ISOPLOT

A Plotting and Regression Program for Radiogenic-Isotope Data

Version 2.53
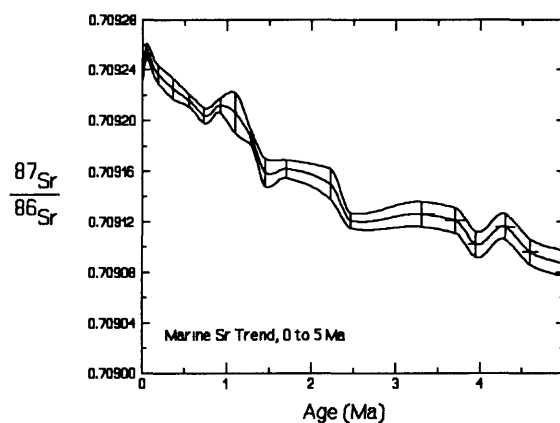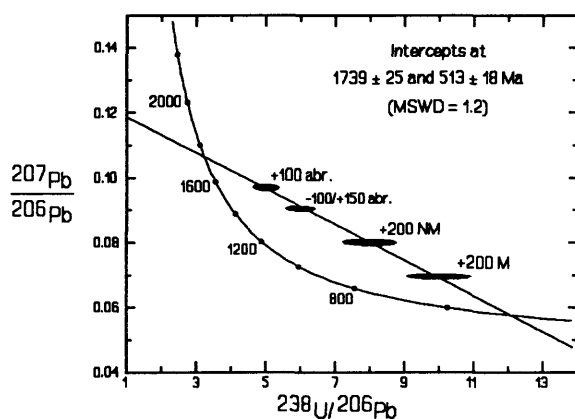
$$\frac{207Pb}{206Pb} \quad \text{vs} \quad {}^{238}U/{}^{206}Pb$$

Intercepts at
1739 ± 25 and 513 ± 18 Ma
(MSWD = 1.2)

+100 abr.
-100/+150 abr.
+200 NM
+200 M

$$\frac{87Sr}{86Sr} \quad \text{vs} \quad \text{Age (Ma)}$$

Marine Sr Trend, 0 to 5 Ma

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INTRODUCTION

Isoplot is a program designed primarily for radiogenic-isotope geochemists, but may be useful for plotting or regressing any X-Y data in a simple, flexible manner. Data can be entered either from the keyboard or from ASCII files produced by spreadsheet or word-processing programs, and can be plotted as a variety of symbols, including various error-symbols and polygons. *Isoplot* can regress data using a modification of the most-widely used two-error regression algorithm, and will calculate isochron ages directly from the regression lines. Graphics can be viewed immediately on the screen or dumped as screen graphics to an Epson-compatible dot-matrix printer. For high-quality, hard-copy graphics, HPGL-compatible pen-plotters are supported (with the assistance of commercial programs, laser or dot-matrix printers can also be used for high-quality graphics output).

In addition to the basic X-Y plotting and common-isochron calculation functions, the program can:

◆ Calculate isochron ages for less-common decay schemes, including K-Ar, K-Ca, Lu-Hf, Re-Os, and ^{230}Th/^{232}Th-^{238}U/^{232}Th (p. 15);

◆ Construct U-Pb concordia plots (conventional, Tera-Wasserburg, or Tatsumoto-style) and calculate concordia-intercept ages and errors (p. 18);

◆ Construct projections of 3-dimensional (X-Y-Z) plots, determine best-fit planes to X-Y-Z data, and calculate concordia intercepts and uncertainties for 3-dimensional concordia data (p. 21, 24);

◆ Construct single-stage growth-curves for plots of common-Pb data (p. 21, 24);

◆ Construct ^{230}Th/^{238}U - ^{234}U/^{238}U evolution curves for U-series data (p. 26);

◆ Calculate and construct plots for weighted averages of a single variable (p. 28);

◆ Show histograms of a data-set, with calculated mean, median, and biweight-mean values (p. 28);

◆ Calculate radiogenic ^{207}Pb/^{206}Pb ages, common-Pb model ages, Nd, Sr, Os, and Hf model ages, U-series ages, and ages from the secular global-marine Sr-isotope trend (pp. 30-31);

◆ Do curvilinear (polynomial) regressions for X-Y data (p. 17);

◆ Fit a smooth curve (either precisely or in a least-squares sense) to data of arbitrary complexity using spline curves (p. 17);

To obtain a disk or disks containing *Isoplot*, write directly to K.R. Ludwig (U.S. Geological Survey, Denver CO, 80225) and enclose a 3½" or 5¼" (preferably 1.2 MB capacity) disk formatted on your system. The source-code is also available on request (~400 Kbytes of text files).

HARDWARE REQUIRED BY *Isoplot*

Isoplot was written for IBM-PC compatible computers, and supports CGA, EGA, and Hercules

graphics modes, numeric coprocessors, and HPGL-compatible plotters (all optional). You should have at least 512 kilobytes of RAM (preferably 640 Kb). Printer output is directed to parallel port :LPT1, and plotter-file output to a serial port :COM1. You can redirect output from :LPT1 to any serial port with DOS's **MODE** command. If you have memory problems (generally indicated by either a refusal by DOS to start running the program or by RESUME WITHOUT ERROR crashes while running the program), they may be caused by having too many device drivers and/or terminate-and-stay-resident programs installed. Changing your CONFIG.SYS or AUTOEXEC.BAT files to delete the drivers or TSR programs may be required. It may also help to reduce the number of points that *Isoplot* can take into memory at one time (the default value is 100). To specify the maximum number of data points, invoke the program with **ISOPLOT /N{#points}** (for example, `ISOPLOT /n50`), where **{#points}** is a number corresponding to the maximum number of points. You can also use this switch to *increase* the maximum number of points. Generally out-of-memory errors will crash *Isoplot* if you specify more than about 400 data-points, though you can increase this limit slightly by invoking the program with the /C switch. /C followed by a number restricts the number of columns accessible from a datafile to that number.

If your monitor is a monochrome display that emulates a color display with different shades of gray (or green, amber...), you should force *Isoplot* to start in true monochrome mode by invoking the program with the /M switch.

Use the /? switch when invoking *Isoplot* to get a list of all valid switches and their syntax.

ISOPLOT WITH *WINDOWS 3*

WINDOWS 3 running in 386 Enhanced Mode will trash *Isoplot*'s EGA-mode graphics screens. To get around this, you can either (1) run *WINDOWS* in the *real* mode, (2) disable *Isoplot*'s graphics and use *Isoplot* only for calculations, (3) specify that *Isoplot* use lower-resolution CGA graphics (press **ALT-S** from *Isoplot*'s starting screen), or (4) wait until I get around to writing the *WINDOWS* version of *Isoplot*.

GETTING STARTED

LOADING THE PROGRAM

If you have a hard disk, transfer all of the files on the original *Isoplot* disk to a subdirectory on the hard disk. If there is an UNPACK.BAT file, you'll need to run it to un-compress *Isoplot*'s files. Set the default disk and directory to be that of *Isoplot*. Type *Isoplot* plus any switches (/N, /M, /P) that you want, then press ◄── to start. The /P switch is used to specify the default path for data-files (e.g., /P C:\LOTUS). You can also restrict the types of files displayed in *Isoplot*'s file-access routine by starting *Isoplot* with the /F switch (see p. 2, 11).

USING THE *Esc* KEY

Isoplot tries to allow you to gracefully back out of most of the situations that you might mistakenly stumble into. In almost all cases, you can do this by pressing the *Esc* key. The *Esc* key will make the program back up at least one level -- probably to where you were before you made your error.

SETTING UP X-Y PLOTS

The first screen of the program will look like this:

```
▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷▷  ISOPLOT  ◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁◁

                                        ┌─────────────────────┐
                                        │     K.R. Ludwig     │
   Enter  X-Y or Isochron Plot          │ U.S. Geol Survey    │
                                        │     Ver. 2.53       │
      C   Conventional Concordia Plot   └─────────────────────┘

      T   Tera-Wasserburg/Tatsumoto Concordia Plot

      A   Weighted Averages Calculation     ┌──────────────────────┐
                                            │ Printer.... Off      │
                                            │ Screen...   Color    │
      H   Histogram Plot                    │ Graphics... On       │
                                            │ HPGL File.. None     │
      L   List of Radiogenic-isotope Utilities │ Errors...         │
                                            │          2-Sigma, %  │
      Esc Exit Isoplot                      │ Speed....    27/12   │
                                            └──────────────────────┘


                              F4 Dos Shell
   F1 HPGL File?    F2 Axes?  F3 1-Sigma Errors   F5 Absolute Errors
   F6 No Graphics   F7 Mono   F8 Datafile         F9 Use Printer
```

First, select whether you want the output sent to the screen or the printer with the **F9** key. Look at the lower-right of the screen to see what the current status is. Notice that the function-key labels will always be the *opposite* of the status display, because the function key labels indicate what the key will do when pressed, *not* what the current status is.

Isoplot will automatically select the graphics display-type when the program is started, searching for the presence of EGA, CGA, and Hercules graphics capability. *For systems with Hercules-compatible graphics cards, you must run HERCULES.COM (supplied with Isoplot) before invoking Isoplot.* If your system has a graphics board capable of using more than one display mode, you can select alternate modes from the starting screen by pressing **ALT-S.** For color screens, select whether you want your display in color or monochrome (**F7**). For some CGA-graphics screens, and for all monochrome Compaq computers, the display will be more legible with monochrome output. Use the **/M** switch when invoking *Isoplot* to specify monochrome mode at the start.

If you don't want a graphical display of your data, press **F6** to cancel the graphics. The output will be more rapid, take less memory, and, for CGA screens, be more legible if no graphics are used.

In the box at the right of the starting screen, the assumed error-format is shown. The default format is for errors to be entered in percent, and at the 2σ (or 95%-confidence) level. You can toggle between percent and absolute errors with the **F5** key, and between 1σ and 2σ errors with the **F3** key. Regardless of whether the errors are entered and plotted at the 1σ or 2σ level, though, isochron-age and concordia-intercept errors will be calculated at the 95%-confidence limit.

The "Speed" numbers at the lower-right of the screen, incidentally, refer to the relative speed of the computer for non-numeric and numeric tasks, from left to right respectively (the higher the number, the faster the relative calculation-speed).

SELECTING AXES AND GRIDLINES

Though the default mode for plotting is to show the data in a "plot-box" defined by all four of the lower-X, left-Y, upper-X, and right-Y axes (e.g. Figure 1), you can specify any combination of these with **F2** from the starting screen. *Isoplot* will then query:

```
Enter axes to show (e.g. 1,2,3,4 = all) ?
```

Enter up to four numbers, separated by commas, where the numbers indicate the axes of the plot-box in a clockwise direction, starting with the lower X-axis. For example, if you wanted to show only the lower-X and left-Y axes, you would enter **1,2**.

You can specify gridlines in the plot (at every axis-tick location), in either the X- or Y- directions. To specify gridlines parallel to an axis, enter the axes to show as described above, but enter axes for which you want parallel gridlines as a negative number. For example, entering axes as **-1, -2, 3, 4** would result in a plot with both X- and Y-gridlines.

CHOOSING THE AXIS NAMES

When you've finished selecting the physical parameters of the plot with the function keys, as described above, press either X or ←— . The screen will then show:

```
                            X-Y PLOT

                   X-Axis Label ==> X
                   Y-Axis Label ... Y

               Lower Limit of X ... 0
               Upper Limit of X ... 10

               Lower Limit of Y ... 0
               Upper Limit of Y ... 10


 F1 206/204-207/204     F2 206/204-208/204     F3 Rb/Sr         F4 Sm/Nd
 F5 Re/Os        F6 Lu/Hf        F7 K/Ar          F8 K/Ca         F10 Th/U
 F9 Recall       Esc Exit Form       ENTER Enter response    CTRL-ENTER Done
```

To fill out this "form", move the cursor with the arrow-keys, enter your responses, and press ←—. When you've entered all the values, press CTRL ←— to "submit" the "form".

The X- and Y-axis labels are the labels that will appear below the X-axis and to the left of the Y-axis; the X- and Y- limits define the minimum and maximum limits of the plot's X- and Y-dimensions.

You can specify some of the more-common axis names with the F1 - F10 keys, giving you the axis names for a $^{207}Pb/^{204}Pb$ versus $^{206}Pb/^{204}Pb$ plot, a $^{208}Pb/^{204}Pb$ versus $^{206}Pb/^{204}Pb$ plot, an Rb-Sr isochron plot, an Sm-Nd isochron plot, et cetera. The plotter output of isotope names (such as ^{87}Sr) will usually automatically show the numerals as superscripts.

If data from a datafile (p. 9) were already loaded into memory when the "form" appeared, the default axis names will be the column-headings for the datafile, and the axis limits will be the extreme values from the datafile. In this case, you might not need to enter anything into the form yourself -- just press CTRL ←—.

ENTERING DATA FROM THE KEYBOARD

After you've specified the axis-names for the plot, *Isoplot* will ask to enter a set of data for plotting. The screen will look something like:

```
   Enter datafile sets as first#, last#, *; break series w. semicolon
        (example: 2,12;14,16* for sets 2 thru 12 + 14 thru 16)

                Errors are 2-sigma, in percent; XY Data

Set#    Name    87Rb/86Sr    %err          87Sr/86Sr    %err    Rho




 SET# 1: ENTER X [,%err], Y [,%err [,err-corr.]]   (ENTER when done)


F1 HELP                                          F7 All Points
F5 XYZ Data                                      F8 Data File
F9 Recall                                        F10 Alpha/Graphics
```

The axis names and plotting symbols shown above are only examples, of course. Also, note that the information about datafile sets will appear only if you've loaded a datafile into memory.

To enter the X- and Y-values for your data points, type in the two numbers, separated by a comma[1], then press ◄—┘. To include the errors with the points (you'll need to include errors for plotting symbols that reflect errors or for Yorkfits), enter 4 values separated by commas, in the format X, X-error, Y, Y-error. Remember to use the correct error-format (percent or absolute, at the $2\sigma/95\%$-confidence level or 1σ), which you specified from the starting screen. If no error correlations are entered (as the optional 5th value), they're assumed to be zero. If the errors for all of the points are going to be the same, don't bother entering them at this point -- you can enter them as a group later (when *Isoplot* requests errors for data points without assigned errors). You can look at the last several entries you've made, incidentally, by pressing the **RECALL** key (F9).

When you've entered all of the points that you want plotted with a given plotting-symbol or color, press ◄—┘. The screen will then display a list of the data-point values that you just entered, and query:

```
       ENTER Set# to be edited   (ENTER when done):
```

Check the displayed list for mistakes. If there are any, enter the set# (shown to the left of the X- and Y-values) of one of the incorrect data-points. Enter the correct values, when requested, then continue with the editing process until all of the values are correct. Press ◄—┘, and the data points will be plotted.

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[1]In addition to commas, you can also use spaces or slashes as the delimiter for multiple entries (though you can't delimiter characters in the same response). So an entry of *1,2,3,4* is equivalent to both *1 2 3 4* and *1/2/3/4*.

SELECTING PLOTTING-SYMBOLS

Before the data points that you've just entered can be plotted, you'll need to select a plotting-symbol for them. The screen will show:

```
           Select Symbol to Start Plotting

     E Error Ellipse              P Polygon

     B Error Box                  C Error Cross

     S Square Box                 X + * O . ALT A-Z

     Symbol-Color# 14             (change with U/D arrows)
     Plotter-Pen# 1               Symbol-size: 1     (open)



     F1 Help                      F4 DOS Shell

     F2 Solid symbols             F3 Change char.-symbol size
```

➪ *The "Symbol Color#" option is displayed only if you have an EGA color screen, and the "Change Char.-Symbol Size" and "Plotter-Pen#" options only if you're creating an HPGL-command file.*

Select a plotting-symbol (see Figure 1) by pressing E, C, B, P, S, X, +, *, O, a period (for a dot-symbol), ALT plus a letter key (for letter-symbols), or the space-bar (no symbol). The O key gives a circle as the plotting-symbol. Use the up/down arrows to change the screen-color and plotter-pen of the plotting symbol, and the **PageUp** - **PageDown** keys to change the background color of the plot on the screen. The open/solid toggle (**F2**) affects all but the character and error-cross symbols. Use **F3** to specify the size of the plotting symbols[1]. See Figure 1 for examples of some of the possible plotting symbols.

Because errors for conventional concordia plots and for common-Pb isotope plots are *always* significantly correlated, the only error-symbol offered for these plots is an error ellipse.

If you selected an error-symbol (error box, error cross, or error ellipse) as the plotting symbol, and didn't enter error-values for some or all of the samples, *Isoplot* will now ask you for blanket errors:

```
     ENTER X-errs,Y-errs [,Err.-Corr.] for sets with unassigned errors
```

Enter the 2 or 3 values requested. Note that, again, the error correlation is an optional value, and that the assigned errors *must* be nonzero. If you don't know how to estimate an error correlation, use this equation:

---

[1]Symbols reflecting data-point errors, as well as screen output for letter-symbols, will not be affected by specifying the symbol-size.

$$\rho_{x,y} = \frac{E_x^2 + E_y^2 - E_{x/y}^2}{2E_x E_y}$$

or:

$$E_{x/y}^2 = E_x^2 + E_y^2 - 2\rho_{x,y}E_x E_y$$

where $\rho_{x/y}$ is the correlation between the X and Y errors, E_x, E_y, and E_z are the percent errors in X, Y and Z, and where Z=Y/X. For example, if X were $^{206}Pb/^{204}Pb$ and Y were $^{207}Pb/^{204}Pb$, then Z would be $^{207}Pb/^{206}Pb$. Or, if X were $^{207}Pb/^{235}U$ and Y were $^{206}Pb/^{238}U$, then Z would be $R*^{207}Pb/^{206}Pb$ (R = natural $^{235}U/^{238}U$). Error correlations are zero if the error in Y doesn't tend to increase with the error in X. If the error correlations are much greater than about 0.5, don't use error box or error cross symbols, because these symbols will convey a misleading impression as to the actual area of uncertainty around the data point.

If you selected a polygon plotting-symbol, *Isoplot* will ask you to define the polygon:

```
POLYGON SYMBOL:

ENTER #Sides [,Size (mm)   [,Rotation (0-360)]]...
          (defaults: 3, 3, 0)



    F9 Recall          F3 Star-shaped symbol
```

The parameters in brackets represent optional input, so you can enter either 1, 2, or 3 values (or press ◄──┘ to specify the values that were used last). The number of sides can vary from 3 (a triangle) to a large number. The SIZE parameter refers to the diameter of the polygon in millimeters. The ROTATION parameter refers to the angular orientation of a vertex of the polygon: 0 gives a vertex at 12 o'clock, 45 a vertex at 3 o'clock, and so on. Press F3 to define a star-shaped symbol with similar parameters. The resulting polygon will be open or solid (filled) depending on the status of the open/solid toggle from the previous screen.

THE *MORE POINTS* SCREEN

After the data points are plotted, a display something like this will appear:

```
    ENTER   Plot more points (new data-set)

    A         "     "    "     (add to existing set)

    Esc     Start a new plot

    E       End ISOPLOT
_____

    Y       Yorkfit (unforced)

    F       Yorkfit (forced through specified age)
_____
 F4 DOS Shell                                    ^F2  Send HPGL
 F6 Splines                    F7 Connect Symb    F9  Polynomial Fit
 F3 Label      F5 Dump Graphics    F8 Datafile   F10  Alpha/Graphics
```

The details of this screen -- which I'll call the "MORE POINTS" screen -- will vary according to the type of plot you're constructing and the number of points already plotted. You have the option at this point of (1) starting a new plot, (2) adding more points to the existing plot, (3) calculating a Yorkfit (with associated isochron or concordia ages), (4) accessing new data from a datafile, or (5) performing various operations on the plotted data. You can toggle between the graphics display and the alphanumeric display (shown above) with the **F10** key.

If you press ◄——┘ , the program will return to the data-input screen, and any additional data-points that you enter will be counted as a new batch for any subsequent regressions or operations. But if you want to plot more points (perhaps with a different plotting-symbol or color) that are to be pooled with the just-plotted points for a later Yorkfit (or other regression), press **A**.

If you're creating an HPGL command-file as you plot, you can send the current contents of that file to the plotter at :COM1 by pressing **CTRL F2** (or you can wait until you've returned to the starting screen). You can view the contents of the HPGL file without sending it to the plotter with **ALT F2**.

CONNECTING DATA POINTS WITH A LINE

You can connect each data point on your plot with a straight line by invoking the "Connect-the-dots" function (F7) from the **MORE POINTS** screen. The data points will be connected from the smallest X-value to the largest X-value. To connect the points in the order that they were entered into *Isoplot*, press **SHIFT F7**; or in the order of their Y-values, press **ALT F7**.
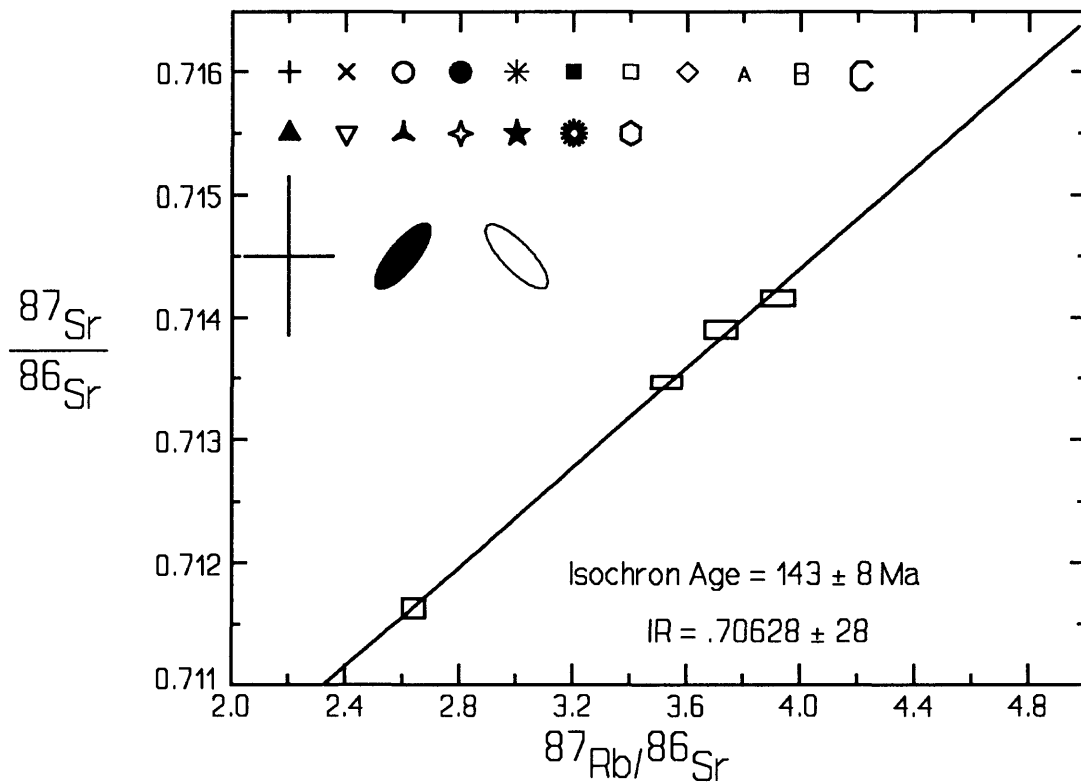
Figure 1: Example of isochron diagram (with error boxes), together with some of the other plotting symbols supported by ISOPLOT.

LABELING WORDS OR PHRASES ON THE PLOT

You can have *Isoplot* put a phrase anywhere on the plot by pressing **F3** from the **MORE POINTS** screen. Type in the phrase, then locate the phrase using the arrow-keys (shifted for gross movement, unshifted for fine movement; if the shifted arrow-keys don't work with your keyboard, use **Page-Up/PageDown** and **Home/End** instead). Press ◄—┘ to put the label on the plot, or **Esc** to exit without any action. If you're creating an HPGL command-file, use **F2** to select the character-size, character-slant, and line-thickness of the label. Note that though the size and shape of the characters on the *screen* won't be affected by this procedure, the position on the screen of the lower-left corner of the label is valid, regardless of the character size). To get the ± symbol included in your labels, use the +/- characters.

STORING AND RETRIEVING DATA FROM DATA FILES

You can use text files to store data that *Isoplot* can read, provided that you use one of the following formats.

SPACE-DELIMITED FILES

Space-delimited files can be created by most DOS word-processing programs, or by LOTUS as a

*.PRN (print-to-disk) file. *Isoplot* requires that:

✧ the data must use a row-column format where the rows are used for data for different samples, and the columns for different parameters or measurements for those samples;

✧ column-widths must all be 9 characters (the LOTUS default);

✧ for the automatic column-name selection feature to work (see below), column names must appear *above* any data, and directly overlie a line of repeating equals-signs (=========). There must be 9 equals-signs for each column;

✧ column names may occupy either 1 or 2 cells directly above the repeating-equals signs;

✧ remember to store the file with a right margin large enough to include all of the columns of data plus the left margin.

TAB-DELIMITED FILES

Tab-delimited files are the text files created by some DOS programs such as EXCEL, and most Macintosh programs. Use a row-column format, where rows contain data for a given sample, and columns the different values for that sample. Columns are delimited by the TAB character. For the automatic column-name selection feature to work (see below), the column names must occupy the first 1 or 2 rows directly above the first numeric-data row, and the first numeric data row must be the first row that is *completely occupied with numeric data* (not counting the optional sample-name column). To meet this criterion, make sure that all of the columns in your first row contain numbers (zero is OK), and that there are no extra tabs to the right of the columns of interest.

SAMPLE NAMES IN DATAFILES

Isoplot will load and display sample names for your data if you wish. To include sample names in a tab-delimited datafile, put them in the leftmost column. For a space-delimited file, put sample names in the leftmost one or two columns (18 characters max.). When you access the file, you must specify whether sample names are present, using the F7 toggle from the datafile screen. *Any numeric data in the first column (tab-delimited files) or first 18 characters (space-delimited files) will not be accessible unless the sample-name toggle is turned off.*

ACCESSING DATAFILES

Selecting a file: To get data from a datafile, press the function key labeled **GET DATAFILE** from either the starting screen or the **MORE POINTS** screen. The screen will then show a catalog of the first 250 files in the current directory, using the file extension or wildcards specified during the last use of the program. When the screen shows a list of the files for the drive or path that you specified, select a file with the cursor keys or by pressing the key of the first letter of the file; then press ◄─┘ .

The file catalog will also show all of the paths accessible from the current path[1]. Path names are distinguished from file names by a back-slash following the name. The "parent directory" (the directory, if any, that contains the current directory) will be shown with the usual DOS notation (..\). You can select

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[1]You can specify an arbitrary default path for data-files when you invoke **ISOPLOT** by using the /P switch. For example, to specify C:\LOTUS\SIERRA as the default data-file path, invoke **ISOPLOT** by typing **ISOPLOT /P C:\LOTUS\SIERRA**. Otherwise, **ISOPLOT**'s default datafile-path will be the last one used by the last user of the program.

one of these paths in the same way as a file.

Use **F2 (Path or filespecs?)** to change disks or paths (directories), or to restrict which files are displayed in the file-list. You can use the usual DOS wildcard characters to restrict which files are shown in the file catalog. Press **F2 (Path or filespecs?)**. Enter the characters indicating the files to be displayed, for example:

.	all files in the current directory.
D:\ISO*.TXT	files with the TXT extension in the \ISO directory of disk D:.
C:CALIF??.ZR*	files in the default directory of drive C: whose first 4 characters are CALIF, and whose extensions have ZR as their first 2 characters.

You can have a quick look at the contents of any text file by putting the file-cursor on the file of interest, then pressing **F3 (FILE PREVIEW)**. *Isoplot* will use the screen as a window to display the contents of the file. You can use the cursor keys to move the screen "window" anywhere in the file, then return to the **DATAFILE** screen by pressing **Esc**. This is a good way of troubleshooting problems with datafile access, incidentally. For tab-delimited files, only the first 9 characters after each tab will be shown.

Isoplot can access a file automatically when you start the program, using the **/F** switch. After **/F**, add the full path and file name of the file you wish to access. For example, to start *Isoplot* and access the file WINDRIV.TXT from path \DATA\ZIRCONS on disk B:, you would invoke the program with **ISOPLOT /F B:\DATA\ZIRCONS\WINDRIV.TXT**. You can also use **/F** with file-wildcards (* or ?) to restrict *Isoplot*'s file-display. For example, invoking the program with **/F *.TXT** would restrict the file-display to only those files with **TXT** extensions.

Selecting data columns: If the data file you wish to access was stored according to the requirements above for automatic column-name selection, *Isoplot* will extract the column names from the file automatically when you press ◄┘.

If the data file wasn't created with *Isoplot*'s auto column-name selection in mind, you'll need to press the **Cancel Auto Col.-Names** toggle (**F6**) before you select the file. Then, after you've selected the file, answer the query "What row contains the last (or only) column-header row?". If you're not sure, press **F3** to look at the file with **FILE PREVIEW** (but note that any blank rows at the top of the datafile will be ignored in the row-count).

Once you've chosen a datafile, the computer will display a list of the column-names (=column headings) for that file. Select either 2 columns (X and Y; or, if doing weighted averages, Y and Y-error), 4 columns (X, X-error, Y, Y-error), or 5 columns (X, X-error, Y, Y-error, X-Y error-correlation).

If your datafile contains data for a Concordia plot ($^{206}Pb/^{238}U$ versus $^{207}Pb/^{235}U$) and/or a Pb-Pb plot ($^{207}Pb/^{204}Pb$ versus $^{206}Pb/^{204}Pb$), with or without associated errors and error-correlations, you may be able to select the appropriate columns (which will be emphasized in the display) by simply pressing **F7 (Pb-Pb Cols)** or **F8 (Concordia Cols)** in response to the column-query. The file needn't have the errors for *Isoplot* to recognize the correct columns, though they will be used if present. The column-recognition feature of *Isoplot* depends on the column-names being recognizable and unambiguous, so it may not be successful in all cases. If *Isoplot* is unable to find the columns for either of the above types of plots, the **F7** and/or **F8** keys will be undefined.

Isoplot will retrieve the data for the specified columns from the disk, and display the data on the screen[1]. If **F4** (**PRINTER OUTPUT**) were pressed before loading the file, the data would also be printed out.

USING DATA FROM DATAFILES

To plot from a datafile, the data-points to be plotted are specified with "set numbers", where the set number of a data point corresponds to its row in the spreadsheet (the first row below the double-equals signs is for set number 1), and is printed out when the datafile is first accessed by the program. For example, after you've loaded a datafile into memory, the data-input screen will show:

```
Enter datafile sets as first#, last#, *; break series w. semicolon
        (example: 2,12;14,16* for sets 2 thru 12 + 14 thru 16)
```

To plot the data for set number 5, enter **5***. To plot data for sets 5, 6, 7, 8, and 9, enter **5,9***. To plot data for sets 5, 6, 7, 8 and 11 and 15, 16, 17, enter **5,8;11;15,17***. In other words, indicate continuous sequences of sets with a comma, separate different continuous sequences (or individual sets) with a semicolon, and always add an asterisk at the end. It's OK to mix data from datafiles and typed-in input. You can also plot data from several different datafiles by pressing **A**(dd) after each plot, then switching datafiles.

If you want to plot *all* of the datafile's data, press **F7** (**All Points**) or **F6** (same as **F7**, but doesn't display the data for the points on the screen).

YORKFITS OF DATA

YORKFIT "MODELS"

A "Yorkfit" refers to a linear regression using the general algorithm developed by Derek York (York, 1969). This algorithm weights each point according to both its X- and Y-errors, and also takes into account the X-Y error-correlations. *Isoplot* starts with the original York algorithm, but may also use some modified approaches, depending on the type of data you're working with and the amount of scatter of the data. The different approaches, called MODELS by the *Isoplot*, make different assumptions about the reason for the scatter of the points about a straight line.

Model-1 Yorkfits: -- The MODEL-1 Yorkfit is York's original algorithm, and assumes that the *only* cause for scatter from a straight line are the assigned errors. The points are therefore weighted proportional to the inverse square of these errors. A test of the MODEL-1 assumption is provided by the PROBABILITY OF FIT value calculated by the program. If this value is reasonably high (more than 15% to 20%), then the MODEL-1 assumptions are probably (but not certainly) justified. If this probability is low (less than 20% or so), however, you may choose another model.

If you select the MODEL-1 fit even though the PROBABILITY OF FIT is close to zero, you are in effect requesting that the actual errors be calculated from the observed scatter (thus invoking the use of the

---

[1]To save time after recovery of a long file, you can suppress the display of the sample names and data by pressing any key as the data are being displayed. If you want to look at parts of a large file, you can pause the scrolling of the display by pressing the P key.

Student's-t multiplier to convert from estimated errors to 95%-confidence errors), *and you are also specifying that the true errors and error-correlations of the data points are for some reason directly proportional to the ones you have assigned to them*. This is an important point, though seldom acknowledged.

Isoplot will always attempt a MODEL-1 fit first. In the printout, the *A Priori* errors are the errors in the slope and intercept calculated by propagating only your assigned errors for the points; 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 1σ level, are provided mainly for comparison purposes with the output of other implementations of York's algorithm. The only geologically useful errors are the ones given as *95% Confidence-Limit* errors.

How the 95% confidence-limit errors are calculated depends on the probability that the assigned errors for the points can account for the observed scatter. If the probability is greater than .15, the 95% confidence-limit errors are simply 1.96 (Student's-t for ∞ points) times the *A Priori* errors (the reason for this is discussed by Brooks and others, 1972).

Model-2 Yorkfits: -- A MODEL-2 Yorkfit 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 on Model-1 regressions) when it is clear that, in fact, some other cause of scatter is involved. The 95% confidence-limit errors are calculated from t_{n-2} times the *Including Scatter* errors. If you know little or nothing about the dominant cause of the scatter of the points, and about the statistical form of that cause, you should probably use this model.

Model-3 Yorkfits: -- A MODEL-3 Yorkfit 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 a good example of such a case, see Juteau and others, 1984.

MODEL-3 is offered as an option if the program recognizes, from numbers in the axis names, that you're plotting isochron data (Rb-Sr, Sm-Nd, U-Pb, Th-Pb, Lu-Hf, Re-Os, K-Ar, or K-Ca). The 95% confidence-limit errors are calculated from t times the *INCLUDING SCATTER* errors.

Model-4 Yorkfits: -- A MODEL-4 Yorkfit is used only for U-Pb isotope data on a conventional concordia diagram. This model, inspired by Davis' (1982) approach to the problem, assumes that the points scatter due to a combination of the assigned errors plus "geological" errors in the $^{207}Pb/^{206}Pb$ ratios. These "geological" errors are assumed to increase linearly from the upper concordia-intercept to the lower concordia-intercept (or vice-versa; see below). MODEL-4 may be appropriate for cases where a multi-episodic disturbance is suspected (in which case the closer the point to the *upper* intercept the greater its weight), and for cases where a significant degree of inheritance of older zircons is suspected (in which case the close the point to the *lower* intercept the greater its weight). You may choose whether the lower concordia-intercept (press L for **Model-4 LI**) or the upper concordia-intercept (press U for **Model-4 UI**) is to be the age of interest.

The MODEL-4 Yorkfit is offered only for data sets with 6 points or more. The 95% confidence-limit

errors are calculated by multiplying the *Including Scatter* errors by the t value for N'-2 degrees of freedom, where N' is a number that is in general *less* than the actual number of points. This approach is necessary because of the way in which the MODEL-4 algorithm weights the points -- the more concordant that point, the greater its weight. In the extreme case, with 2 nearly-concordant points plus any number of much- less concordant points, the algorithm will in effect pay attention only to the two most-concordant points and ignore the others. Obviously, in this case the true degrees of freedom are much less than the apparent degrees of freedom. To compensate for this effect, N' is calculated by assigning each of the two most-concordant points a "point value" of 1, and assigning the remaining points a fractional "point value" based on their MODEL-4 weights; the less their MODEL-4 weight, the smaller a fraction of a whole "point' is assigned.
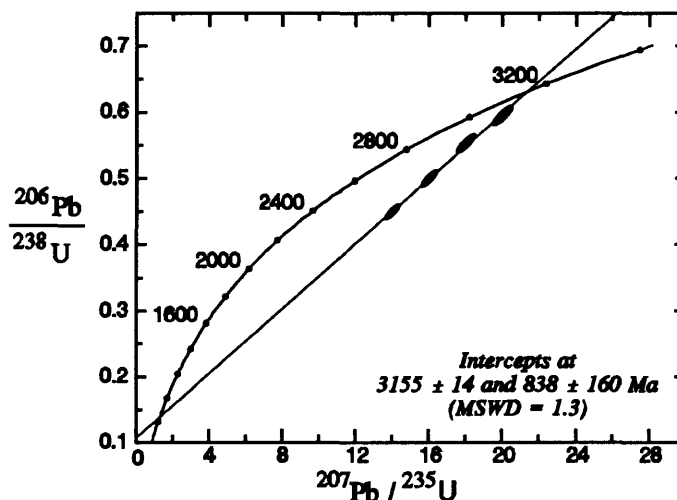
Figure 2: Example of concordia plot with Yorkfit line (and associated concordia intercepts) after enhancement by a commercial drawing program.

The effect of this procedure is to drastically reduce the degrees of freedom assigned to many data sets, especially if 1 or 2 of the points in the set are much more concordant than the rest. So the data sets which are most appropriate for the MODEL-4 approach are those with a large number of points that are relatively evenly-spaced along a linear trend. Data sets with few points may have MODEL-4 errors that are very large, due to the large (up to several tens or even hundreds) Student's-t multiplier invoked. You can tell the value of N' used by the algorithm from the printout, which refers to the *Number of Equivalent "Points"*.

ERROR ENVELOPES FOR YORKFIT LINES

Once the Yorkfit regression line has been plotted, you can request that the 95%-confidence limit error-envelope about the line be plotted by pressing E (Figure 3). The true regression line will fall somewhere in the area defined by this envelope 19 times out of 20.

⇨ *Don't use the error envelope for evaluating outliers.* The error envelope has nothing to do with the expectation of finding individual *data points* within it (a common misconception). This should be
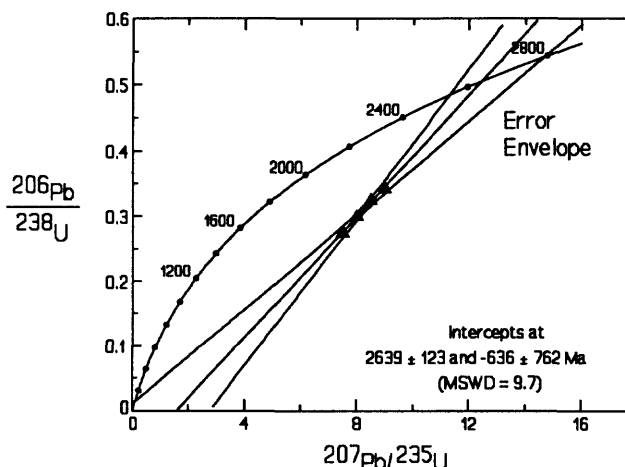
Figure 3: Conventional concordia plot with error envelope about Yorkfit line.

clear if you realize that for an infinite number of points, the error-envelope will contract until it is infinitely thin, excluding all of the points no matter how small their scatter.

OBTAINING ISOCHRON AGES FROM YORKFIT LINES

If your plot is an isochron plot (including Rb/Sr, Sm/Nd, Pb-Pb, U-Pb, Th-Pb, Re-Os, Lu-Hf, K-Ar, K-Ca, and $^{230}Th/^{232}Th$-$^{238}U/^{232}Th$), the computer will automatically calculate an isochron age and error from the Yorkfit results. The decay constants used are those recommended by the I.U.G.S. Subcommission on Geochronology (Steiger and Jäger, 1977), though you can change them if you wish (see the section on *CHANGING DECAY CONSTANTS AND MODEL-AGE PARAMETERS*). Sm-Nd isochron regressions will also yield the calculated ε_{CHUR} for the initial ratio. $^{230}Th/^{232}Th$-$^{238}U/^{232}Th$ isochron regressions will request a value for the $^{234}U/^{238}U$ activity ratio of the samples before calculating an isochron age.

A WORD ABOUT 3-POINT ISOCHRONS

You should be aware that the actual uncertainties of isochron ages for regression lines with only 3 or 4 data points and no apparent "geological" scatter can be significantly greater than the uncertainties calculated by most regression algorithms, including that of *Isoplot*. The reason for this is that with only 1 or 2 degrees of freedom (3 or 4 data points), the probability of getting an MSWD[1] of close to 1 even though some "geological" scatter exists in the population is significantly greater than zero. 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. For this reason, you should avoid the use of 3-point isochrons or concordia chords if possible.

COMMENTS ON *Isoplot*'S CONCORDIA-INTERCEPT ERRORS

Occasionally, a user will comment that the concordia-intercept errors from *Isoplot* seem unreasonably high, especially compared to published errors calculated by other methods. The reason is usually one of the following:

✧ **Confusion between whether a given regression program is asking for 1σ or 2σ/95%-confidence errors.**

If one responds with 1σ errors when the program is expecting 2σ errors, and if the MSWD of the regression is not much more than one, the resulting errors will be too low by a factor of 2.

✧ **Incorrect assignment of error correlations.**

Normally, data on the conventional concordia diagram are *very* highly correlated - typically in the range of 0.97 to 0.99999. If some arbitrary value such as 0.7 or 0.9 or even (God forbid) 0 is used, the mathematics of the York algorithm will, in effect, assume a much larger radiogenic $^{207}Pb/^{206}Pb$ than is probably the case. For example, if X- and Y-errors of 1% and an error-correlation of 0.7 are assigned, the implicit error in the radiogenic

---

[1]MSWD = <u>M</u>ean <u>S</u>quare of <u>W</u>eighted <u>D</u>eviates. This does not refer to porcine perverts; it is a measure of the ratio of the mean *observed* scatter of the points from the best-fit line to the scatter *predicted* by the assigned errors (and error correlations) of the points. 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.

$^{207}Pb/^{206}Pb$ is 0.77% -- much larger than the typical errors of .05% - .10%. As a result, the MSWD of the regression may be grossly underestimated (with especially dramatic possible effects on 3- or 4-point chords). Note that the printout for a (conventional) concordia-plot Yorkfit always shows the $^{207}Pb/^{206}Pb$ errors corresponding to the assigned $^{206}Pb/^{238}U$-$^{207}Pb/^{235}U$ errors and error-correlations, so you can judge for yourself if your assigned error-correlations are reasonable.

Pb-isotope data are also usually very highly correlated, with the exception of data for those 207/206-204/206 plots where the 204/206 ratio is much less precise than the 207/206 ratio. Note that this is *not* the case for 207/206-204/206 data for common Pb, where almost all of the errors generally arise from mass-fractionation uncertainty.

✦ **Use of *2σ* (or even worse, *1σ*) regression uncertainties instead of 95%-confidence limit for regressions with excess scatter.**

1σ regression errors for small ($N<\sim10$) data-sets with significant non-analytical scatter do *not* in themselves say anything about a confidence limit. They are not even the "true" standard deviations of the regression parameters (slope, intercept...) -- just the *best estimate* of the standard deviations for that data set, and in fact have a significant uncertainty in themselves. The smaller the data set, the larger this uncertainty becomes.

The solution to this problem is the use of confidence limits for small data-sets. Confidence limits are obtained by multiplying the *estimated* "1σ" errors by a numerically-derived fudge-factor ("Student's-*t*"). Student's-*t* factors are a function of the degrees of freedom of the data-set (N-2 for a linear regression) and the confidence level of interest. For a large number of points, the 95%-confidence limits and the 2σ errors become very similar. By convention, this confidence limit is usually at the 95% level (so the true value will lie outside the 95%-confidence limits only 1 time out of 20). It is my contention, as well as that of many other workers, that use of "1σ" regression errors for small data-sets with excess scatter borders on deliberate deception. In the worst case (a 3-point regression), the 1σ errors are a factor of almost 13 smaller than the 95%-confidence errors, and offer little in the way of useful geologic constraints.

✦ **Calculation of the concordia-intercept uncertainties from only the *slope* error, while ignoring the contribution from the *intercept* or *centroid* error.**

In the past, some workers have estimated concordia-intercept uncertainties by calculating the intercepts of the upper and lower extremes of the slope of the best-fit line when constrained to pass through its centroid. This procedure ignores the effect of the uncertainty of the location of the centroid itself, resulting in an underestimate of the concordia-intercept uncertainties that is greatest for data points whose centroid is nearly concordant. Note that if one ignores the centroid uncertainty, then no matter how much scatter exists for an array of points whose centroid lies close to concordia, the calculated intercept-error will be zero.

✦ **Calculation of the slope- and intercept-errors from only the propagated analytical errors but ignoring the scatter of the points.**

If one is sure that analytical errors can be the sole reason for point scatter, then it is true that the appropriate way of estimating the regression-line errors are by simply propagating the analytical errors, without even the application of the Student's-*t* factor (though Student's-*t* should have been used in the calculation of the analytical errors). In many real-world instances, however, it is quite clear that the analytical errors are not the cause of most of the scatter (the probability figure shown in *Isoplot*'s printout can be used as a guide). In such

cases, it is evident that the precision of the regression line should reflect the actual scatter of the points, for example by multiplying the *A Priori* errors by the square root of the MSWD parameter. There are programs in use, however, which ignore the scatter of the points even when this scatter grossly exceeds that predicted by the analytical errors. Such a procedure makes little sense.

FITTING A CURVE TO DATA

POLYNOMIAL CURVES

To request a polynomial regression on data you've just plotted, press F9 from the *MORE POINTS* screen and specify the order of the polynomial for regression. This regression weights the points equally, uses the Y values as the dependent variables and the X values as the independent variables. *Note: Isoplot doesn't offer the polynomial-regression option for either concordia plots or common-Pb isotope plots.*

SPLINE CURVES

If a polynomial curve doesn't adequately describe the trend of the data, you may want to try fitting a spline curve (F6 from the *MORE POINTS* screen, *except for concordia and common-Pb plots*). Examples of spline curves are shown in Figures 4 and 5. The SPLINES menu offers the options below:

```
F1  HELP                F2  Akima Spline        F3  Normal Spline
F4  Smooth Spline        F5  Sr Ages            F10 Alpha/Graphics
```

A spline curve is a collection of cubic polynomials that connect a set of X-Y points without breaks in slope. Two disadvantages of spline curves are that (1) there is no convenient analytical expression for them (because they're a collection of many different polynomials), and (2) there is no really satisfactory analytical expression for the error of the curve.
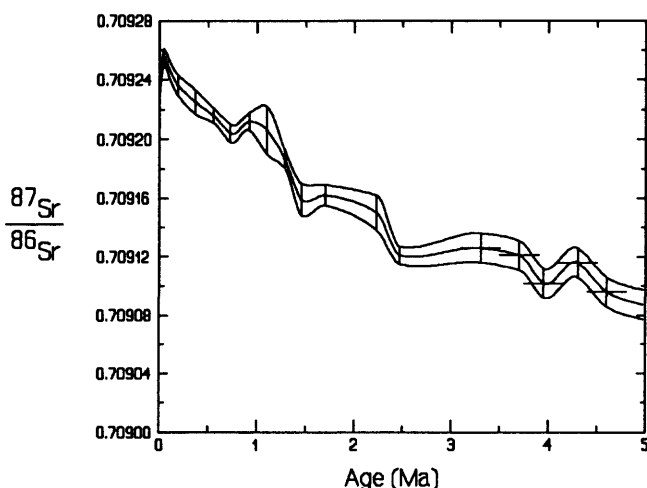
Akima Splines (Akima, 1970) will yield a curve that may bend sharply towards the next point, as the curve proceeds from left to right. This type of curve is especially suitable if you believe that data-points strongly constrain the local location of the curve. The **Akima Spline** option will also construct curves through the upper and lower Y-error limits if errors were entered when you plotted the data. The X-errors will be ignored, though.

Figure 4: Example of Akima-method splines, with error envelope.

Normal Splines tend to curve less sharply than the **Akima Splines**, though at the expense of possible overshoots and oscillatory artifacts. Try both types of splines to see which is the most useful for your data.

Smooth Splines are useful if you don't want the spline to be forced through every point, because you've plotted a large number of points that scatter about any reasonable curve. A **Smooth Spline** is constructed through the points in a least-squares sense, and is especially useful for data sets with significant scatter due to geological or analytical error.
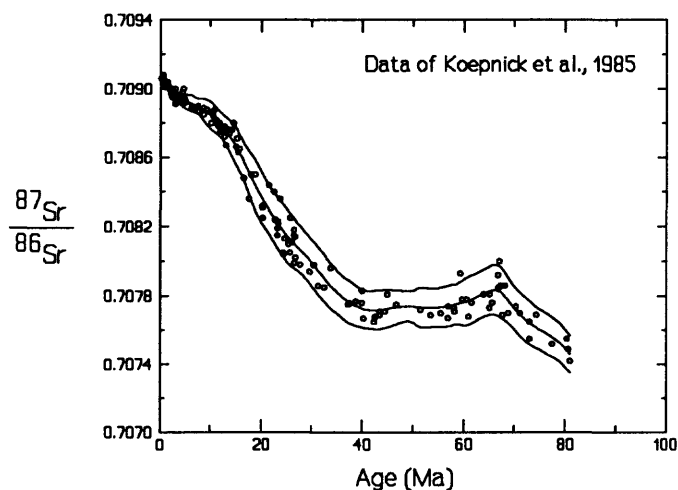
Figure 5: Example of smoothed spline, with error envelope.

For a smooth spline, you'll have to specify the minimum X-interval over which the curve-segments will "pay attention" to the data, and the minimum number of points to be used for each segment. The curve is constructed as a sort of moving average, in which only a quarter of the curve-segment is drawn for each least-squares fit. The larger the X-interval specified and the larger the minimum number of points for each interval, the more smoother the curve will be. Experiment.

You also have the option of plotting the "error-envelope" of the smoothed spline. This "error envelope" is another pair of spline curves that should enclose most of the data points defining the smoothed spline, and will pinch and swell according to the local scatter of points along the spline. This envelope does not have rigorous statistical significance, however, and should be used mainly as a *visual* guide to the relative precision of the curve.

CREATING U-Pb CONCORDIA PLOTS

If your plot is a U-Pb isotope concordia plot (Figures 2, 3, 6, 7), you'll find a few differences from the normal X-Y plotting routines. To select a conventional ($^{206}Pb/^{238}U$ vs. $^{207}Pb/^{235}U$) concordia plot, press C from the starting screen. To select either a Tera-Wasserburg ($^{207}Pb/^{206}Pb$ vs. $^{238}U/^{206}Pb$) or a Tatsumoto-style ($^{206}Pb/^{207}Pb$ vs. $^{235}U/^{207}Pb$; Tatsumoto et al., 1972) concordia plot, press T from the starting screen. You can then either specify the plot limits in terms of minimum and maximum *ages* to be shown, or (by pressing F2) define the limits of the concordia plot in terms of its X- and Y-limits.

When you request a Yorkfit through data on a Concordia plot, the program will automatically calculate the intercepts of the Yorkfit line with the concordia curve, and the uncertainties of those intercepts. These uncertainties are calculated using the algorithm developed by Ludwig (1980), and are printed out in two forms: symmetrical but approximate uncertainties, and the more accurate, asymmetric intercepts of the error-hyperbola. You can choose which to use.

FORCING A YORKFIT LINE THROUGH A SPECIFIED AGE

You can force a Yorkfit through a specified age on the conventional concordia curve from the **MORE POINTS** screen by pressing **F** (forced Yorkfit) instead of **Y**. *Isoplot* will ask you through what age (in Ma) to force the next Yorkfit line, and what uncertainty to assign to this forcing age. The uncertainty value is optional -- if you enter only one value, the uncertainty in the forcing age will be assumed to be zero. If you do enter an uncertainty value, the program will calculate the Yorkfit line and concordia intercepts three times, forcing the line through not only the forcing age but also the forcing age plus and minus its assigned uncertainty. The propagated uncertainties in the *unforced* intercept arising from this procedure will be included in the final age-uncertainties of the unforced intercept.

The uncertainty in the forcing age is assumed to be symmetric; that is, you can't enter a forcing age with uncertainties of +100 Ma and -50 Ma.

After any Yorkfit regression, the program will calculate the concordia intercepts of the Yorkfit line and its associated uncertainties, using the algorithm of Ludwig (1980). These intercepts will be labeled on the lower-right corner of the plot. Labels for each successive solution for a given plot will be stacked on top of the previous labels.

TERA-WASSERBURG AND TATSUMOTO-STYLE U-Pb CONCORDIA PLOTS

For the conventional concordia diagram, with radiogenic $^{206}Pb/^{238}U$ versus $^{207}Pb/^{235}U$, the X- and Y-errors in the data are generally highly correlated, and must be accurately estimated for a valid Yorkfit. In the Tera-Wasserburg concordia diagram (Figure 6; Tera and Wasserburg, 1972), however, radiogenic $^{207}Pb/^{206}Pb$ is plotted against $^{238}U/^{206}Pb$: if the common-Pb correction is not large, the errors in these values are only slightly (anti-) correlated. Thus the analyst can use an approximation of zero for the error correlations without much effect on the Yorkfit line or errors. Another advantage is that even for relatively young age-segments, the Tera-Wasserburg diagram is sufficiently
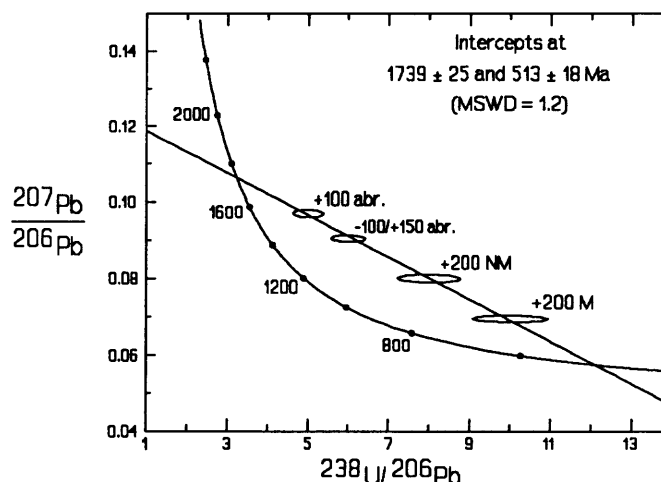
Figure 6: Tera-Wasserburg concordia plot.

curved to allow discordant points to be evident. A variation on the Tera-Wasserburg concordia plot is the Tatsumoto-style concordia plot (Tatsumoto et al., 1972), wherein radiogenic $^{206}Pb/^{207}Pb$ is plotted against $^{235}U/^{207}Pb$ (Figure 7). This type of plot is particularly suited to the plotting of data for Phanerozoic uranium ores, for which continuous-diffusion loss of ^{238}U radioactive daughters affects all ratios for ^{206}Pb. In the Tera-Wasserburg plot, ^{206}Pb appears in the ratios for both axes, whereas in both the conventional and Tatsumoto-style plots, ^{206}Pb is restricted to only one axis. Note, however, that though the error correlations for the Tatsumoto style plot are less than for the conventional concordia plot, they can still be significantly nonzero (even close to 1, if the common-Pb corrections were large).

Differences in the use of the non-conventional concordia plots include:

❖ Error-box and error-cross plotting-symbols are permitted, as the errors may be sufficiently uncorrelated to make these a valid representation;

♦ Rigorous comparison of Yorkfit calculations for the two types of concordia diagrams is logical only for Model-1 fits; even then, you'll have to use the correct errors and error-correlations. The formulae for transforming conventional-plot errors to the Tera-Wasserburg or Tatsumoto-style errors and error-correlations are:

$$X = {}^{207}Pb/{}^{235}U \qquad Y = {}^{206}Pb/{}^{238}U$$

$$X' = {}^{235}U/{}^{207}Pb = \frac{1}{X} \qquad X'' = {}^{238}U/{}^{206}Pb = \frac{1}{Y}$$

$$Y' = {}^{206}Pb/{}^{207}Pb = \frac{137.88\,Y}{X} \qquad Y'' = {}^{207}Pb/{}^{206}Pb = \frac{X}{137.88\,Y}$$

$$E_{Y'} = \sqrt{E_X^2 + E_Y^2 - 2\rho_{X,Y}E_X E_y}$$

$$\rho_{X'',Y''} = \frac{E_Y - E_X \rho_{X,Y}}{E_{Y''}}$$

$$\rho_{X',Y'} = \frac{E_X - E_Y \rho_{X,Y}}{E_{Y'}}$$

where E refers to the error in percent, and ρ to the error correlations. Note that the equations for ρ given in Ludwig (1980, p. 216) are wrong. Sorry about that.

CONTINUOUS-DIFFUSION CURVES FOR COUPLED LEAKAGE OF RADIOGENIC-Pb AND ^{238}U RADIOACTIVE DAUGHTERS

Some systems -- notably low-temperature uranium ores and low-temperature uraninite (pitchblende) and coffinite -- continuously leak both radiogenic-Pb and one or more of the several radioactive daughters of uranium. For many such systems, the ratio of the leakage of Pb to the radioactive daughters was evidently roughly constant over the age of the material, so that a particular type of continuous-diffusion curve can be useful in evaluating the age of the material (Ludwig, Simmons, and Webster, 1984).

To construct such a curve (Figure 7), press F9 from the MORE POINTS screen. *Isoplot* will ask you to specify the age of the system and the ratio of diffusion constants for Rn compared to Pb, divided by 10^{10}. Radon may not, in fact, have been the actual daughter that was leaking out of the system (Radium seems to be the dominant wanderer in many cases), but the shape of the curve is the same for any daughter. Try diffusion-constant ratios in the range of 0.5 to 10 ($x10^{10}$) to get a feeling for the shape of the curves. For any specific set of data points, you'll have to find the best-fit curve by a trial-and-error process of varying the assumed age of the system and the assumed diffusion-constant ratio. There is no provision for estimating errors.

FITTING A PLANE TO X-Y-Z DATA

Though *Isoplot* can only plot data on the X-Y plane, you can enter data as 3-dimensional, X-Y-Z values, and have *Isoplot* determine the corresponding best-fit plane. The algorithm of Kent *et al.* (1990) is used for the plane-fit: this method weighs the points according to the X-Y-Z errors of the points *and* the 3 corresponding error-correlations.

ENTERING X-Y-Z DATA FROM THE KEYBOARD

Select an X-Y or concordia plot as usual from the starting screen, and define the X-Y plot (or concordia age) boundaries. From the data input screen, press the XYZ Data key (F5). Enter the data-point values in two parts for each point.

Figure 7: Tatsumoto-style concordia plot with coupled diffusion-loss curve for radioactive and stable daughters of uranium.

First, enter the X-Y-Z values and errors as either 3 (X-Y-Z values only) or 6 (X-Y-Z values and X-Y-Z errors) numbers. If the errors are the same for all of the points, you can enter just the X-Y-Z values now, and the errors as a single entry for all of the points later. Next, enter 0, 1, 2, or 3 numbers to define the X-Y, Y-Z, and X-Z error-correlations, respectively. If you enter just 1 number, it will be assigned as the X-Y error-correlation, and the Y-Z and X-Z correlations will be assigned a value of zero. If you enter 2 numbers, they will be assigned to the X-Y and Y-Z correlations, respectively, and the X-Z correlation will be zero. Or, press ◄─┘ without any numbers to assign values of zero to all 3 correlations (you can enter group values later, if you wish).

ENTERING X-Y-Z DATA FROM A FILE

From the Datafile screen, press the XYZ Data key (F5) before you select a file. Select a file, and choose the columns for X, X-error, Y, Y-error and X-Y error-correlation as usual. A second query will than ask you for columns of the Z, Z-error, Y-Z error-correlation, and X-Z error-correlation. Enter 1, 2, 3, or 4 values. Unspecified parameters will be assigned values of zero, as usual.

REGRESSING

Once the X-Y values of 4 or more points are plotted, press P (Plane Fit) from the MORE POINTS screen to request a best-fit plane to the points. *Isoplot* will calculate the least-squares solution to the equation

$$Y = aX + b + cZ$$

including errors and error-correlations for a, b, and c. The MSWD parameter is the same as for linear regressions (Yorkfits), and indicates how closely the scatter of the data-points from the best-fit matches the scatter predicted by the assigned errors and error-correlations. The weighted residuals given by *Isoplot* for

each point are the ratios of the observed scatter from the plane to the predicted scatter from the plane. The line drawn on the X-Y plane by *Isoplot* is the intersection of the best-fit plane with the X-Y plane, and the error-envelope the intersection of the error-hyperboloid with the X-Y plane.

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 more than 15%, 1.96 times the 1-σ *a priori* errors will be used as the 95%-confidence error-estimate for the plane parameters. If less than 15%, the 1-σ *a priori* errors will be expanded by the Student's-*t* factor for N-3 degrees of freedom. The latter case is equivalent to expanding the analytical errors until they predict precisely the actual amount of scatter, but keeping the weighting of the points proportional to the analytical errors.

You may want to plot the *projection* of the X-Y-Z points on the X-Y plane. To do so, enter any value to the query:

```
Z-value of projection-pt. on Y-Z plane (ENTER for parallel to Z)?
```

The subsequent screen asks you to select a plotting-symbol for the projected points. Unless you enter a nonzero value in response to the query above, the points will be projected to the X-Y plane parallel to the Y-Z plane (Figure 8). If you enter a nonzero value, the points will be projected through a point on the Y-Z plane with the Z value specified, and a Y-value that lies above (or below) the best-fit plane by the same amount as the actual data-point. This feature is useful in the case of Tera-Wasserburg-style 3-dimensional concordia plots, where you might want to see the shift of the points in both the X and the Y directions as if you knew the actual $^{204}Pb/^{206}Pb$ of the initial Pb.

SOLUTIONS FOR 3-DIMENSIONAL CONCORDIA-PLOT DATA

Two-dimensional (X-Y) concordia plots assume that the initial-Pb of the system is both precisely known and invariant. This assumption is essentially fulfilled for cases where the Pb is very radiogenic, or where the analyst has great confidence in the choice of initial Pb (perhaps from a cogenetic feldspar that is known to have been undisturbed -- a rare case, incidentally). But if the ratio of radiogenic Pb to common Pb is low (say, $^{206}Pb/^{204}Pb < 100$), or the isotopic composition of the initial Pb is suspected to be strange, the 3-dimensional concordia approach can provide significant benefits (Levchenkov and Shukolyukov, 1970; Neymark and Levchenkov, 1979; Wendt, 1984; Zheng, 1989).

Briefly, the 3-dimensional concordia-plot approach involves adding a third, Z-axis which contains ^{204}Pb to the X-Y concordia-plot axes. The three possible concordia-plots are then:

$$^{207}Pb/^{235}U - {}^{206}Pb/^{238}U - {}^{204}Pb/^{238}U,$$

$$^{238}U/^{206}Pb - {}^{207}Pb/^{206}Pb - {}^{204}Pb/^{206}Pb,$$

and

$$^{235}U/^{207}Pb - {}^{206}Pb/^{207}Pb - {}^{204}Pb/^{207}Pb.$$

Unlike 2-dimensional concordia plots, the Pb-isotopic abundances for the above axes must be *un*corrected for initial Pb (a correction for blank Pb should be applied, though, unless blank Pb accounts for essentially all of the common Pb, and its composition is poorly known).
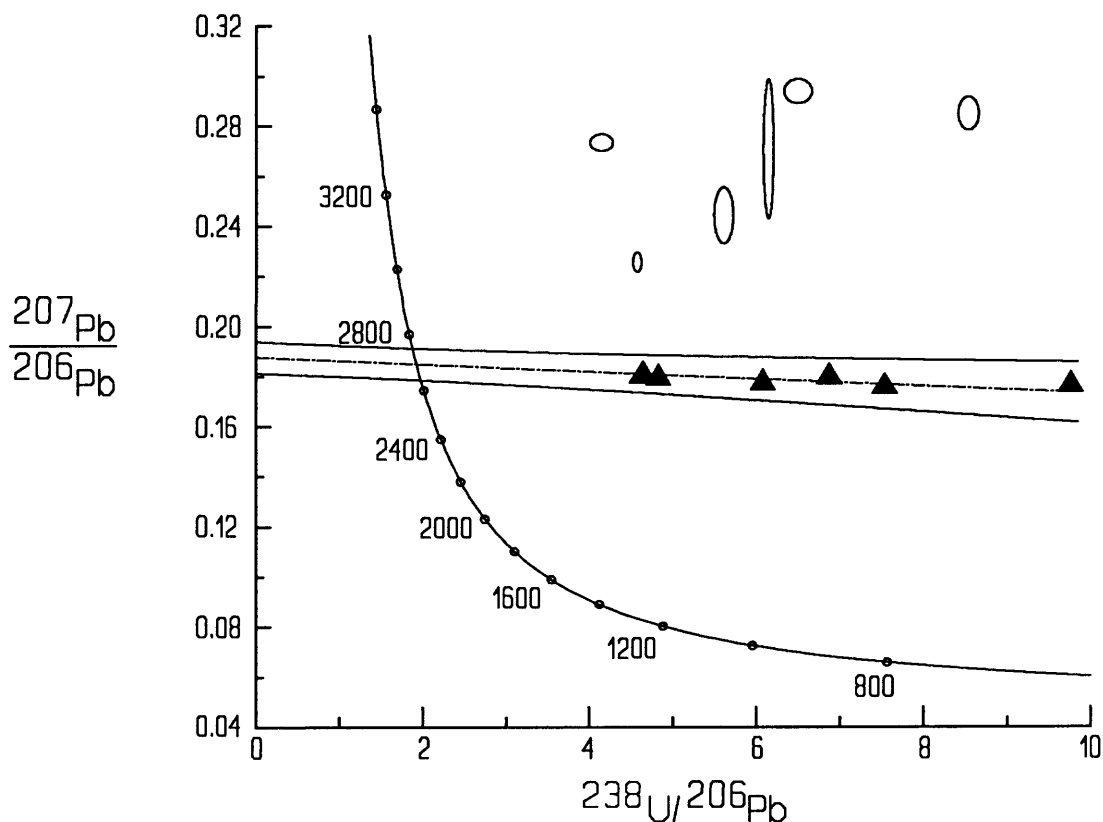
Figure 8: Planar solution to 3-dimensional concordia-plot data (ellipses), with projected points (triangles) and error-envelope.

If the data-points on the 3-dimensional concordia plot represent systems that have

(1) experienced no more than 1 disturbance involving U/Pb fractionation,

(2) have no inherited, older component (except for special cases), and

(3) have either an initial-Pb isotopic composition that is common to all points, or an initial-Pb isotopic composition that falls along a straight line on a ^{206}Pb - ^{207}Pb - ^{204}Pb diagram but with no secondary-disturbance event,

then the points will define a plane. As for the 2-dimensional concordia diagram, the intersection of the best-fit plane with the concordia curve on the X-Y plane of the 3-dimensional concordia diagram defines the primary age and disturbance age. The intersection of the best-fit plane with the Y-Z plane (^{204}Pb/^{206}Pb - ^{207}Pb/^{206}Pb) of the Tera-Wasserburg style 3-dimensional concordia diagram (Figure 8) defines the possible loci of the best-fit initial-Pb to the data, so that the user can evaluate whether the 3-dimensional concordia-plot solution is geochemically realistic. In other words, if the planar solution required the initial Pb to have a ^{207}Pb/^{204}Pb of 10 at a ^{206}Pb/^{204}Pb of 18, one would have cause to doubt the results.

If the plot is a concordia plot, *Isoplot* will determine the concordia-intercept ages and uncertainties for the best-fit plane. If a Tera-Wasserburg style concordia plot, the intercepts of the best-fit plane with the currently-defined single-stage Pb-isotope growth curve will also be given.

For 3-dimensional concordia-plot solutions, it is essential that the user evaluate the reasonableness of the fit of the plane, as given by the MSWD parameter and the weighted residuals of the points. If the MSWD is so large (more than 5 or 10) that there must be a significant amount of non-analytical scatter, you should consider using the 2-dimensional plot instead (with accurately calculated errors and error-correlations!), to guard against the possibility that the planar-fit procedure achieves its fit only by demanding a physically unreasonable isotopic composition for the initial Pb. Such a spurious solution is quite possible if the data come from a population with significant multi-episodic disturbance and/or inheritance.

Error correlations for 3-dimensional concordia-plot data: If you're plotting 3-dimensional data for a Tera-Wasserburg concordia plot, you may be able to approximate the X-Y-Z error-correlations by zero *providing that*:

(1) The (external) precision on the $^{204}Pb/^{206}Pb$ and $^{207}Pb/^{206}Pb$ measurements is *not* dominated by the variability in mass fractionation (generally true if the $^{204}Pb/^{206}Pb$ is very low). Otherwise, (e.g. for high $^{204}Pb/^{206}Pb$) the $^{204}Pb/^{206}Pb$ and $^{207}Pb/^{206}Pb$ ratios can be highly anti-correlated; and

(2) Blank-Pb corrections on the $^{204}Pb/^{206}Pb$ and $^{207}Pb/^{206}Pb$ ratios are small (less than a few percent). Otherwise, the uncertainty in the amount and composition in the blank Pb will cause the uncertainty in the blank-corrected $^{204}Pb/^{206}Pb$ and $^{207}Pb/^{206}Pb$ ratios to have a significant *positive* correlation. Note that in the case of analyses of very small amounts of zircon, this situation is quite common.

For the conventional 3-dimensional concordia plot ($^{207}Pb/^{235}U$ - $^{206}Pb/^{238}U$ - $^{204}Pb/^{238}U$), all 3 error correlations are generally very high. Despite claims to the contrary, ignoring the error correlations for even Tera-Wasserburg concordia plots can have a significant effect on the results -- especially the MSWD value. Versions of *PBDAT* (Ludwig, 1988) later than 1.20 will calculate the error correlations for 3-dimensional concordia data.

OBTAINING GROWTH CURVES FOR Pb-ISOTOPE PLOTS

If your plot is either for $^{207}Pb/^{204}Pb$-$^{206}Pb/^{204}Pb$ or for $^{208}Pb/^{204}Pb$-$^{206}Pb/^{204}Pb$, and you want *Isoplot* to construct a single-stage Pb-isotope growth curve on the plot (Figure 9), press **F9 (Growth Curve)** from the **MORE POINTS** screen. You must then select:

```
S        Stacey-Kramers Growth-Curve

O        Other Growth-Curve (you specify)

Esc      No Growth-Curve
```

If you press S, the program will draw a single-stage Pb-isotope growth-curve using the constants suggested by Stacey and Kramers (1975). If you press O, the program will ask you to define your own single-stage growth curve, requesting: (1) the starting age of the system, (2) the initial isotope ratios, (3) the μ^1 of the source, and, for $^{208}Pb/^{204}Pb$-$^{206}Pb/^{204}Pb$ plots, (4) the Th/U of the source. The screen will look like this:

---

[1]μ (Mu) is defined as the $^{238}U/^{204}Pb$ of the system, normalized for U-decay to the present day.

```
╔═══════════════════════════════════════════════════════════════════╗
║          SINGLE-STAGE Pb-ISOTOPE GROWTH-CURVE                      ║
║                                                                   ║
║              206/204 AT START OF GROWTH ... 11.152                 ║
║              208/204 AT START OF GROWTH ... 31.230                 ║
║        Mu (present-day 238/204) of source ==> 9.74                 ║
║              present-day 232/238 of source ... 3.78                ║
║       Time before present (Ma) at growth-start ... 3700           ║
║        (add an asterisk to specify a starting-                    ║
║         age on the current growth-curve)                          ║
║                                                                   ║
╠═══════════════════════════════════════════════════════════════════╣
║ F5 Restore Stacey-Kramers            ENTER Enter response          ║
║ F9 Recall          Esc Exit Form     CTRL-ENTER done              ║
╚═══════════════════════════════════════════════════════════════════╝
```

Use the arrow-keys to move the cursor to the value you want to change, type in the value and press ←─┘. You needn't change values which are already acceptable. To restore the values in the form to the standard Stacey-Kramers values (Stacey and Kramers, 1975), press **F5**.

If you want to start a new growth curve at some particular age on the growth curve defined by the parameters first appearing on the screen, you can have the program calculate the appropriate 206/204 and 207/204 or 208/204 ratios for this age by entering the age with an asterisk in the "Time... at start of growth" cell. For example, if you wanted to construct a growth curve that started from the Stacey-Kramers curve at 2700 Ma and evolved with a μ of 12, you would:

1) press **F5** to restore the Stacey-Kramers values (if the initial values on the screen were not the Stacey-Kramers values);

2) type in **2700*** in the "Time..." cell and press **CTRL ←─┘**. The 206/204 and 207/204 or 208/204 values immediately change to the values defined by a 2700 Ma age on the Stacey-Kramers growth curve;

3) enter a value of 12 in the "Mu" cell and press **CTRL ←─┘**.

Once you select a growth curve the screen will show:

```
┌─────────────────────────────────────────────────┐
│                                                 │
│    T  Suppress ticks and tick-labels            │
│                                                 │
│    L  Suppress tick-labels only                 │
│                                                 │
│    C  Draw a complete curve with labelled ticks │
│                                                 │
│   Esc  No growth-curve                          │
│                                                 │
└─────────────────────────────────────────────────┘
```

Because the plot may become too cluttered if the age-ticks and age-tick labels of the growth curve are included, you can select how much labeling you want to include.

If you request a Yorkfit for data on a $^{207}Pb/^{204}Pb$ - $^{206}Pb/^{204}Pb$ plot that contains a growth curve, *Isoplot* will solve for the growth-curve intercepts as well as the $^{207}Pb/^{206}Pb$ age of the Yorkfit line.
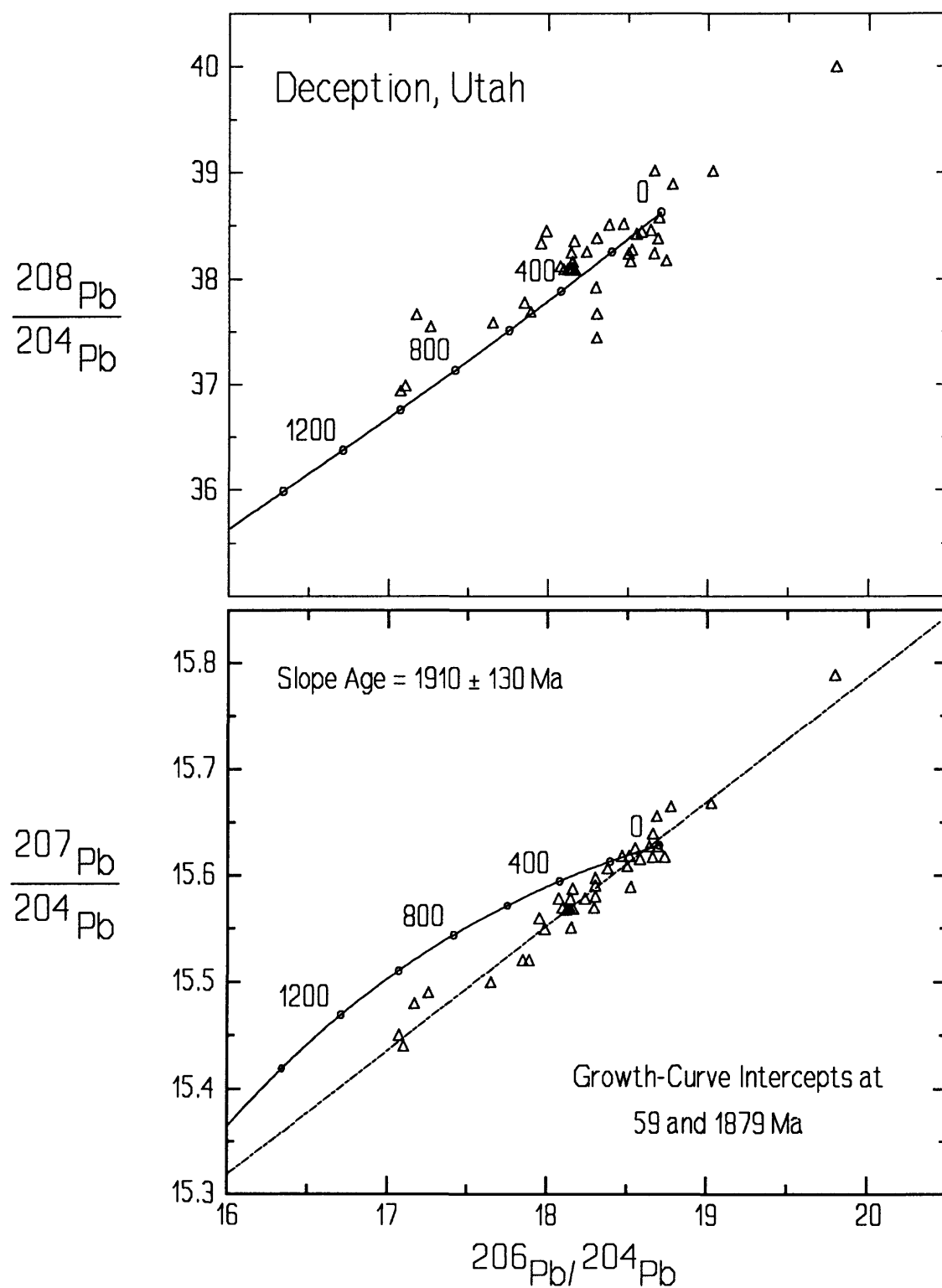
Figure 9: Common-Pb plot with single-stage growth curves. Created by stacking two plots with the ADD PLOT option.

OBTAINING ^{230}Th/^{238}U - ^{234}U/^{238}U CONCORDIA CURVES

If *Isoplot* recognizes from the X- and Y-axis names that you may be plotting ^{234}U/^{238}U activity ratios against ^{230}Th/^{238}U activity ratios, **F2** will be labeled as **Draw Concordia** in the "Select Plotting-Symbol" screen. Pressing **F2** will bring up this FORM:

Enter the ages at which the evolution curve is to start and end, and specify the locations of the age ticks for the curve. If you don't want any age ticks, enter 0 for the age-tick interval. Enter all ages in ka (thousands of years).

```
            Th-230/U-234 Concordia Curve

                Starting Age (ka) ==> 0
                  Ending Age (ka) ... 250

                First Age-Tick (ka) ... 0
            Age-Tick Interval (ka) ... 50

Initial U-234/U-238 Activity Ratio ... 1.1479

            Label Age-Ticks (Y/N)? ... Y
```
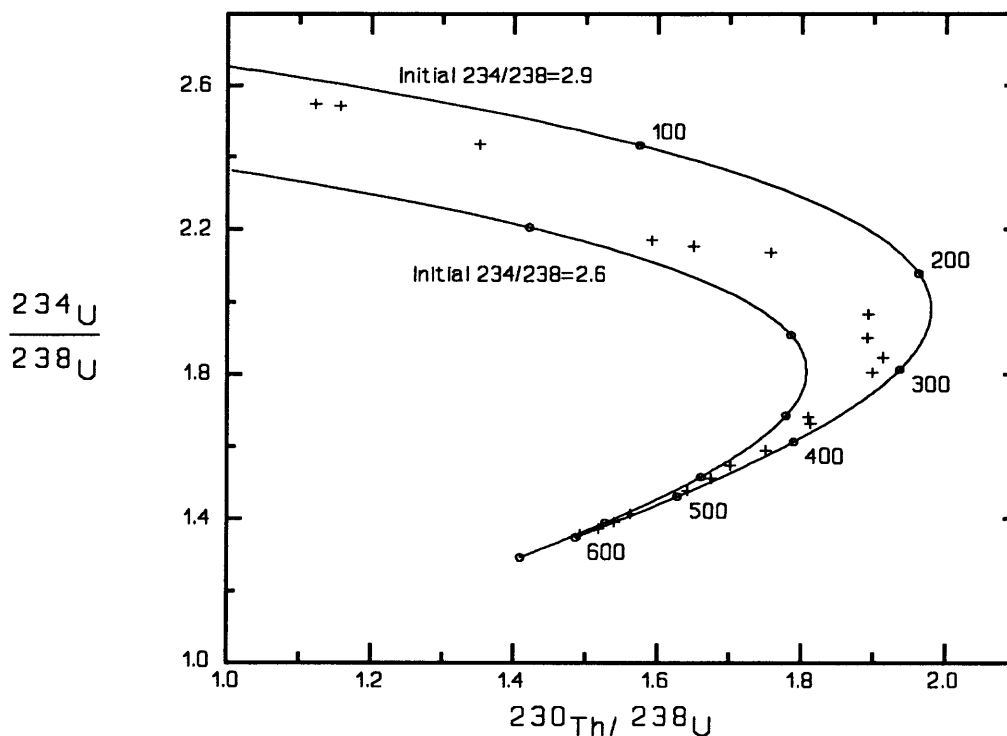

Figure 10: U-series evolution curves for two different initial ^{234}U/^{238}U values.

CALCULATING WEIGHTED AVERAGES OF A SINGLE VARIABLE

You can use *Isoplot* to calculate weighted averages of a single variable by pressing A from the starting screen. *Isoplot* will then ask for data and errors for only one variable rather than two, will use the Y-axis to show that variable, and use the X-axis to show the "set number" of the data points (Figure 11).

You can use data from a datafile just as for X-Y plots, except that you'll be asked to specify only two columns (the values and their errors) of data. Request datafile access *after* you've specified a weighted-averages plot (otherwise, the datafile's Y-values will be mistakenly used as the errors for the weighted averages).

If there is no excess scatter of the data being averaged (that is, the MSWD is not much greater than 1), the weighted averages algorithm simply weights each point by its inverse variance and calculates the uncertainty in the average value from the assigned uncertainties for each point. *If there is excess scatter (MSWD significantly >1), the average is*

Weighted Average = 2611 ± 6.5 (.25%)   95% Confidence Limit

external population error = 3.2 (1.2%)

M.S.W.D. = 2.9   Probability = 0

Robust (Biweight/9) "Average" = 2610.2 ± 7.5   (Gaussian)

Figure 11: Example of weighted averages plot, with optional biweight-statistics calculation.

calculated by assuming that the data scatter due to a combination of their assigned errors plus an unknown, "external" variance that has a normal (Gaussian) distribution[1]. In these cases, the most probable value of the "external sigma" arising from the external variance is also calculated.

Unless outlier rejection is specifically disabled with the F2 toggle (from the data-input screen), the weighted averages algorithm will reject outliers that are distinguishable from the weighted average value at the 95%-confidence level. Multiple passes of rejection are permitted by the algorithm, but the criteria for rejection become more stringent with each pass so that excessive outlier rejection is minimized. You can also request "robust" (Tukey's Biweight) data-averaging with the F3 toggle from the data-input screen, though you would normally do this with the **Histogram** option (see below). Note that this procedure ignores (and does not need) both the assigned errors and the outlier-rejection toggle.

OBTAINING A HISTOGRAM PLOT

If you want to look at one-dimensional data (that is, only X- or only Y-values, as opposed to X-Y pairs) *without* regard to assigned errors, you should use the Histogram Plot option (Figure 12): press H from the starting screen of *Isoplot*. The resulting FORM will be:

The first 3 parameters of the FORM specify the upper- and lower-limits of the values to be shown on the histogram, and the width of the histogram cells. If you don't have specific requirements in mind, press F2 and *Isoplot* will scale the histogram for you.

---

[1]The algorithm for this approach was developed by Brent Troutman of the U.S. Geological Survey.

```
                    HISTOGRAM PLOT

                    Lower limit of data ==> ??
                    Upper limit of data ... ??
                            Cell-width ... ?
                             Data name ... ?

      Gaussian Statistics [mean/sigma] (Y/N) ... N
                          Median/MAD  (Y/N) ... N

                    Biweight Statistics:
        Specify tuning constant of 6 or 9
                        (0 to decline) ... 9

 F1 HELP
 F2 Autoscale                               ENTER Enter response
 F9 Recall               Esc Exit Form      CTRL-ENTER Done
```

You can select one or all of 3 different ways of calculating "mean" and "standard deviation" for the data. The first (**Gaussian Statistics**) is the usual mean and estimated standard deviation. *Isoplot* will also evaluate whether the data conform to a Gaussian distribution, at the 95%-confidence limit. The second calculates the median of the data, and the *M*edian *A*bsolute *D*eviation from the median (**MAD**).

The third invokes the Tukey's Biweight algorithm (Hoaglin, Mosteller, and Tukey, 1983), which yields a very robust (insensitive to outliers or distributions with heavy tails) estimate of the "average" for most data sets. Outlier rejection is neither necessary nor desirable with this approach. You must select a "tuning constant" of 9 or 6: the latter value gives results that are the least sensitive

Mean = 2610 ± 7.5   Std. Dev. = 21   May be Gaussian
Median = 2614.5 ± 6.6   MAD = 11
Biweight "Mean" = 2610.5 ± 7.5   "Sigma" = 20

Figure 12: Example of histogram plot and calculations.

to outliers, at the expense of efficiency for near-normal distributions. If you invoke the Biweight procedure, *Isoplot* will also determine whether the distribution being "averaged" is a non-Gaussian one, at the 95%-confidence limit.

Note that the plus-or-minus values calculated for both the median value and the Biweight value are valid *only* if a dominant component of the data conforms to a normal distribution (note that the Gaussian distribution test examines only the entire data-set). That is, you should pay attention to the calculated uncertainties only if the data set can be regarded as from dominantly normal distribution, perhaps contaminated by one or more values that do not belong to the dominant distribution.

UTILITY FUNCTIONS FOR ISOTOPIC DATA

Several utility functions can be invoked from the starting-screen of *ISOPLOT*. These functions (press *L* to see a list) include:

Calculation of Radiogenic $^{207}Pb/^{206}Pb$ ages: -- Press **R**. Enter the radiogenic $^{207}Pb/^{206}Pb$ ratio together with the percent error in the ratio (optional) and the time that radiogenic Pb-isotope growth ended (also optional). If the second optional value is not entered, a value of zero is assumed (yielding the usual radiogenic 207/206 age).

Another way of obtaining a $^{207}Pb/^{206}Pb$ age with this function is to simply enter the observed $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$ ratios, separated by a comma. *Isoplot* will detect this type of input, and automatically calculate the age by assuming that the initial-Pb lies on the Stacey-Kramers Pb-evolution curve.

Calculation of Model-Pb age and μ: -- Press **P**. Enter the $^{206}Pb/^{204}Pb$ and $^{207}Pb/^{204}Pb$ ratios of the isotopic composition of interest. The program will calculate a model age and μ^1 assuming a Stacey-Kramers single-stage growth-curve.

Calculation Sm/Nd, Rb/Sr, Lu/Hf, or Re/Os Model-ages: -- Press **N, S, H,** or **O**, respectively. For Sm/Nd model ages, both CHUR and depleted-source model ages will be calculated, where the time-dependence of the depleted-source 143/144 ratio is modeled with a quadratic function. Enter the parent/daughter isotope ratio and the radiogenic-isotope ratio of the sample. You can change the source's assumed isotope ratios and depleted-source coefficients by pressing ALT-C from the starting screen.

Calculation of U-Series Ages: -- Press **U**. You can enter 1, 2, 3, or 4 values, corresponding to: the measured $^{234}U/^{238}U$ ratio, error in that ratio, the measured $^{230}Th/^{238}U$ ratio (or $^{230}Th/^{234}U$ ratio -- press F4 to toggle), and error in that ratio, respectively. You can enter the ratios either as *activity* ratios or as *atomic* ratios -- use the F2 key to toggle between the two formats. Enter the errors as either percent errors or absolute errors, depending on which option was invoked from the starting-display with F5. *Isoplot* will then calculate up to 4 values and associated errors:

1) a 234/238 age, assuming that the initial 234/238 was that of modern seawater;
2) a 230/238 (or 230/234) "undefined initial" age, using the observed 234/238 value;
3) the initial 234/238 activity ratio corresponding to the 230/238 "undefined initial" age, and
4) a 230/238 (or 230/234) "seawater initial" age, which assumes that the initial 234/238 was that of modern seawater.

For "undefined initial" 230/238 ages, there may be two solutions for 230/238 activity ratios greater than 1. If so, both solutions will be given.

The half-lives and seawater 234/238 activity-ratio used by these calculations can be changed from the **Decay Constants** screen (press ALT-C from the starting screen).

$^1\mu$ is $^{238}U/^{204}Pb$ normalized for decay of ^{238}U to the present day.

CALCULATION OF AGES FROM MARINE-CARBONATE SR-ISOTOPE RATIOS

One more utility function can be invoked from the **Splines** menu (p. 17), provided that you've just plotted data for a global-marine trend of Sr-isotope ratios versus age. These data can be either in the form of $^{87}Sr/^{86}Sr$ versus age, or as some simple function of $^{87}Sr/^{86}Sr$ (such as δ-values relative to modern seawater) versus age. The data-set for this trend is of your own choosing.

For examples, data selected from Koepnick and others (1986), Hess and others (1986), DePaolo (1986), and Capo and DePaolo (1986) have been put on the *Isoplot* disk and stored as files named MOBIL~SR, HESS~SR, and UCLA~SR, respectively. The latter file contains combined data from DePaolo (1986), Capo and DePaolo (1986), and Richter and DePaolo, 1987 (diffusion-corrected data). The Sr-isotope data are expressed in two ways in these files -- as measured $^{87}Sr/^{86}Sr$, and as δ^{87}Sr, where the latter is the difference in parts per thousand between the sample $^{87}Sr/^{86}Sr$ and modern-seawater $^{87}Sr/^{86}Sr$.

From the SPLINES menu, select the **SR AGES** option (F5). Specify a **Perfect Fit** or a **Smoothed Curve** to the global-marine trend data.

If you specify a **Perfect Fit**, the routine will fit an Akima-method spline to the data, where the curve is forced through each data-point on the trend. This is appropriate for relatively sparse, very-high precision data-sets. You should include the analytical errors of the reference data-set if you specify a **Perfect Fit**.

For large global-marine-trend data-sets with resolvable non-analytical scatter, such as those of Koepnick and others (1985) or Hess and others (1986), you should specify a **Smoothed Curve**. For a **Smoothed Curve**, the analytical errors of the reference data-set are ignored. The attributes of both of these curve-types are briefly described in p. 17).

Isoplot will ask you to enter the $^{87}Sr/^{86}Sr$ value of the unknown-age sample and the uncertainty in that value. Again, you can use other ways of expressing the $^{87}Sr/^{86}Sr$ ratio such as δ-values, so long as the form of the ratio is the same as that used for the global-marine trend. The procedure is as follows:

1) All ages (intercepts) along the global-marine trend (spline curve) that have the $^{87}Sr/^{86}Sr$ ratio of your unknown are determined. If there is only one such age, it is used as the best age-estimate. If there are several such ages, their average is used.

2) The intercepts of the upper and lower limits (from your assigned error) on the sample $^{87}Sr/^{86}Sr$ ratio with the global-marine trend are located. The differences between the resulting maximum and minimum ages and the best age-estimate are used to calculate variances in the positive and negative age directions, and assigned to a sample-error variance.

3) The intercepts of the sample δ^{87}Sr with the spline curve constructed through all of the upper limits of the calibration curve are determined, then the intercepts of the spline curve constructed through all of the lower limits of the calibration curve. In the case of a normal spline or Akima spline calibration curve (that is, a curve passing through each of the calibration points), the upper and lower limits are taken to be spline curves constructed though the upper and lower error-limits of the points. In the case of a smooth spline, the limits reflect the 2σ statistical error about the curve. The differences between the maximum and minimum ages from these intercepts and the best age estimate are used to calculate variances in the positive and negative age-directions, and assigned to a global-marine-trend variance.

4) The upper and lower errors on the best age-estimate are determined by taking the square

roots of the sums of the variances from sample error and from global-marine-trend error. Because the upper and lower errors are determined separately, they will generally not be symmetric about the best age estimate.

CREATING PLOTTER FILES FOR HIGH-QUALITY GRAPHICS OUTPUT

Isoplot can create a file of HPGL graphics-commands as it constructs the screen graphics. Though this will slow down operation of the program somewhat due to intermittent disk access, you can then obtain high-quality graphics output on any device that can read HPGL commands, such as a Hewlett-Packard pen-plotter. You can also obtain high-quality graphics using a laser printer or even an ordinary dot-matrix printer if you have one of the commercial programs that will translate the HPGL commands to the appropriate printer-graphics commands[1]. Another way of using *Isoplot*'s HPGL files is to import the HPGL files into a commercial program which can recognize or convert HPGL files, such as WordPerfect (used for this documentation), Microsoft Word, or many drawing programs. WordPerfect's DrawPerfect program has proven to be particularly useful in modifying *Isoplot*'s HPGL-file plots.

Press **F1** (**HPGL File**) from the starting-screen, to invoke the FORM that specifies HPGL file parameters:

```
                                                              Slow Plot

                    PLOTTER-FILE SPECIFICATIONS

            No file (0), New file (1), or
                   Add to existing file (2)  ==> 0

                 Disk\Path for HPGL file ... C:\ISOPLOT
                      Name of HPGL file ... HPGL

             Whole-Plot Left-limit (mm) ... 20
                    ''      Right-limit (mm) ... 220
                    ''      Bottom-limit (mm) ... 15
                    ''         Top-limit (mm) ... 186
        Suppress X-Axis Tick-Labels (Y/N) ... N

                          Default Pen#  ... 1
            Plot-Box Pen# (or line-width, mm) ... 1
          Axis-Label Pen# (or line-width, mm) ... 1
               Curve Pen# (or line-width, mm) ... 1
                        User-Label Pen#  ... 1
                      Pen-width assumed (mm) ... .3


F1 Help        F4 COM port settings
F2 Define limits of Plot-Box only                       F3 Fast Plot
F9 Recall    Esc Exit       ENTER Enter response        CTRL-ENTER Done
```

---

[1]For example, FPLOT (Fplot Corporation, Suite 605, 24-16 Steinway Street, Astoria, NY 11103). This inexpensive program permits virtually any dot-matrix or laser printer to function as a high-quality plotter, and also permits rapid screen previews of the plot.

If you answer *1* or *2* to the first item, the rest of the FORM will specify where to store the file containing the graphics (HPGL) commands, what size to make the plot (as defined by the margins), and what pens to use for various parts of the plot (a response of *0* to the first item makes the rest of the form irrelevant). Unless you want the plotter-plot to be added to a previous plot on the same piece of paper, you'll want to specify a different file-name for each plot and specify *New File*. The plot-limits requested by the form can refer to either the whole plot (including axis labels), or to the plot-box alone. Press **F2** to toggle from one to the other. The limits are locations on the plotter-paper, where the lower-left hand corner of the paper is defined as the origin, and the right-limit and upper-limit are located at 279 and 216 mm, respectively, from the origin.

SPECIFYING PEN NUMBERS AND LINE WIDTHS

The pen numbers can refer either to the actual pens of a pen plotter, or, for the Plot-Box, Axis-Label, and Curve pen-numbers, to the line-width for these features in millimeters. To specify a line-width for the latter, enter a non-integral number such as .1. The *Pen-Width* parameter refers to the assumed, invariant line-thickness of the plotting device itself - typically about 0.3 mm for a pen-plotter, or as little as .025 mm for a laser printer. The *Line Width* should not be less than the *Pen Width* for any of the features, unless you really want the plotter pen to repeatedly fill in the same lines. Specifying the *Line-Width* for the plot-box, axis-label, or curves is mainly of use for plots that will be produced on a dot-matrix or laser printer rather than an actual pen-plotter, as thick lines will slow down the latter considerably.

PUTTING MORE THAN ONE PLOT ON A PAGE

Occasionally, you may want to stack one plot on top of another, or have two plots side-by-side, but on the same piece of paper. The best way to do this is to:

(1) Make the first plot as usual, but specify the plot-limits for the plot-box only (F2). Leave enough room on the paper for the second plot.

(2) After finishing the first plot, bring up the **HPGL File** menu and select *Add to existing file*. Specify the same file as for the first plot.

(3) Keep either the Left/Right limits (for vertically-stacked plots) or the Bottom/Top limits (for side-by-side plots) the same as before, and change the other pair of limits to correspond to the desired position for the second plot.

(4) If you want a vertically-stacked plot, position the second plot on top of the first one (with the Top/Bottom limits). If the upper plot is to share the same X-axis label and X-axis limits, specify *Suppress X-axis labels*.

(5) Enter the plotter-file FORM and start the second plot. For vertically-stacked plots with a shared X-axis, make sure that the X-limits are exactly the same as for the lower plot.

(6) Proceed as usual.

Figure 9 is an example of a stacked plot with a shared X-axis.

SELECTING THE PEN SPEED

If your plot will be created by a pen-plotter, you can toggle the pen-speed from fast to slow with F3. The pen-speed toggle will have no effect for laser or dot-matrix printer outputs.

CONFIGURING THE PLOTTER'S *COM* PORT

Press F4 to customize the settings of the COM port that the plotter is connected to. The default settings are for COM1, 2400 baud, parity=space, 7 data-bits/byte, 1 stop-bit. These correspond to DIP-switch settings on the plotter as follows:

<div align="center">

Switch#: *1 2 3 4 5 6 7 8*
Setting: *0 0 0 1 1 0 0 0*

</div>

SENDING THE PLOTTER-COMMAND FILE TO A PLOTTER

You can use DOS's PRINT command to send the HPGL file to the plotter once you have exited *Isoplot* (use the DOS SHELL function from the starting-screen if you intend to re-enter *Isoplot* after sending the HPGL file). While running *Isoplot*, you can send the current HPGL file by pressing SHIFT F1 or CTRL F1 from either the starting screen (if you've just generated an HPGL file with *Isoplot*) or from the ADD POINTS screen.

CHANGING THE DECAY CONSTANTS AND MODEL-AGE PARAMETERS

The default decay constants used by *Isoplot* are those recommended by the I.U.G.S. Subcommission on Geochronology (Steiger and Jäger, 1977). You can change those constants, however, as well as the Rb-Sr, Sm-Nd, Lu-Hf, and Re-Os model-age parameters. From the starting screen, switch to the Radiogenic-Isotope Utilities screen by pressing *L*. Press *ALT-C* to bring up the form containing the decay constants and model-age parameters being used by *Isoplot*. Select the parameters that you want to change with the Up/Down arrows, type in the new values, and press ◄─┘ . Press CTRL ◄─┘ when you've completed the changes.

Isoplot will query if you want to store the changed constants (in the CONSTS.ISO file). If you do, the new values will be used by *Isoplot* from now on. Make sure, though, that the CONSTS.ISO file is on the same disk and path as the *Isoplot* program itself.

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Isoplot uses several algorithms that were adapted in whole or in part from other sources. The polynomial regression and "normal" spline algorithms, as well as the routines for calculating probabilities from M.S.W.D. values, were adapted from Numerical Recipes (Press and others, 1987). The "Akima" spline algorithm was adapted from Akima (1970), and sorting is done with a modified version of the Shell Sort subprogram supplied with the Quick Basic 4.0 language. Jim Quick of the U.S.G.S. supplied the Epson printer-dump algorithm, and Brent Troutman of the U.S.G.S. developed the analytical expression for the external variance of a weighted average. The algorithm for construction of error ellipses is based in part on a method provided by George Cumming, and David Ward supplied the routine for Hercules

graphics dumps. The Model-1 Yorkfit is, of course, modified from York (1969), and the Model-2 Yorkfit is a modification of the "equal weight" model of McSaveney (Faure, p. 427-434). The robust data-averaging algorithm is an adaptation of the Tukey's Biweight method described in Hoaglin and others (1983), except for the 95%-confidence error-estimator, which is based on Monte Carlo simulations by myself (using a tuning-constant of 9) on contaminated normal distributions. The planar-fit solution makes use of the marvelous algorithm of Kent et al. (1990), with suitable corrections for a couple of nasty typos in that paper.

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