plotted as error bars calculated from the input data, only the data specified for the regression will be used to calculate the error-bar size.

If you re-scale the Y-axis of the Probability Plot, the X-axis ticks and labels will be stranded in their original position. To put them back on the X-axis, select Rescale Filled Symbols from the *Isoplot* drop-down menu (or click on the Rescale toolbar-button).

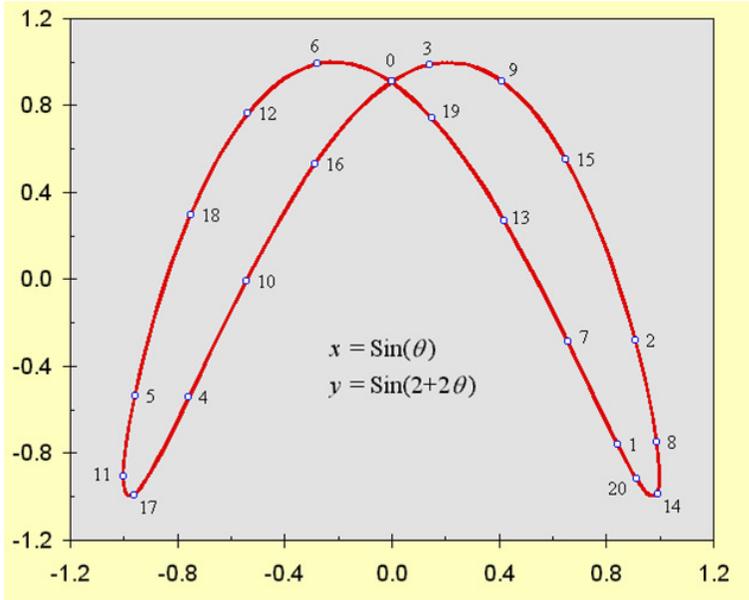


Once a data-range has been selected, a linearized probability plot can be invoked directly from the worksheet after data-selection, using the toolbar-button. If the input range includes only one column, a (small) probability plot will be generated immediately, and placed directly on the data-sheet next to the input-data range.



For all regressions (including weighted averages), *Isoplot* will place a small linearized probability plot of the regression's weighted residuals next to the input -data range if you check *Include Wtd Residuals* in the appropriate "Results" dialog box.

### Adding an Algebraically-Defined Curve to an Existing Plot



Once you've created a plot with *Isoplot*, you can easily add any curve that can be defined with *Excel's* comprehensive list of mathematical functions. With the plot sheet open, select **Add any curve** from the *Isoplot* drop-down menu (or click on the *add curve* toolbar button). You will be asked to define the curve using the dialog box shown below and, if a parametric curve, if you want ticks and tick labels included in the plot (leave the **Curve ticks** edit-boxes blank if you don't want any). If the position of the curve-tick labels isn't what you want for every label, don't worry – with a little practice, you can click and drag the individual tick-labels anywhere you want.



User-Specified Curve

Type of curve

Nonparametric  
e.g.  $Y = 0.12 + 3.4 * X - 5.6 * X^2$

Parametric  
e.g.  $X = \text{Exp}(0.155E-3 * T) - 1, Y = \text{Exp}(0.984E-3 * T) - 1$

---

Algebraic Formula

Formula for X-values, using "@" as the parametric variable

4.39+(@/3)\*3-exp(@\*0.879E-4)

e.g.  $\text{Exp}(0.984E-3 * @) - 1$

Formula for Y-values, using "@" as the parametric variable

Sin(@/3.14159)-Ln(@-7.772)

e.g.  $\text{Exp}(0.155E-3 * @) - 1$

OK

Cancel

Range of parametric variable to plot

Starting:  Ending:

Curve ticks (in parametric units)

Starting:  Interval:

Tick label position

top

left  right

bottom

The entries in the dialog box at left are just examples – they aren't the ones used to generate the plot above.

## Age Limits for a Series of Dated, Stratigraphically-Ordered Units

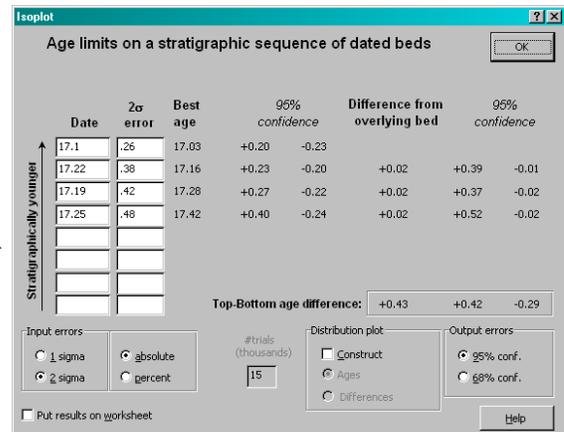
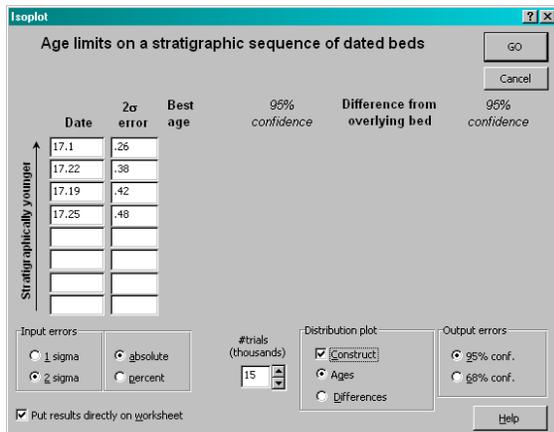
### Stratigraphically-constrained Dates with close to Gaussian uncertainties

The isotopic dates obtained on a sequence of geologic units in close stratigraphic proximity may overlap within their assigned errors. In such cases, there may even be apparent reversals of age with stratigraphy which are the logical result of the finite precision of the dates. Because the stratigraphic constraint of a decrease of age with stratigraphic height is an absolute one (provided the stratigraphy is unquestionable), this overlap can be used together with the analytical errors of the dates to increase the precision of the dates on the individual beds, using a Monte Carlo implementation of a Bayesian approach<sup>8</sup>.

Unit	Elevation (m)	Ar-Ar Date (Ma)	$\pm 2\sigma$
A	321	17.10	$\pm 0.26$
B	325	17.22	$\pm 0.38$
C	327	17.19	$\pm 0.42$
D	330	17.25	$\pm 0.48$

For example, consider the sequence of four tuffs and Ar-Ar dates at right. The apparent ages of units B and C are reversed, but within their assigned errors. We can use the stratigraphic constraints to provide

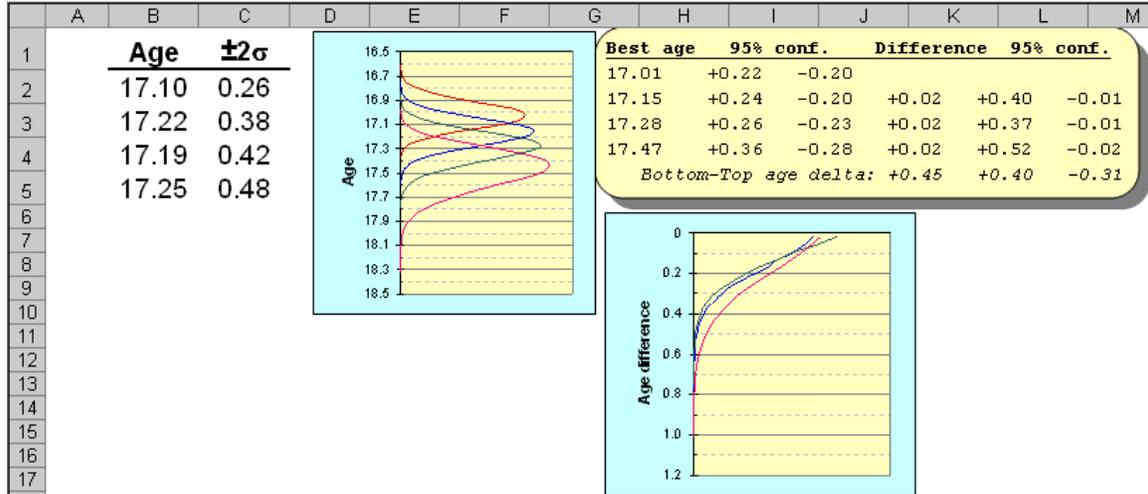
better age-estimates and tighter age uncertainties using *Isoplot's* Ages of Stacked Beds utility. Enter the ages and uncertainties into a  $4 \times 2$  (row  $\times$  column) range in a worksheet, select the range, and either click on the Stacked Beds button of the *Isoplot 3 Charts & Isochrons* toolbar, or invoke *Isoplot* and select Ages of Stacked Beds from the Isochron or Plot Type drop-down menu. Check and edit the ages and errors in the resulting dialog box, and specify the type and sigma-level of the age errors. Select the number of Monte Carlo trials for the calculation (fewer trials for faster results, more for better accuracy) and click Go. The results will either appear in the original dialog box (below) or, if the Put results directly on worksheet box were checked, directly on the worksheet next to the original data. If Construct is checked, a plot showing the probability distributions for either the ages themselves or their differences will also be added to the worksheet. As in the example (below), the uncertainties of the resulting "Best ages" will generally be somewhat better than the original analytical uncertainties on the individual dates. Note that the "Best ages" are the *mode* rather than the *mean* of the (smoothed) distribution from the Monte Carlo trials, and that it is not impossible for the "Best ages" to violate stratigraphic order if these distributions are highly skewed. The "Mean difference from overlying bed" values (the average differences in the ages for stratigraphically adjacent beds), however, will always be positive.



In addition to the differences in ages between adjacent beds, *Isoplot* will also display (numerically, but not graphically) the age difference between the top (youngest) and bottom (oldest) beds. As for all of the other

<sup>8</sup> See, for example, p. 440 of Bernardo and Smith (1994). For examples of archaeometric applications with radiocarbon dating, see Buck *et al.* (1996).

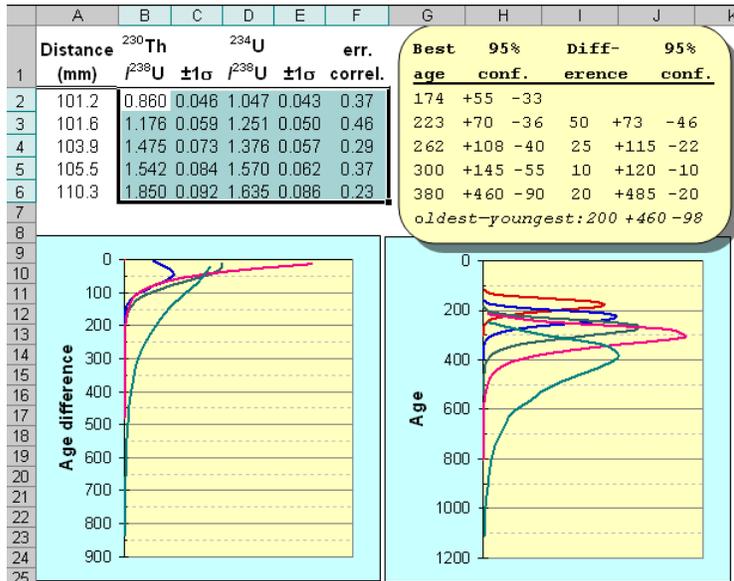
results of this calculation, the youngest-oldest age difference will be a function of *all* of the dates, not just those of the top and bottom beds.



**Figure 11:** Example of worksheet with data for the *Stacked Beds* routine after solving for best ages with both the "Put results directly on worksheet" and "Include small plot on worksheet" boxes checked. The "Age" and "Age difference plots" are both shown for illustration.

### Stratigraphically-constrained Dates from <sup>230</sup>Th/U Analyses

As mentioned earlier (p. 40), uncertainties for dates by the <sup>230</sup>Th/U method can be significantly asymmetric and non-Gaussian, especially for dates approaching the upper limit of the method (say >200 ka for alpha-spectrometric analyses, or >350 ka for TIMS or ICP-MS analyses). Because of this complication, for relatively "old" suites of <sup>230</sup>Th/U dates you should use the Ages of Stacked U-series utility instead of the Ages of Stacked Beds utility described above (you can use the *Isoplot 3 Charts & Isochrons* toolbar-button at left). The input data for Ages of Stacked U-series are the <sup>230</sup>Th/<sup>238</sup>U and <sup>234</sup>U/<sup>238</sup>U activity ratios, errors, and error correlation (see example at right). As usual, the errors can be specified as 1- or 2σ, percent or absolute. If the <sup>230</sup>Th/<sup>238</sup>U – <sup>234</sup>U/<sup>238</sup>U error correlation is small (e.g. for TIMS/ICP-MS data), it can be omitted from the data range. The results (both graphically and numerically) are displayed in a format similar to the Ages of Stacked Beds utility.



## Deconvolution of Multiple Age Components Using the Sambridge-Compston Algorithm

*Isoplot* includes a partial implementation (Gaussian distributions only) of the Sambridge and Compston (1994) "mixture modeling" method for deconvoluting a suite of dates obtained on single-crystal (or smaller) samples that contain multiple age components. *Isoplot* asks the user to specify the number of components present; starting guesses as to component age and proportion can either be made by the user or left to *Isoplot*. In the latter case, a slightly different guess is made for each trial, so the stability of any solution can be assessed by pressing the Calculate button repeatedly.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Age	±1σ														
2	136.84	0.56														
3	139.53	1.45														
4	136.45	1.13														
5	135.52	0.79														
6	131.98	0.92														
7	134.51	1.21														
8	135.57	0.54														
9	138.11	1.19														
10	135.94	0.52														
11	141.42	1.47														
12	131.55	0.67														
13	135.68	1.44														
14	131.47	1.40														
15	130.73	1.07														
16	140.61	0.67														
17	136.63	1.15														
18	136.26	0.70														
19	139.73	0.65														
20	130.06	1.15														
21	132.29	0.91														
22	135.38	0.52														
23	139.63	1.31														
24	135.50	0.76														
25	139.96	0.90														
26	130.61	0.95														
27	137.98	0.87														
28	138.75	1.39														
29	135.64	1.20														
30	140.12	0.65														
31	131.35	0.54														
32	132.77	1.06														
33	134.39	1.18														

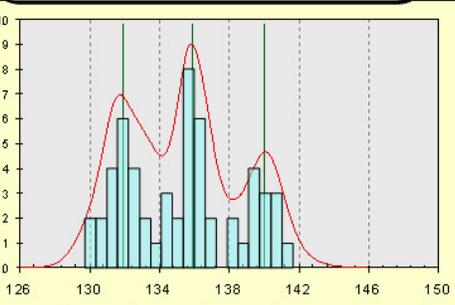
  

Age	±1σ	fraction	±1σ
131.93	0.22	0.38	0.08
135.92	0.19	0.40	0.09
140.01	0.28	0.22	---

relative misfit = 0.322

Sigma-Rho Matrix						
	f1	f2	t1	t2	t3	
f1	0.085	-0.060	0.105	0.084	0.007	
f2	-0.060	0.089	-0.094	-0.013	0.069	
t1	0.105	-0.094	.216	0.147	0.012	
t2	0.084	-0.013	0.147	.191	0.128	
t3	0.007	0.069	0.012	0.128	.278	

**Unmixing of Superimposed Gaussian Distributions**

# components:  [Calculate Again]

Let *Isoplot* guess the trial ages [Construct Output and Exit]  
 Let *me* guess the trial ages [Cancel]

Trial Age	Relative fraction	Calculated Age	±1σ	Fraction	±1σ
132.9	.479	131.93	0.22	0.38	0.08
136.6	.169	135.92	0.19	0.40	0.09
139.3	.352	140.01	0.28	0.22	---

1 sigma    absolute    1 sigma   **Relative misfit**  
 2 sigma    percent    2 sigma   **0.322**

Show numeric results with data    Include error-rho matrix with results  
 Show chart with data    Show chart as separate sheet   [Help]

To invoke the procedure, either select Unmix Ages from *Isoplot's* drop-down menu, or click on the toolbar button for Unmix Ages Using Gaussian Deconvolution. 

You must guess at the number of age components present in the mixture (*Isoplot* offers the solution for 2 components as a starting point). If you're not sure, increase the number of components until adding one either yields a negligible decrease of the Relative Misfit parameter (as defined by Sambridge and Compston, 1994), or yields two components of essentially equal age. You can guess at trial components and fractions yourself (you can leave the final fraction blank, as *Isoplot* knows that they must sum to 1), or have *Isoplot* do so for you. In the latter case, each subsequent calculation starts with a randomly different set of guessed-at component ages and fractions, so you test the stability of the solution is by repeatedly pressing the Calculate button.

If you check the Show Chart next to Data box, *Isoplot* will put a small histogram and cumulative-Gaussian curve plot next to the source-data (see above). To have a text-box containing the ages, fractions, and errors placed next to the source-data on the worksheet, check the Show Numeric Results with Data box. Check the Include Error-Rho Matrix with Results to see the full matrix of 1-sigma errors and error correlations for the various ages and fractions. Note that there is no error associated with the fraction of the last component, since by definition its value is 1 minus the sum of the fractions of the other components.

The Sambridge-Compston algorithm can produce surprisingly accurate and precise results, but only when: (1) the number of components can be specified *a priori* with reasonable confidence, and (2) the errors of the input-data are accurate and truly Gaussian. When one or both of these conditions are absent, the method is best suited for *qualitative* exploration and evaluation of data.

### Youngest Zircon in a Suite of Detrital Zircons

Given a suite of (usually U-Pb) dates on a large number of zircon crystals, it is often useful to know what the youngest true age is of the suite. If one can assume that:

- The errors assigned to each date are normally distributed as well as accurate, and
- The analyzed crystals all come from the same sample – that is, no contamination during mineral separation or mounting has occurred,

then one of the few (or perhaps only) approaches that can be statistically justified is to ::

1. Perturb each date randomly by its (Gaussian) assigned error,
2. Select the youngest of the suite of perturbed dates,
3. Repeat steps 1-2, say, 10,000 times,
4. Sort the suite of 10,000 youngest dates,
5. From this sorted set of youngest dates, select the mode (or mean, if desired), upper limit on the mode (i.e. the date for which only 2.5% of the youngest dates are older), and the lower limit on the mode (i.e. the date for which only 2.5% of the youngest dates are younger)
6. Use the mode (or mean) as the best estimate of the youngest age, with the upper/lower limits defining the uncertainties at 95% confidence.

If you want to take into account the possibility of contamination by younger zircons during mineral separation, select the degree of contamination that you want to guard against using the "Change degree of "youngest" spin-button (right), then click OK again.

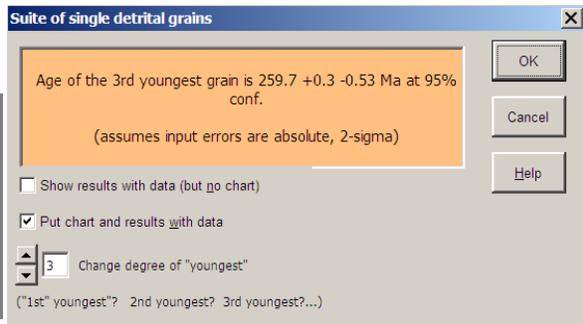


Figure 11: The *Youngest detrital zircon* routine results-box.

For rather large suites of analyses (say >50), you can speed up the calculation by selecting only those grains whose dates obviously cannot overlap with any reasonable credible guess at the youngest age at, say, the 4-sigma error level. Thus in the example below, selecting only those grains younger than, say, 120 Ma should produce the same result as selecting all grains, with a several-fold decrease in calculation time.

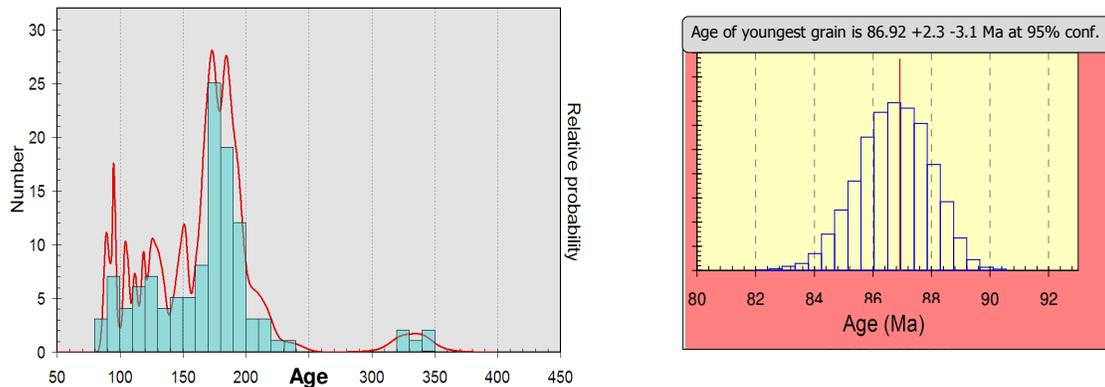


Figure 12: *Left:* Distribution of dates for a suite of detrital zircons. *Right:* Isoplot's output for youngest detrital grain. Vertical red line shows mode, blue boxes show distribution of Monte Carlo simulations.

## Utility Functions for Isotopic Data

Many of the numeric routines used by *Isoplot* are made available to the user as a set of additional spreadsheet functions, which can be used like any other *Excel* function. For example, to insert the  $^{207}\text{Pb}/^{206}\text{Pb}$  age of the  $^{207}\text{Pb}/^{206}\text{Pb}$  ratio in cell G3 into cell H3, just enter =AgePb76(G3) into cell H3, where AgePb76 is one of the *Isoplot* “user-defined” functions (in this case, “user” is me, not you). Note that for functions that return errors, where the level of the input errors can be specified as either  $1\sigma$  or  $2\sigma$ , the default input errors are always  $2\sigma$  and the default output errors are always  $2\sigma/95\%$ -conf.

### Accessing Isoplot’s User Functions

Press the Function button on the Standard Toolbar (the button containing the  $f_x$  symbol). Select *User Defined* from the Function Wizard’s Function Category. The list at the right will show the *Isoplot* functions available, with a brief description of each function at the bottom (as the cursor is moved). Select the desired function, click NEXT. A dialog box with more-detailed explanation will appear, in which you can enter the required arguments as either numeric values (e.g. 1.234), calculated values (e.g. 123.4/100) or ranges (e.g. D5). As soon as you have entered the required arguments, the result of the function will appear at the upper-right of the Function Wizard. When you click Finish, your entries will appear on the Formula line of *Excel*.

Once you already know how the function works and the arguments it requires, you can use it like any other *Excel* function – for example, entering

=AgePb76(0.123)

will calculate the  $^{207}\text{Pb}/^{206}\text{Pb}$  age for the ratio 0.123. When a function requires the use of geochemical constants such as decay constants, *Isoplot* will use the constants defined in the Options/Consts screen.

Because you won’t be able to remember the syntax of all of *Isoplot*’s functions, one of the best ways to invoke a function is to first type in its name in the relevant cell, e.g.

=AgeErPb76

then press the  $f_x$  symbol in either the formula bar or one of the toolbars. If you typed the function name in correctly, *Excel* will present a dialog box in which you can enter the function’s arguments, e.g.

**Function Wizard - Step 2 of 2**

**AgeErPb76** Value: 2.535250518

Error in Pb7/6 age, input err is abs. 2sigma unless SigmaLevel=1 or PercentErrsIn=True.  
t2 is end of Pb growth (default=0); output errs always 2sigma.

**Pb76rad (required)**

Pb76rad	<input type="text" value=".08432"/>	0.08432
Pb76er	<input type="text" value=".00011"/>	0.00011
t2	<input type="text"/>	
withLambdaErrs	<input type="text" value="FALSE"/>	FALSE
SigmaLevel	<input type="text" value="2"/>	2

Buttons: Help, Cancel, < Back, Next >, Finish

Some of the *Isoplot* functions are *array* functions, which are a bit tricky to use. The output of an array function occupies a range of cells rather than a single cell, so you need to know in advance how large a range to select before invoking the array function. For example, the worksheet output for the WtdAv function looks like:

25.159	Wtd Mean (using ext. err)
0.029	95%-conf. err. of mean
0.051	Required external 2-sigma
1.873	MSWD
1	#rejected
0.059	Probability of fit

with the numeric output in the left column of the 6-row by 2-column range and the explanation (which is part of the function output) in the right. You could select a smaller range — for example 6 rows by 1 column — in which case the explanation column would not be shown.

To enter an array function, select the output range as discussed above, type in the equals sign followed by the function name and arguments (or use the function wizard), then press *Ctrl-Shift-Return* instead of simply *Return*.

If you create a workbook with *Isoplot* functions on one computer and open a copy of that workbook on another, the second computer's *Excel* must also have *Isoplot* loaded. In addition, you must update the references to the *Isoplot* functions using the *Renew Isoplot References* toolbar-button.



## Uranium-Lead Functions

### Age7corr (TotPb6U8, TotPb76, Comm76)

Returns the “207-corrected age” often-used by SHRIMPsters. Variables are the total (that is, uncorrected for common Pb)  $^{238}\text{U}/^{206}\text{Pb}$  and  $^{207}\text{Pb}/^{206}\text{Pb}$ , and the assumed common  $^{207}\text{Pb}/^{206}\text{Pb}$ . The age returned is calculated by assuming that the true radiogenic  $^{238}\text{U}/^{206}\text{Pb}$  and  $^{207}\text{Pb}/^{206}\text{Pb}$  ages are precisely concordant.

### Age8Corr (TotPb6U8, TotPb8Th2, Th2U8, CommPb68)

Returns the “208-corrected age”, also mainly used by SHRIMPkins. Variables are the total (that is, uncorrected for common Pb)  $^{238}\text{U}/^{206}\text{Pb}$  and  $^{208}\text{Pb}/^{232}\text{Th}$ , and the assumed common  $^{206}\text{Pb}/^{208}\text{Pb}$ . The age returned is calculated by assuming that the true radiogenic  $^{238}\text{U}/^{206}\text{Pb}$  and  $^{208}\text{Pb}/^{232}\text{Th}$  ages are precisely concordant.

### AgeEr7Corr (Age, TotPb6U8, TotPb6U8err, TotPb76, TotPb76err, CommPb76, CommPb76err)

Returns the error in the “207-corrected age” calculated by Age7corr. Variables are the 207-corrected age, total  $^{238}\text{U}/^{206}\text{Pb}$ , error, total  $^{207}\text{Pb}/^{206}\text{Pb}$ , error, common-Pb  $^{207}\text{Pb}/^{206}\text{Pb}$ , error. Because the sigma-level of input errors is unspecified, the output error is at same sigma-level as the input error.

### AgeEr8Corr (T, TotPb6U8, TotPb6U8err, TotPb8Th2, TotPb8Th2err, Th2U8, Th2U8err, CommPb68, CommPb68err)

Returns the error in the “208-corrected age” calculated by Age8corr. Variables are the 208-corrected age, total  $^{238}\text{U}/^{206}\text{Pb}$ , error, total  $^{208}\text{Pb}/^{232}\text{Th}$ , error, common-Pb  $^{206}\text{Pb}/^{208}\text{Pb}$ , error. Because sigma-level of input errors is unspecified, output error is at same sigma-level as input error.

### AgeErPb76 (Pb76rad, Pb76er, Optional t2, Optional withLambdaErrs, Optional SigmaLevel, Optional PercentErrsIn)

Returns the error in the  $^{207}\text{Pb}/^{206}\text{Pb}$  age calculated by AgePb76 (also available via *Isoplot*'s toolbar button: see p. 66) Required variables are the radiogenic  $^{207}\text{Pb}/^{206}\text{Pb}$  and error (absolute or percent); optional variables are:



t2	The time at which Pb-isotope evolution ceased, zero if unspecified;
withLambdaErrs	TRUE if the $^{238}\text{U}$ and $^{235}\text{U}$ decay-constant errors are to be propagated in the age-error calculation, FALSE if unspecified;
SigmaLevel	Relevant only if withLambdaErrs=TRUE; 2 if unspecified; must be either 1 or 2;
PercentErrsIn	If Pb76er is in percent, must be TRUE.

Output errors are always  $2\sigma$  (even if input is  $1\sigma$ ), absolute.

### AgePb6U8 (Pb6U8)

Returns the  $^{206}\text{Pb}/^{238}\text{U}$  age. Input is the radiogenic  $^{206}\text{Pb}/^{238}\text{U}$ .

**AgePb76** (Pb76rad, Optional t2)

Returns the classical  $^{207}\text{Pb}/^{206}\text{Pb}$  age (also available via *Isoplot*'s toolbar button: see p. 66). Variables are the radiogenic  $^{207}\text{Pb}/^{206}\text{Pb}$  and the time at which the system ceases to evolve (zero if not specified).

**AgePb7U5** (Pb7U5)

Returns the  $^{207}\text{Pb}/^{235}\text{U}$  age. Input is the radiogenic  $^{207}\text{Pb}/^{235}\text{U}$ .

**AgePb8Th2** (Pb208Th232)

Returns the  $^{208}\text{Pb}/^{232}\text{Th}$  age. Input is the radiogenic  $^{208}\text{Pb}/^{232}\text{Th}$ .

**Concordia** (Pb7U5, Pb7U5err, Pb6U8, Pb6U8err, ErrCorrel, Optional withLambdaErrs, Optional PercentErrs, Optional SigmaLevel)

An array function that returns the “Concordia” age for the conventional-Concordia ratios, errors, & error-correlation (see Ludwig, 1998). Input values are  $^{206}\text{Pb}^*/^{238}\text{U}$ , error,  $^{207}\text{Pb}^*/^{235}\text{U}$ , error, error-correlation, withLambdaErrs (TRUE to propagate the  $^{235}\text{U}$  and  $^{238}\text{U}$  decay-constant errors), and two optional Boolean variables (PercentErrs and SigmaLevel specifying the type of error input (default is absolute,  $2\sigma$ ). Output is a 2-row x 4-col range containing the Concordia Age,  $2\sigma$  *a priori* age error, MSWD, and probability-of-concordance. The second row of cells contains captions for the values in the first row. Remember that the *a priori* error propagates only the assigned  $^{206}\text{Pb}/^{238}\text{U}$  and  $^{207}\text{Pb}/^{206}\text{Pb}$  errors, and so is invalid/irrelevant for low probabilities. For Tera-Wasserburg Concordia data, use ConcordiaTW.

**ConcordiaTW** (U8Pb6, U8Pb6 err, Pb76, Pb76 err, Optional ErrCorrel, Optional withLambdaErrs, Optional PercentErrs, Optional SigmaLevel)

Same as the Concordia function, but with Tera-Wasserburg Concordia ratios.

**ConvertConc** (InputRange, TeraWassIn, Optional PercentErrs)

An array function that converts Tera-Wasserburg concordia ratios, errors, and error correlations to Conventional concordia ratios, errors, and error correlations — or vice-versa. The input ratios can be either 2-dimensional ( $X=^{238}\text{U}/^{206}\text{Pb}$ ,  $Y=^{207}\text{Pb}/^{206}\text{Pb}$  to/from  $X=^{207}\text{Pb}/^{235}\text{U}$ ,  $Y=^{206}\text{Pb}/^{238}\text{U}$ ) or 3-dimensional ( $X=^{238}\text{U}/^{206}\text{Pb}$ ,  $Y=^{207}\text{Pb}/^{206}\text{Pb}$ ,  $Z=^{204}\text{Pb}/^{206}\text{Pb}$  to/from  $X=^{207}\text{Pb}/^{235}\text{U}$ ,  $Y=^{206}\text{Pb}/^{238}\text{U}$ ,  $Z=^{204}\text{Pb}/^{238}\text{U}$ ).

For converting Tera-Wasserburg ratios to Conventional ratios (TeraWassIn = TRUE), the input range must be structured as:

$X$ ,  $X$ -error,  $Y$ ,  $Y$ -error [ $\rho_{xy}$ ] for 2-dimensional data, or as  
 $X$ ,  $X$ -error,  $Y$ ,  $Y$ -error,  $Z$ ,  $Z$ -error or as  
 $X$ ,  $X$ -error,  $Y$ ,  $Y$ -error,  $\rho_{xy}$ ,  $Z$ ,  $Z$ -error [ $\rho_{xz}$ ,  $\rho_{yz}$ ]

for 3-dimensional data, where  $\rho_{xy}$  is the  $X$ - $Y$  error correlation, and the brackets indicate an optional parameter.

For converting Conventional ratios to Tera-Wasserburg ratios (TeraWassIn = FALSE), the input-range must be

$X$ ,  $X$ -error,  $Y$ ,  $Y$ -error,  $\rho_{xy}$  for 2-dimensional data, or as  
 $X$ ,  $X$ -error,  $Y$ ,  $Y$ -error,  $\rho_{xy}$ ,  $Z$ ,  $Z$ -error,  $\rho_{xz}$ ,  $\rho_{yz}$

for 3-dimensional data. The output range is always

$X$ ,  $X$ -error,  $Y$ ,  $Y$ -error,  $\rho_{xy}$  [ $Z$ ,  $Z$ -error,  $\rho_{xz}$ ,  $\rho_{yz}$ ]

The errors can be input either as absolute (default) or percent (add TRUE as a third parameter). Output errors are the same form as input errors.

**DisEq68age** (Pb206U238, init234238ar, init230238ar)

Returns the  $^{206}\text{Pb}/^{238}\text{U}$  age (in Ma) for the specified  $^{206}\text{Pb}^*/^{238}\text{U}$  ratio, and initial  $^{234}\text{U}/^{238}\text{U}$  and  $^{230}\text{Th}/^{238}\text{U}$  activity ratios.

**DisEq68ratio** (AgeMa, init234238ar, init230238ar)

Returns the  $^{206}\text{Pb}^*/^{238}\text{U}$  ratio for the specified age (in Ma), and initial  $^{234}\text{U}/^{238}\text{U}$  and  $^{230}\text{Th}/^{238}\text{U}$  activity ratios.

**DisEq75age** (Pb207U235, init231235ar)

Returns the  $^{207}\text{Pb}/^{235}\text{U}$  age (in Ma) for the specified  $^{207}\text{Pb}^*/^{235}\text{U}$  ratio and initial  $^{231}\text{Pa}/^{235}\text{U}$  activity ratio.

**DisEq75ratio** (AgeMa, init231235ar)

Returns the  $^{207}\text{Pb}^*/^{235}\text{U}$  ratio for the specified age (in Ma) and initial  $^{231}\text{Pa}/^{235}\text{U}$  activity ratio.

**DisEq76ratio** (AgeMa, init234238ar, init230238ar, init231U235ar)

Returns the  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ratio for the specified age (in Ma) and initial  $^{234}\text{U}/^{238}\text{U}$ ,  $^{230}\text{Th}/^{238}\text{U}$ , and  $^{231}\text{Pa}/^{235}\text{U}$  activity ratios.

**DisEqPbPbAge** (R76, Init234238ar, Init230238ar, Init231235ar)

Returns the  $^{207}\text{Pb}/^{206}\text{Pb}$  age (in Ma) for the specified  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ratio and initial  $^{234}\text{U}/^{238}\text{U}$ ,  $^{230}\text{Th}/^{238}\text{U}$ , and  $^{231}\text{Pa}/^{235}\text{U}$  activity ratios.

**La232** ( )

Returns the  $^{232}\text{Th}$  decay constant, in decays per year per atom, as specified in *Isoplot's* **Consts** dialog box.

**La235** ( )

Returns the  $^{235}\text{U}$  decay constant in decays per year per atom, as specified in *Isoplot's* **Consts** dialog box.

**La238** ( )

Returns the  $^{238}\text{U}$  decay constant in decays per year per atom, as specified in *Isoplot's* **Consts** dialog box.

**Pb76** (AgeMa)

Returns the radiogenic  $^{207}\text{Pb}/^{206}\text{Pb}$  ratio for the specified age, assuming initial secular equilibrium of the radioactive uranium daughters.

**SingleStagePbMu** (Pb206Pb204, Pb207Pb204)

Returns the Mu-value defined by the specified  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$ , assuming single-stage Pb-isotope evolution using the Stacey and Kramers (1975) parameters.

**SingleStagePbR** (Age, WhichRatio)

Returns the  $^{206}\text{Pb}/^{204}\text{Pb}$ ,  $^{207}\text{Pb}/^{204}\text{Pb}$ , or  $^{208}\text{Pb}/^{204}\text{Pb}$  ratio (WhichRatio = 0, 1, 2, respectively) for the specified age, assuming single-stage Pb-isotope evolution using the Stacey and Kramers (1975) parameters.

**SingleStagePbT** (Pb206Pb204, Pb207Pb04)

Returns the age defined by the specified  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$ , assuming single-stage Pb-isotope evolution using the Stacey and Kramers (1975) parameters.

**U238U235** ( )

Returns the present-day natural  $^{238}\text{U}/^{235}\text{U}$  atomic ratio (e.g. 137.88) as specified in *Isoplot's* **Consts** dialog box.

## Uranium Series Functions

### AlphaMS (Ratios, Optional PercentErrs)

An array function that converts Osmond-type U-series isochron ratios ( $X=^{238}\text{U}/^{232}\text{Th}$ ,  $Y=^{230}\text{Th}/^{232}\text{Th}$ ,  $Z=^{234}\text{U}/^{232}\text{Th}$ ) to Rosholt-type ratios ( $X=^{232}\text{Th}/^{238}\text{U}$ ,  $Y=^{230}\text{Th}/^{238}\text{U}$ ,  $Z=^{234}\text{U}/^{238}\text{U}$ ). “Ratios” is a 6- or 9-cell range of X, x-error, Y, y-error, Z, Z-error [,  $\rho_{xy}$ ,  $\rho_{xz}$ ,  $\rho_{yz}$ ]. The error correlations ® are optional, *but should always be included when converting from Rosholt to Osmond ratios*. Errors are assumed to be in percent, unless the optional PercentErrs parameter is FALSE.

Output is a 9-cell range containing the converted X, x-error, Y, y-error, Z, Z-error,  $\rho_{xy}$ ,  $\rho_{xz}$ ,  $\rho_{yz}$ , with the errors in the same form as the input errors.

### CorrThU (Detritus, Sample, Optional PercentIn, Optional PercentOut)

An array function that corrects measured  $^{230}\text{Th}$ - $^{232}\text{Th}$ - $^{234}\text{U}$ - $^{238}\text{U}$  ratios for a detrital component, using  $^{232}\text{Th}$  as an index isotope. Detritus is a 6- or 9-cell range containing  $^{232}\text{Th}/^{238}\text{U}$ , err,  $^{230}\text{Th}/^{238}\text{U}$ , err,  $^{234}\text{U}/^{238}\text{U}$ , err (all as activity ratios) and, optionally, the error correlations for  $^{230}\text{Th}/^{238}\text{U}$ - $^{232}\text{Th}/^{238}\text{U}$ ,  $^{234}\text{U}/^{238}\text{U}$ - $^{230}\text{Th}/^{238}\text{U}$ , and  $^{234}\text{U}/^{238}\text{U}$ - $^{232}\text{Th}/^{238}\text{U}$  (assumed to be zero if not specified). Sample is another 6- or 9-cell range with the same ratios, but for a measured, detritally-contaminated sample. The two optional Boolean variables specify the form of the input and output errors (default is FALSE for both). Output is a 5-cell row containing the detritus-corrected  $^{230}\text{Th}/^{238}\text{U}$ , error,  $^{234}\text{U}/^{238}\text{U}$ , error, error-correlation.

### InitU234U238 (AgeKyr, U234U238ar)

Returns the initial  $^{234}\text{U}/^{238}\text{U}$  activity ratio for the specified age (in kiloyears) and present-day  $^{234}\text{U}/^{238}\text{U}$  activity ratio.

### Th230238ar (AgeKyr, InitialU234U238ar)

Returns the  $^{230}\text{Th}/^{238}\text{U}$  activity ratio for a closed system of AgeKyr kiloyears with an initial  $^{234}\text{U}/^{238}\text{U}$  activity-ratio of InitialU234U238ar.

### Th230Age (Th230U238ar, U234U238ar)

Returns the age in kiloyears for a closed system with present-day activity ratios for  $^{230}\text{Th}/^{238}\text{U}$  and  $^{234}\text{U}/^{238}\text{U}$  of Th230U238ar and U234U238ar.

### Th230AgeAndInitial (Th230U238, Th230Err, U234U238, U234Err, Optional RhoThU, Optional PercentErrs, Optional SigmaLevel, Optional WithLambdaErrs, Optional AtomRatios)

An array function whose input are the  $^{230}\text{Th}/^{238}\text{U}$ , error,  $^{234}\text{U}/^{238}\text{U}$ , error, and error-correlation (in activity ratios) of a closed-system sample. If the error correlation is not specified, it is assumed to be zero (OK for mass-spectrometric, but *not* for alpha-spectrometric analyses). By default, the errors are assumed to be absolute,  $2\sigma$ ; use the optional, Boolean PercentErrs and SigmaLevel to specify otherwise. If withLambdaErrs is specified as *TRUE*, the  $^{230}\text{Th}$  and  $^{234}\text{U}$  decay-constant errors will be propagated in the age-error calculation (default is without decay-constant errors). If the activity ratios were calculated by multiplying measured atomic ratios times the decay-constant ratios, you must specify AtomRatios as *TRUE* to correctly propagate the decay-constant errors.

### U234age (U234U238ar, InitialAR)

Returns the  $^{234}\text{U}/^{238}\text{U}$  age, in ka, for the specified present-day and initial  $^{234}\text{U}/^{238}\text{U}$  activity ratios.

### U234U238ar (AgeKyr, InitialU234U238ar)

Returns the present-day  $^{234}\text{U}/^{238}\text{U}$  activity ratio for the specified age, in ka, and initial  $^{234}\text{U}/^{238}\text{U}$  activity ratio.

## Other Radiogenic-Isotope Functions

### **Lambda** (RadiogenicNuclideMass)

Returns the decay constant (in decays/year/atom) of the geochronologically-useful nuclide with that (integral) mass. For example, `Lambda(147)` returns the decay constant of  $^{147}\text{Sm}$ .

### **HalfLife** (RadiogenicNuclideMass)

Returns the half life (in years) of the geochronologically-useful nuclide with that (integral) mass. For example, `HalfLife(147)` returns the half life of  $^{147}\text{Sm}$ .

### **ModelAge** (RockParent, RockRad, Optional Mtype, Optional Depleted, Optional SourceParent, Optional SourceRad, Optional DecayConst)

Returns an Rb/Sr, Sm/Nd, Re/Os, or Lu/Hf model age (Mtype = 1 to 4, respectively; default = Sm/Nd). The two required arguments are the parent-isotope and radiogenic-isotope ratios of the rock, relative to the daughter-element normalizing-isotope (e.g.  $^{147}\text{Sm}/^{144}\text{Nd}$  and  $^{143}\text{Nd}/^{144}\text{Nd}$ ); Mtype specifies what system (default is Sm/Nd); Depleted specifies calculation of a depleted-mantle age; SourceParent and SourceRad are the corresponding ratios for the source; DecayConst is the decay constant of the parent isotope, in decays per year. If Depleted is specified, Mtype must be 2 (=Sm/Nd), the DePaolo (1981) quadratic constants are used, and the function becomes an array function whose 1x3-cell output is the depleted-mantle age, initial ratio, and Epsilon CHUR (assuming that the Source ratios are CHUR ratios). If SourceRad, SourceParent, or DecayConst are unspecified, the stored *Isoplot* values are used (from the Options/Consts dialog box).

## Statistical Functions

### **Biweight** (NumRange, Optional Tuning)

An array function that returns the Tukey's biweight robust mean, "sigma", and 95%-conf. error in a 3-row x 2-col range (the right-hand column contains captions for the 3 numbers). NumRange is the Worksheet range containing the data to be averaged; Tuning affects how robust the algorithm is against outliers, and must be either 9 (default) or 6 (more robust). The biweight mean self-weights the points according to their deviation from the (robust) mean; values more than Tuning deviations from the mean are ignored. The 95%-conf. error returned is only valid for slightly-contaminated normal distributions.

### **ChiSquare** (MSWD, DegFree As Integer)

Returns the "probability of fit" for a regression.  $\chi^2$  is the Mean Square of Weighted Deviates (expectation=1 if the assigned data-point errors are the only cause for scatter in the regression), DegFree is the degrees of freedom in the regression (e.g.  $N-1$  for a 1-dimensional weighted average,  $N-2$  for a 2-dimensional linear regression...). The result is the probability that the assigned data-point errors will yield the observed amount of scatter or more.

### **GaussCorr** (X, SigmaX, Y, SigmaY, RhoXY)

An array-function that generates a pair of X-Y values with random, Gaussian distributions about the specified errors, with the specified error correlation. Output is a 2-cell range in the same row.

### **Gaussian** (Mean, Sigma)

Generates a random, Gaussian-distributed value with the specified mean and standard deviation.

### **MAD**(Values)

Returns the Median Absolute Deviation from the Median. The MAD is a robust estimator of variability — use MAD with medians in the same way that standard deviations are used with averages.

### **StudentsT** (DegFree)

The Students-*t* value for the specified degrees of freedom (2-tailed, 5% confidence).

**WtdAv** (ValuesAndErrors, Optional PercentOut, Optional PercentIn, Optional SigmaLevel, Optional CanReject, Optional ConstantExternalErr)

An array function that returns the error-weighted mean of a set of values and assigned errors. The required argument ValuesAndErrors must be a range that includes the measured values in the left-hand column, and their associated errors in an immediately adjacent right-hand column. The errors are assumed to be  $2\sigma$ , absolute unless the optional PercentIn and SigmaLevel arguments specify otherwise. Similarly, the output error will be absolute, unless the optional PercentOut variable is *TRUE* (output errors are always  $2\sigma$ /95%-confidence). If the optional CanReject is *TRUE*, outliers will be identified and rejected. Weighting of the data points is by the inverse-square of their errors, unless 1) the probability-of-fit is less than 15%, and 2) the optional ConstantExternalErr is *TRUE*. Also invocable (in modified form) from *Isoplot's* toolbar button.

For ConstantExternalErr weighting, the data are assumed to scatter because of a combination of the assigned errors and some unknown but constant error. The constant ("external") error that, together with the assigned errors, would yield an MSWD=1 is found iteratively, and the data-points appropriately reweighted.

For ConstantExternalErr weighting, or if the probability-of-fit from the assigned errors is less than 10%, the error of the mean includes a Student's-*t* factor, as well as the square root of the MSWD (since the assigned errors are unlikely to be responsible for the observed scatter).

Output is a 2-column x 6-row (internal-error weighting) or 2-column x 7-row (weighting by internal+external errors) range, where the left column contains values and the right column the captions for the output. If CanReject, is *TRUE*, the sixth or seventh row in the output range contains the index numbers of any rejected values in the input range.

**xyWtdAv** (XYrange, Optional PercentErrors, Optional SigmaLevel)

An array function that calculates the weighted mean of a set of *N* measured X-Y data pairs whose errors are more or less correlated, using the algorithm given in Ludwig (1998). Input is an *N*-row by 5-column range containing X, X-error, Y, Y-error, Error-correlation. By default, the errors are absolute,  $2\sigma$ . Use the optional PercentErrors and SigmaLevel arguments to specify otherwise.

Output is either 1 or 2 rows of up to 7 columns. The first row contains: Mean X,  $2\sigma$  error, Mean Y,  $2\sigma$  error, Error correlation of mean X-Y pair, MSWD, Probability-of-fit. The second row contains captions for these values. Note that the output errors are *a priori* errors — that is, they are propagated from the input errors only, and ignore the actual scatter from a single X-Y point. Obviously, when the probability-of-fit becomes small (say less than 5%), the data-points are *not* equivalent, and the *a priori* errors are an irrelevant underestimate.

**YorkSlope** (xyValuesAndErrs, Optional PercentErrors, Optional SigmaLevel)

Returns the slope of the *x-y* error-weighted regression ("Yorkfit"; York, 1969 – but see also the "put Yorkfit" function described on p.68) of the xyValuesAndErrs range. This range must be a contiguous set of cells whose columns contain, in order, the *x* values, *x* errors, *y* values, *y* errors, and (optional) *x-y* error correlation (if the latter is omitted, it is assumed to be zero). The *x-y* errors are assumed to be at the  $1\sigma$  level and absolute, unless the optional PercentErrors and SigmaLevel parameters specify otherwise. If specified, PercentErrors must be either True or False.

**YorkSloperErr95**

**YorkInter**

**YorkInterErr95**

**YorkMSWD**

**YorkProb**

All have the same input parameters as YorkSlope, and return other parameters of the same 2-error regression. The errors (YorkSloperErr95 and YorkInterErr95) are returned at the  $2\sigma$  level, propagated from the *x-y* input-errors alone, if the probability-of-fit of the regression is greater than 15%. If the probability-of-fit of the regression (YorkProb) as calculated from its MSWD (YorkMSWD) is less than 15%, the slope and intercept errors are expanded by Student's-*t*  $\times \sqrt{\text{MSWD}}$  and thus returned at the 95%-confidence level.

## **Rounding Functions**

### **Drnd** (Number, SigFigs As Integer)

Returns Number rounded to SigFigs significant figures.

### **Ernd** (Value, PlusOrMinus, Optional Short)

Returns Value whose significant figures are justified by its error, PlusOrMinus, at 3 significant figures for the latter. Specify Short = TRUE if you want only 2 significant figures.

## **Acknowledgments**

*Isoplot* uses several algorithms that were adapted or extended from other sources. The Model 1 Yorkfit is, of course, modified from York (1969), except that errors are calculated using the maximum-likelihood estimation algorithm of Titterton and Halliday (1979). The Model 2 Yorkfit is a modification of the “equal weight” model of McSaveney (Faure, p. 427-434). The Tukey’s Biweight algorithm is from Hoaglin and others (1983), except for the 95%-confidence error-estimator (based on Monte Carlo simulations by KRL). The planar-fit solution uses the algorithm of Kent and others (1990, with corrections for typographical errors), and the solution for unconstrained 3-D linear regressions would not have been possible without the help of Michael Titterton. Regressions for 3-D lines and Total-Pb/U Isochrons make use of a downhill simplex algorithm modified from Press and others (1987), from which the one-dimensional minimization algorithm used by the Concordia Age solution was also adapted. This material is based upon work supported in part by the National Science Foundation under Grants No. 22719 and 0125705, and also by the Ann and Gordon Getty Foundation. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author and do not necessarily reflect the views of the National Science Foundation.

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### **Appendix I: Tips on Minimizing Plot-Construction Time**

- Use **Filled Symbols** instead of outline symbols for error ellipses and error boxes;
- Leave **Minimum Sheet Margins** unchecked (Options/Lines);
- Leave **Superscript Isotopes In Axis Labels** unchecked (Options/Fonts);
- Leave **Show Results With Data** and **Show Results With Plot** unchecked;
- Leave **Rescale When Done** unchecked (Preferences/Graphics/Lines);
- Select **Coarse Error Ellipses & Curves** from Options/Lines (generally a small effect on speed).

### Appendix II: Toolbar-Only Functions

Four of the toolbar buttons in the *Isoplot* toolbar offer functions that can only be accessed via these buttons. All of these four buttons put results of an operation on a range immediately on the worksheet.



Places the  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ages corresponding to the  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ratios of the selected range one column to the right of the selected range. The selected range can be a single cell or a columnar-range of cells. For example, if the selected input range were

0.1142
0.1058
0.1079
0.1091
0.1148
0.1154
0.1128
0.1151
0.1069

the result would look like

0.1142	1868
0.1058	1728
0.1079	1765
0.1091	1785
0.1148	1878
0.1154	1887
0.1128	1845
0.1151	1881
0.1069	1747



Places the  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ages and age-errors corresponding to the  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ratios and ratio-errors of the selected range one column to the right of the selected range. The selected range must be two columns of cells where the left-hand column contains  $^{207}\text{Pb}^*/^{206}\text{Pb}^*$  ratios and the right-hand columns their corresponding errors, either absolute or percent (*Isoplot* will recognize which). For example, an input range of:

0.1142	0.210
0.1058	0.093
0.1079	0.158
0.1091	0.057
0.1148	0.073
0.1154	0.143
0.1128	0.097
0.1151	0.077
0.1069	0.205

will fill the right-hand columns so the result would be as shown at right (note that in this case the errors were interpreted by *Isoplot* as percent).

0.1142	0.210	1868	±4
0.1058	0.093	1728	±2
0.1079	0.158	1765	±3
0.1091	0.057	1785	±1
0.1148	0.073	1878	±1
0.1154	0.143	1887	±3
0.1128	0.097	1845	±2
0.1151	0.077	1881	±1
0.1069	0.205	1747	±4



Places the weighted-average values, errors, and statistics below the selected range of values and errors. Assumes that the selected range consists of a left-hand column of cells containing the values of interest, with a right-hand column containing their errors. The errors can be either absolute or percent, 1-sigma or 2-sigma. If there is a header-cell just above the first cell in the error column, *Isoplot* will attempt to decide the error type based on the contents of that cell (e.g. whether it contains the word “percent” or the % character, or the characters “1-s”, “1 s”, “2-s”, or “2 s”). So an input range of

Age	±1 sigma
1127.5	6.6
1127.7	8.1
1123.4	6.3
1119.6	5.2
1116.5	5.4
1122.7	5.3
1131.7	8.8
1127.6	8.1

will give the output at right:

Age	±1 sigma	
1127.5	6.6	
1127.7	8.1	
1123.4	6.3	
1119.6	5.2	
1116.5	5.4	
1122.7	5.3	
1131.7	8.8	
1127.6	8.1	
1123.0535	Wtd Mean (from internal errs)	
4.39023303	2-sigma err. of mean	
0.56798512	MSWD	
0	rejected	
0.7825495	Probability of fit	
<u>User specifies</u>		
FALSE	% out	
FALSE	% in	
1	Sigma level	
TRUE	Can reject	
FALSE	Const. ext. err	

Note that under the User specifies cell there are 5 parameters that you can change at any time, and which will be reflected in the output above as soon as the worksheet is recalculated (that is, upon pressing the Recalculate key (F9) or immediately if Calculation is set to Automatic). The output errors are always given at 2-sigma of 95%-confidence regardless of the input-error level.



Puts the median of the values in the selected 1-column range below the selection, together with their upper and lower error-bounds. The median is an extremely robust measure of central tendency, and the error calculation (following Rock *et al.*, 1987) makes no assumption about the distribution of the scatter of the data. The confidence limit of the errors is shown with the calculation (see right), as it is not always 95%.

27.3	
30.6	
27.7	
27.1	
32.7	
27.4	
28.5	
27.6	
28.5	
28.6	
33.9	
28.2	
30.0	
29.4	
28.8	
28.5	Median
1.5	+error
1.0	-error
96.5% conf.	



Puts the results of a Yorkfit (2-error regression) calculation for the selected X-Y values and errors below the selection. The selected range must be contiguous, and column-wise in the column-order of X-values, X-errors, Y-values, Y-errors [,X-Y error correlation] (the fifth column is optional; if missing, error correlations are assumed to be zero). By default, the errors are assumed to be 2-sigma, percent; this can be changed by including the word or symbol for percent and/or word or symbol for 2-sigma in a header-row above the selected data.



Puts the results of a robust (nonparametric) x-y regression for the selected X-Y values below the selection. The algorithm used is that discussed in Rock and Duffy (1986), ultimately derived from Vugrinovich (1981).



Changes the font of all isotope numbers in the selected range to superscripts. To recognize an isotope number, it must precede an element symbol. For example, selecting a range containing  $^{87}\text{Sr}/^{86}\text{Sr}$   $^{87}\text{Rb}/^{86}\text{Sr}$  would yield  $^{87}\text{Sr}/^{86}\text{Sr}$   $^{87}\text{Rb}/^{86}\text{Sr}$ .



Replaces appropriately-delimited, spelled-out Greek letters in the selected Worksheet cells (e.g. "alpha" or "sigma") with their corresponding symbols in a worksheet. Besides spaces and hard returns, and numbers, recognized delimiters can be any of the following characters: % ( ) ; , - ± . The Greek letter will be lower case, unless all of the characters in the spelled-out letter are uppercase (e.g. ALPHA).



Updates references to *Isoplot* functions for workbooks that were originally saved on another computer (if not updated, imported workbooks with cells containing *Isoplot* functions cannot be calculated, even though they worked fine on the source computer).



Plot and regress data for a conventional U-Pb concordia plot.



Plot and/ regress data for a Tera-Wasserburg U-Pb concordia plot.



Plot and regress data for a Total-Pb/U (concordia-constrained  $^{238}\text{U}/^{206}\text{Pb}$  -  $^{207}\text{Pb}/^{206}\text{Pb}$  -  $^{204}\text{Pb}/^{206}\text{Pb}$  linear) isochron.



Plot and regress data for a planar fit on the  $^{238}\text{U}/^{206}\text{Pb}$  -  $^{207}\text{Pb}/^{206}\text{Pb}$  -  $^{204}\text{Pb}/^{206}\text{Pb}$  Concordia diagram.



Plot and regress data for a "Normal" Ar-Ar isochron ( $^{40}\text{Ar}/^{36}\text{Ar}$  versus  $^{39}\text{Ar}/^{36}\text{Ar}$ ).



Plot and regress data for an "Inverse" Ar-Ar isochron ( $^{36}\text{Ar}/^{40}\text{Ar}$  versus  $^{39}\text{Ar}/^{40}\text{Ar}$ ).



Plot data and extract a Plateau age for an Ar-Ar stepwise-release age spectrum.



Plot and determine the "Ar-Ar PlateauChron" age for an Ar-Ar stepwise-release age spectrum.



Plot and regress data for an Rb-Sr isochron.



Plot and regress data for an Sm-Nd isochron.



Plot and regress data for an Re-Os isochron.



Plot and regress data for a "Normal" Pb-Pb isochron ( $^{207}\text{Pb}/^{204}\text{Pb}$  versus  $^{206}\text{Pb}/^{204}\text{Pb}$ ).



Plot and regress data for an "Inverse" Pb-Pb isochron ( $^{207}\text{Pb}/^{206}\text{Pb}$  versus  $^{204}\text{Pb}/^{206}\text{Pb}$ ).



Plot and regress data for a "Normal"  $^{238}\text{U}$ - $^{206}\text{Pb}$  isochron ( $^{206}\text{Pb}/^{204}\text{Pb}$  versus  $^{238}\text{U}/^{204}\text{Pb}$ ).



Plot and regress data for an "Inverse"  $^{238}\text{U}$ - $^{206}\text{Pb}$  isochron ( $^{204}\text{Pb}/^{206}\text{Pb}$  versus  $^{238}\text{U}/^{206}\text{Pb}$ ).



Plot and regress data for any type of  $x$ - $y$  data.



Construct and plot data on a  $^{230}\text{Th}/\text{U}$  evolution plot ( $^{234}\text{U}/^{238}\text{U}$  versus  $^{230}\text{Th}/^{238}\text{U}$ , with evolution curves for specified initial  $^{234}\text{U}/^{238}\text{U}$ ).



Plot and regress data for a  $^{230}\text{Th}/\text{U}$  3-D isochron ( $^{230}\text{Th}/^{238}\text{U}$  -  $^{234}\text{U}/^{238}\text{U}$  -  $^{232}\text{Th}/^{238}\text{U}$  activity ratios).



Plot and calculate a weighted (and robust) average.



Deconvolute ("unmix") a suite of dates or other parameters with overlapping errors, using the Sam-bridge-Compston algorithm.



Determine best estimates of ages of dated samples in known stratigraphic order but with overlapping date-errors.



Determine best estimates of ages of samples in known stratigraphic order from their  $^{230}\text{Th}/\text{U}$  isotope ratios and errors.



Construct a linearized probability plot for the selected data.



Construct a probability density ("cumulative Gaussian") plot and related histogram.



Extract the best age-estimate from a complex suite of single-zircon analyses.

### Appendix III – Error Correlations

Error correlations are a statistical index of the tendency of the measurement errors of two values to be in the same direction. For example, if the error in measurements of parameter  $x$  tends to be positive (measured  $x$  higher than true  $x$ ) when the simultaneous measurement error of parameter  $y$  is also positive, and vice versa ( $y$  error negative when  $x$  error negative), the  $x,y$  errors will have a positive error correlation. If the  $y$  errors tend to be negative when the  $x$  errors are positive, the  $x,y$  errors will have a negative error correlation. Error correlations can range from -1 to +1, with +1 indicating a perfect, positive correlation – that is, the  $x$  and  $y$  measurement errors will not only always have the same sign, they will also maintain precisely the same relative size.

Error correlations affect how error ellipses will appear. The major and minor axes of error ellipses for data points having error correlations of zero will be parallel to the  $x$ - and  $y$ -axes. Error ellipses for data points with nonzero, positive (negative) error correlations will appear tilted, with the long axis of the ellipse having a positive (negative) slope.

For error-weighted regressions (e.g. "Model 1" isochrons), the quantitative effect (on the regression line slope, intercept, errors, and *MSWD*) of the data-point error correlations can be as important as the data-point errors themselves, especially for error correlations approaching +1 or -1. Note that in assessing the relative importance of an error correlation to a regression, use  $1/(\rho^2-1)$  rather than  $\rho$  itself, thus showing, for example, that although a  $\rho$  of 0.9999 seems similar to one of 0.99, the  $1/(\rho^2-1)$  values of 50 and 5,000, respectively, do not.

#### How to Calculate an Error Correlation

*By differentiation*

If you know the analytical expressions from which the two (possibly correlated) parameters of interest can be calculated, you can use simple differential calculus to determine the error correlations of the two parameters, provided that each of the variables with errors in the two expressions are either uncorrelated, or whose error correlations themselves are known.

#### Example

Consider parameters  $x$  and  $y$ , which are calculated from measurements of parameters  $a$ ,  $b$ , and  $c$ , such that

$$x = \frac{a}{c} \text{ and } y = \frac{b}{c}. \text{ We first determine the partial derivatives of both equations}$$

$$dx = \frac{1}{c} da - \frac{a}{c^2} dc \qquad dy = \frac{1}{c} db - \frac{b}{c^2} dc$$

which can be rearranged to the more convenient

$$\frac{dx}{x} = \frac{da}{a} - \frac{dc}{c} \qquad \text{and} \qquad \frac{dy}{y} = \frac{db}{b} - \frac{dc}{c}$$

Taking the squares and the cross-products of the above equations and substituting the assigned errors for the differentials (thus obtaining a linear extrapolation of the effect of the assigned errors on the parameters of interest), we obtain

$$\frac{\sigma_x^2}{x^2} = \frac{\sigma_a^2}{a^2} + \frac{\sigma_c^2}{c^2} - 2 \frac{\text{cov}(a,c)}{ac} \qquad (1)$$

$$\frac{\sigma_y^2}{y^2} = \frac{\sigma_b^2}{b^2} + \frac{\sigma_c^2}{c^2} - 2 \frac{\text{cov}(b,c)}{bc} \qquad (2)$$

$$\frac{\text{cov}(x,y)}{xy} = \frac{\sigma_c^2}{c^2} + \frac{\text{cov}(a,b)}{ab} - \frac{\text{cov}(a,c)}{ac} - \frac{\text{cov}(b,c)}{bc} \qquad (3)$$

where  $\text{cov}(x,y)$  is the covariance of  $x$  and  $y$ . The error correlation,  $\rho$ , is defined as

$$\rho_{x,y} \equiv \frac{\text{cov}(x,y)}{\sigma_x \sigma_y}$$

so that

$$\frac{\text{cov}(x,y)}{xy} = \frac{\sigma_x}{x} \frac{\sigma_y}{y} \rho_{x,y}$$

Equations (1-3) can be rearranged (defining  $S_x = \sigma_x/x$ , etc.) to

$$S_x^2 = S_a^2 + S_c^2 - 2S_a S_c \rho_{a,c} \quad (4)$$

$$S_y^2 = S_b^2 + S_c^2 - 2S_b S_c \rho_{b,c} \quad (5)$$

$$\rho_{x,y} = \frac{S_c^2 + S_a S_b \rho_{a,b} - S_a S_c \rho_{a,c} - S_b S_c \rho_{b,c}}{S_x S_y} \quad (6)$$

If the errors of  $a$ ,  $b$ , and  $c$  are all uncorrelated (that is,  $\rho_{a,b} = \rho_{a,c} = \rho_{b,c} = 0$ ), equations (4-6) are simplified considerably, to

$$S_x^2 = S_a^2 + S_c^2 \quad (7)$$

$$S_y^2 = S_b^2 + S_c^2 \quad (8)$$

$$\rho_{x,y} = \frac{S_c^2}{S_x S_y} \quad (9)$$

This general approach can be extended to any pair of analytical expressions, no matter how complex.

#### *By observation*

If the parameters  $x$  and  $y$  can't be described analytically, we can still estimate  $\rho_{x,y}$  using a series of replicate measurements of  $x$  and  $y$ , and calculating the familiar linear correlation coefficient,

$$\rho_{x,y} = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

where  $\bar{x}$  and  $\bar{y}$  are the means of  $x$  and  $y$ , respectively.

### **If You Want to Simplify Plotting and Calculations by Avoiding Correlated Errors**

For  $x$ ,  $y$  regressions of isotope ratios involving 3 isotopes, calculations of error correlations can often be avoided entirely by simply using different ratios of the 3 isotopes. The trick is to sequester the largest component of measurement error in just one of the axes. For example, consider the common  $^{206}\text{Pb}/^{204}\text{Pb}$  -  $^{207}\text{Pb}/^{204}\text{Pb}$  plot and associated isochron. If all of the data are highly radiogenic, so that both  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$  are always very large (say >500), the largest source of error in both ratios will arise from  $^{204}\text{Pb}$  measurement error, and all of the  $^{206}\text{Pb}/^{204}\text{Pb}$  -  $^{207}\text{Pb}/^{204}\text{Pb}$  error correlations will approach unity. The solution here (if avoiding error correlations is the goal, at any rate) is to shift  $^{204}\text{Pb}$  from the denominator of both axes to the numerator of only one of the axes – for example,  $^{207}\text{Pb}/^{206}\text{Pb}$  versus  $^{204}\text{Pb}/^{206}\text{Pb}$ , or  $^{206}\text{Pb}/^{207}\text{Pb}$  versus  $^{204}\text{Pb}/^{207}\text{Pb}$ . The error correlations will then be close to zero, and can comfortably be ignored.

Note that this strategy is ineffective for high-precision analyses of relatively unradiogenic leads – that is, with rather low  $^{206}\text{Pb}/^{204}\text{Pb}$  and  $^{207}\text{Pb}/^{204}\text{Pb}$ , because in these cases (at least for unspiked or single-spiked TIMS analyses) the dominant error in all possible ratios typically arises from the mass fractionation correction, thus forcing significantly nonzero error correlations even for  $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{204}\text{Pb}/^{206}\text{Pb}$  plots.

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