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UISO

A Program for Calculation of ^{230}Th - ^{234}U - ^{238}U Isochron Ages

by

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ABSTRACT

UISO is a small, stand-alone program to calculate uranium-series isochron ages and errors using the maximum-likelihood estimation algorithm of D.M. Titterington (Ludwig and Titterington, 1993). Use of the program and significance of the results are explained.

INTRODUCTION

Ages in the ^{230}Th-^{234}U-^{238}U system are mathematically defined by the $^{230}Th/^{238}U$ and $^{234}U/^{238}U$ isotopic ratios, providing that the material being dated (1) has been a closed system, and (2) contained no ^{230}Th at the time of its formation. It is not uncommon, however, for samples to contain variable amounts of ^{232}Th as a detrital contaminant, in which case the ^{230}Th, ^{234}U, and ^{238}U that always accompany the detrital ^{232}Th must be subtracted from the analysis before a meaningful age can be calculated.

If several cogenetic samples of such material are analyzed, one can arrive at the detrital-corrected Th-U isotopic ratios providing that (1) the detrital Th-U isotopic composition is the same from sample to sample, and (2) the sample have behaved as closed systems for Th and U. The usual way of determining such detrital-corrected Th-U isotopic ratios is to fit regression lines to the data on a pair of isotopic-ratio diagrams that define straight-line mixing trends for the ^{230}Th-^{234}U-^{238}U system. Of relevance to *UISO* are:

1) $^{230}Th/^{238}U$-$^{232}Th/^{238}U$ and $^{234}U/^{238}U$-$^{232}Th/^{238}U$ (referred to as Osmond Type-II diagrams), and

2) $^{230}Th/^{232}Th$-$^{238}U/^{232}Th$ and $^{234}U/^{232}Th$-$^{238}U/^{232}Th$ (referred to as Rosholt Type-II diagrams).

In both diagrams, the ^{230}Th-^{234}U-^{238}U isotope ratios (from which the age of a closed system is calculated) of the ^{232}Th-free end-member are given by either the slope (Rosholt diagrams) or intercept (Osmond diagrams) of the best-fit straight lines. The data will not, in general, fall precisely on the isochron (regression) lines because of analytical error, so a regression procedure is required that takes into account the magnitude of the analytical errors and error correlations for each data-point.

These considerations have been discussed in detail by Ludwig and Titterington (1993), who developed a MLE (maximum-likelihood estimate) algorithm to take into account the facts that:

1) error correlations as well as errors must be considered in weighting the data points,

2) all of the appropriate isochron pairs use some of the same data in each of the two *X-Y* regression lines, and

3) the age-error calculation requires either the slope-slope or the intercept-intercept error correlation for the *X-Y* regression-line pair.

The program *UISO*, written in Microsoft Quick Basic 7 for IBM-PC compatible computers, implements the algorithm developed by D.M. Titterington in Ludwig and Titterington (1993). The standard version of *UISO* requires an 80*x*86 CPU with an 80x87 numeric coprocessor, where *x* is 2 or greater. A version that will run (slowly) on machines lacking a numeric coprocessor and/or with the older 8086/8088 CPU's is also available[2]. The memory required by *UISO* varies according to the number of data-points in the input file (10 data-points requires about 69 kilobytes). The time required for solution of the isochrons and isochron age varies according to the number of data points, but for 5-10 points is typically 1-3 seconds for an 80486/33 CPU. For machines without a coprocessor or with 8086/8088 CPU's, however, the time for such a solution can be greater than 5 *minutes*.

Because *UISO* is a small, single-purpose program that can direct its output to a small disk-file, it can be invoked from other programs via a DOS SHELL call; the calling program can then read the results of the *UISO* calculation from the file, and use those results for its own purposes. A more-flexible implementation of the Titterington isochron-algorithm has been incorporated into *ISOPLOT* (Ludwig, 1991) versions 2.7 and later. *ISOPLOT* is preferable to *UISO* for interactive use or if graphical presentation of the results is required.

USING *UISO*

Command-Line Syntax

When invoking *UISO*, use the syntax

```
UISO   Style(1-3)  Outputs(1-7) FileIn [FileOut]
       [/S]  [/2]  [/A]  [/F#]  [/L#]  [/TOL#]  [/HALF]
```

where brackets indicate optional switches or parameters, and

[2]To obtain the program (no charge), contact the author directly. Include a formatted disk with your request, and specify if the source-code is required.

`Style` specifies which isotopic ratios are present in the input file. Three styles are supported: Style **1** specifies $^{232}Th/^{238}U$-$^{234}U/^{238}U$-$^{230}Th/^{238}U$ ratios (Osmond Type-II); Style **2** specifies $^{238}U/^{232}Th$-$^{234}U/^{232}Th$-$^{230}Th/^{232}Th$ ratios (Rosholt Type-II). Style **3** specifies general (non U-series) X-Y-Z data.

`Outputs` specifies where the results of the isochron calculation are directed. Add together the following values for **Outputs**:

1 = screen
2 = printer (on LPT1:)
4 = file

`FileIn` is the name of the file containing the data, with disk and path specifiers as necessary (example: C:\USERIES\BONNEVILLE.TXT). The required format of the input file is described below.

`FileOut` is an optional parameter that specifies the name of the file (or other device, such as LPT2:) that will receive *UISO*'s output (**FileOut** is ignored if **Outputs** is less than 4). Include disk and path specifiers as necessary. If **Outputs** is 4 or greater and you do not specify **FileOut**, *UISO* will name the file UISO*nnnn*.TXT, where *nnnn* is an arbitrary 4-digit number selected by *UISO*.

`/S` suppresses the output of the input data. If omitted, the input data will be output as parsed by *UISO*, but with no more than 5 significant figures for ratios and error-correlations, and no more than 3 significant figures for errors (the calculations, however, use the input data without rounding).

`/2` specifies 2-sigma error-input. If omitted, errors are assumed to be 1-sigma.

`/A` specifies absolute error-input. If omitted, errors are assumed to be in percent.

`/F#` specifies **#** as the *first* valid data-line of the input file to accept. If omitted, the first data-line accepted will be the first valid data-line in the file.

`/L#` specifies **#** as the *last* valid data-line of the input file to accept. If omitted, the last data-line accepted will be the last valid data-line in the file.

`/TOL#` (normally omitted) specifies **#** as the fractional convergence tolerance for the MSWD of the regression solution (must be no greater than 10^{-9}). If omitted, the convergence tolerance defaults to 10^{-16}. Higher tolerances result in slightly faster calculation times, at the expense of accuracy.

/HALF directs *UISO* to read the ^{230}Th and ^{234}U half-lives from file HALF_LVS (no other name can be used) in the default path, rather than using the default half-lives of 78,381 yr and 244,600 yr, respectively. The HALF_LVS file must be a text file containing only the ^{230}Th and ^{234}U half lives, in years. Separate the two numbers with a comma, tab, or CR/LF.

Entering just the word **UISO** at the DOS command line will invoke a terse HELP screen that explains the *UISO* syntax. Complete documentation is contained in the text file UISO.DOC.

Example:

UISO 1 5 a:pyramid.prn c:\data\pyr_age /S /2 /F3 /L10

Input file is A:PYRAMID.PRN, containing data as ^{232}Th/^{238}U - ^{234}U/^{238}U - ^{230}Th/^{238}U ratios, output directed to the screen and to file C:\DATA\PYR_AGE (output of the input-data suppressed). Input errors are 2-sigma, in percent, and only the third through tenth valid data-rows are to be used. Ages will be calculated using the default ^{230}Th and ^{234}U/^{238}U half-lives of 75,381 and 244,600 years, respectively.

Example:

UISO 2 2 c:\useries\horizb_2 /a /tol1E-8 /half

Input file is C:\USERIES\HORZB_2 containing data as ^{238}U/^{232}Th - ^{234}U/^{232}Th - ^{230}Th/^{232}Th ratios, output to the printer on LPT1: (including the input data). Input errors are 1-sigma, absolute. All of the data in the file will be used, and the iterations of the numerical solution will end when the fractional change in the MSWD between iterations is less than 10^{-8}. Ages will be calculated using the half-lives in the HALF_LVS file.

Input-Data File Format

The input-data file for *UISO* must be a text (ASCII) file with the following characteristics:

1) each sample's data occupies one line (row);

2) the sample data consist of numbers, separated by one or more spaces or by TAB (ASCII 009) characters (do not mix the two delimiters in one line);

3) the numbers are in the order *X*, *X*-error, *Y*, *Y*-error, *Z*, *Z*-error, *X*-*Y* error-correlation, *X*-*Z* error-correlation, *Y*-*Z* error-correlation;

4) for Style-1 data, $X=^{232}$Th/^{238}U, $Y=^{234}$U/^{238}U, $Z=^{230}$Th/^{238}U;

5) for Style-2 data, $X=^{238}U/^{232}Th$, $Y=^{234}U/^{232}Th$, $Z=^{230}Th/^{232}Th$;

6) for Style-3 data, *X*, *Y*, and *Z* can be any parameters (no isochron age will be calculated);

7) errors are 1-sigma, in percent, unless the **/2** (=2σ) or **/A** (=Absolute) switches are set;

8) for Style 1 and 2 data, values for the 3 error correlations must all be nonzero.

The input file can contain any number of non-data lines (rows). Input-file lines that contain 9 numbers (and nothing else) are counted as sample-data. Input-file lines are ignored if they contain less than 9 numbers or contain other, non-numeric characters (besides spaces or tabs). The number of data-points is limited only by available memory.

Input-Data Requirements

Uiso will fail to solve some data sets. The reasons for this failure are generally either: (1) the data do not trend along an X-Y-Z line, or (2) the data show almost no variation along one of the axes. In the former case, you may be able to force a solution by increasing the errors or changing the error correlations. If you do this, of course, the significance of the regression-line parameters will be diminished, and their errors will be meaningless (though if the true input-error correlations are used and the input-errors have all been expanded by a constant factor, you can recover the *a priori* regression line errors by scaling down the *UISO* errors by √MSWD).

An example input-data file is given below (the header lines are entirely arbitrary, and are ignored by *UISO*). If you have trouble creating a legal *UISO* input-data file, try modifying one of the example data-files (XMPL1.TXT and XMPL2.TXT, which contain Style-1 and Style-2 data, respectively) on the *UISO* disk. Estimation of the input errors and error correlations is discussed in detail in Ludwig and Titterington (1993).

Example of Input Data

The output of `UISO 1 7 C:\DATA\TUFA88_7.TXT /F2 /L7` (using the above input-data file) would look like this:

```
Data for Tufa Mound 88-7 (1-sigma, percent errors)

          error             error             error    Correl   Correl   Correl
 232/238    (%)    234/238    (%)     230/238   (%)     48:28    08:28    48:08
=============================================================================
0.086672 3.594625 1.058275 1.301611 0.690156 2.033034 0.186175 0.392868 0.329178
0.172389 2.810219 1.100502 1.286511 0.749392 2.006063 0.239850 0.508587 0.335998
0.235257 2.473362 1.094651 1.224979 0.787719 1.944147 0.258824 0.579004 0.329278
0.291330 2.279726 1.075879 1.179709 0.816791 1.898518 0.268196 0.628749 0.322048
0.322981 2.156432 1.089738 1.113874 0.818452 1.854052 0.269358 0.662057 0.313288
0.386907 2.069444 1.052789 1.114285 0.795402 1.854011 0.276146 0.687239 0.308234
0.410665 2.003231 1.036214 1.073084 0.842250 1.811558 0.272601 0.712597 0.301444
0.443317 1.953095 1.034277 1.047010 0.850629 1.792365 0.272555 0.730534 0.296996
0.470637 1.903287 1.036450 1.010056 0.854561 1.768288 0.270094 0.748534 0.290714
0.504263 1.872168 1.054588 0.991421 0.838958 1.762349 0.271813 0.759078 0.288751
```

Example of *UISO* input file

```
Titterington/Ludwig solution for Th230/U234/U238 isochron
errors are 1-sigma, in percent
 232/238    %err    234/238    %err    230/238    %err rho 28-48 rho 28-08 rho 48-08
 .17239     2.81    1.1005     1.29    .74939     2.01    .23985     .50859     .336
 .23526     2.47    1.0947     1.22    .78772     1.94    .25882     .579       .32928
 .29133     2.28    1.0759     1.18    .81679     1.9     .2682      .62875     .32205
 .32298     2.16    1.0897     1.11    .81845     1.85    .26936     .66206     .31329
 .38691     2.07    1.0528     1.11    .7954      1.85    .27615     .68724     .30823
 .41067     2       1.0362     1.07    .84225     1.81    .2726      .7126      .30144
stored as C:\DATA\TUFA88-7.TXT
MSWD = 1.74                    (6 data-points)
probability of fit = 0.0832
intercept-error correlation = +0.367

 Isochron intercepts       95% conf.          1-sigma a priori
U234/U238  =  1.1561      +/- 0.0645           +/- 0.0212
Th230/U238 =  0.71955     +/- 0.067            +/- 0.022
Age (ka)   =  102.8       +/- 15               +/- 5.0

         Set#    Weighted Residual    (ratio of observed residual to
          1          1.18             residual predicted from
          2          0.337            assigned errors)
          3          1.48
          4          1.6
          5          2.3
          6          1.55
```

Example of *UISO* output

If the regression is not successful, the output will consist of the word FAILED (after the list of input data, if not suppressed), followed on the next line by the reason for failure.

The **MSWD** value reported by *UISO* is the Mean Square of Weighted Deviates of the data from the regression line (McIntyre *et al.*, 1966; Brooks *et al.*, 1972; Wendt and Carl, 1991). If only the assigned data-point errors are responsible for scatter from the regression lines, the **MSWD** will average unity. The square root of the **MSWD** corresponds to the factor by which all of the data-point errors would have to be expanded (or contracted, if <1) for the observed amount of scatter about the isochron lines to agree perfectly with the amount of scatter predicted by the assigned analytical errors and error correlations. The **probability of fit** reported by *UISO* is

the probability that the assigned data-point errors could have resulted in at least the observed amount of scatter. For example, if the **probability of fit** for a regression were 0.373, and if the assigned data-point errors were the only cause of scatter from the regression lines, then 37.3% of the time, re-analyses of the same samples (with the same errors) would exceed the amount of scatter from the regression lines observed in the first analysis, and 62.7% of the time, the amount of scatter would be less.

The **1-sigma a priori** errors reported by *UISO* are the 1-sigma errors propagated only from the assigned data-point errors and error correlations. The **1-sigma a priori** errors ignore how well the data points actually conform to the regression lines.

If the **probability of fit** is *greater* than 15%, the **95%-conf.** errors reported by *UISO* are simply 1.96 times the **1-sigma a priori** errors. If the **probability of fit** is *less* than 15%, *UISO* calculates the **95%-conf.** errors by multiplying the **1-sigma a priori** errors by the square root of **MSWD** and by the Student's-*t* factor for *2N–4* degrees of freedom. The first factor takes into account the fact that the data scatter from the regression line by more than is predicted by the assigned data-point errors; the second factor takes into account the fact that the actual error of the data points must be estimated from the scatter of only the *N* data-points used in the regression. For isochrons with **probability of fit** less than 15%, *UISO* in effect assumes that all of the data-point X-Y-Z errors were underestimated by a constant factor (but with correct error correlations), and determines this factor from the actual scatter of the data.

You should be aware that though this assumption may not be grossly unreasonable for **MSWD** values that are only moderately high (<3-5), it is almost certainly invalid for very high **MSWD**'s and indicates a gross failure of the isochron assumptions (closed system, cogenetic, uniform initial isotope-ratios). The **1-sigma a priori** errors in such cases are entirely irrelevant.

If the isochron $^{230}Th/^{238}U$ - $^{234}U/^{238}U$ error correlation is less than 0.4, *UISO* will check for asymmetric 95%-confidence-limit age-errors. If the age errors are significantly asymmetric, both the symmetric and approximate asymmetric age-errors (95%-confidence only) will be output, such as:

```
Age (ka)    =  132 ka        +/- 71
asymmetric age-errors:       +120 -64
```

Because the asymmetric age-calculation ignores the $^{230}Th/^{238}U$-$^{234}U/^{238}U$ isochron-error correlation, asymmetric age-errors will be slightly too high or too low for positive or negative error-correlations, respectively.

The **Weighted Residuals** of the output are the residuals of each data-point. For the Titterington algorithm, this is the sum of the data point's distance (in the X-direction) to the X-Y regression line plus the data point's distance (in the X-direction) to the X-Z regression line, divided by the distance predicted by the assigned errors and error correlations. If the assigned errors are the only cause for scatter, the average value of each point's **Weighted Residual** will be slightly less than 1. A **Weighted Residual** of 3.22 means that the data point falls 3.22 times further from the regression line than one would predict from its assigned errors and error correlations. Conversely, a **Weighted Residual** of 0.123 means that the data point scatters much less (only 12.3%) from the regression line than would be expected from the assigned errors.

The half-lives for ^{230}Th and ^{234}U used in *UISO*'s age calculations are 75,381 years and 244,600 years, respectively. Age errors are calculated from the equation in Ludwig and Titterington (1993), and will become inaccurate for very large errors on very old systems. If no ^{230}Th-^{234}U-^{238}U age can be calculated from the regression, the age will output as zero. If a ^{230}Th-^{234}U-^{238}U age *can* be calculated but the age-errors are infinite, the age errors will be output as zero.

To obtain the complete regression-line parameters (2 slopes, 2 intercepts) and their errors and error correlations, you must specify the input data as Style **3**.

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