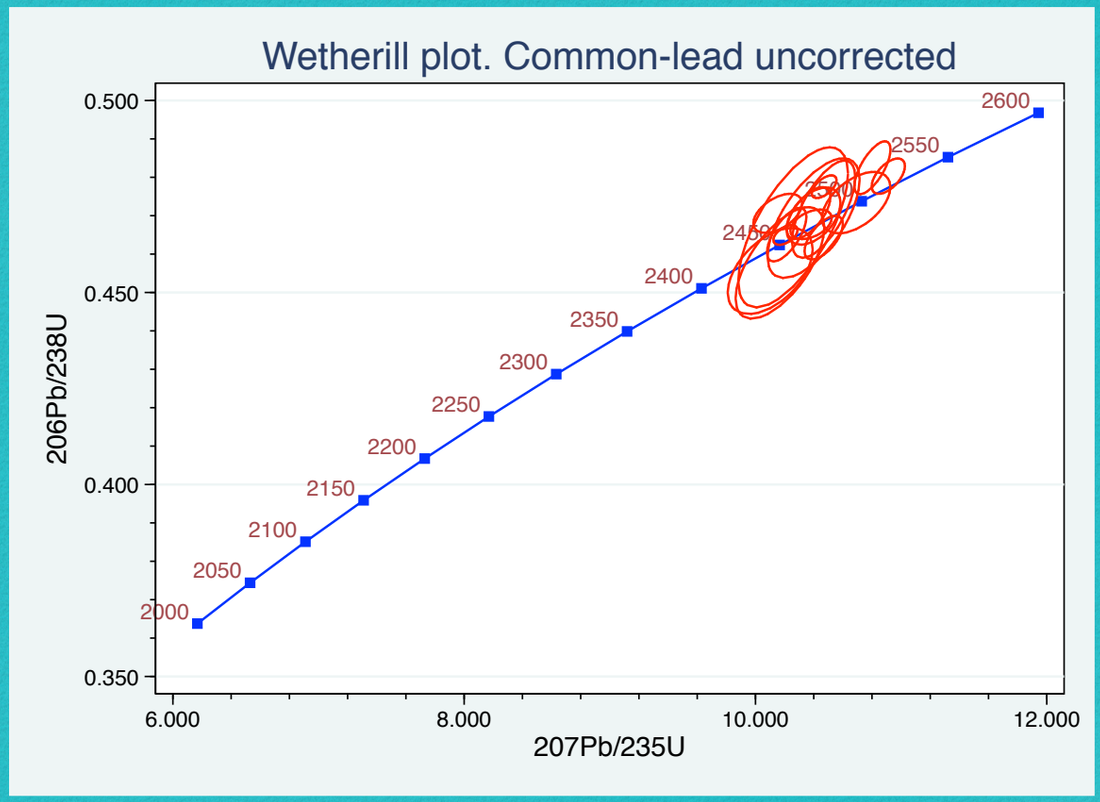
First Edition

SHRIMPTOOLS

SHRIMP data reduction and analysis using STATA™



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Introduction

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Getting Started

1. SHRIMTOOLS, what for?

SHRIMPTOOLS is a home-made software package for reducing and analyzing U-Th-Pb data generated by the SHRIMP II ion microprobe of the IBERSIMS Laboratory at the University of Granada. To a large extent it is a new implementation of the PRAWN data reduction software developed for the SHRIMP I, complemented with some ISOPLOT-like utilities. We have written it using the STATA commercial package which runs in Mac, Windows, or Linux. Data files and program files are fully interchangeable between the three platforms.

SHRIMPTOOLS is free, but STATA is a commercial package (www.stata.com). To download an evaluation license go to: http://www.stata.com/customer-service/evaluate-stata/

SHRIMPTOOLS has been tailored to our requirements. We are happy if other people find it useful, so we have decided to write this manual. The software is as “it is”. Therefore, we accept neither responsibility nor liability for erroneous results or any other problem derived from its use.

SHRIMPTOOLS has been extensively checked and improved since 2010. We think it is reasonably bug-free, but one never knows. If you find a bug, please, report it to us and we shall fix it as soon as possible.

If you believe the program lacks some features you really need, please, drop us an e-mail with your suggestions and we shall see whether we can implement them.

2. Why STATA?

STATA is a powerful statistics, graphics and data analysis package, that is extensively documented and well supported. It is also a programming environment with its own language. There is a huge library of user-made routines available on the internet. STATA programs (ADO files) are truly multi-platform and run independently of the operating system settings (language, date formats, etc.).

3. Which STATA version and flavor?

The current version of SHRIPMTOOLS works well with STATA 13, 12 and 11. STATA comes in different flavors (see www.stata.com) depending on the dataset size it can work with. Even the simplest version (STATA for student) can run SHRIMPTOOLS. We run it with STATA/IC.

4. Useful additional software

SHRIMPTOOLS runs inside STATA. No additional files or packages are required. Nevertheless, users will probably find it useful to have (1) a text processor (2) a spreadsheet program.

A *text processor* is often required to manipulate the .pd files generated by the SHRIMP, especially if these are partially corrupted or contain incomplete analyses. On the Mac we recommend the free application TextWrangler, but any word processor would probably be suitable.

A *spreadheet* program is useful to format the tables made by SHRIMPTOOLS. We provide templates in Apple NUMBERS and Microsoft EXCEL for producing publication-ready tables.

5. SHRIMPTOOLS file format and installation

SHRIMPTOOLS consists of several (currently 24) ADO files. These are text files with the extension .ado, which STATA interprets as compilable code files. The user does not need to consider the number or the name of these ADO files. This task is automatically undertaken by STATA. The only thing the user must check carefully is the place where the files are installed, this must be the personal subdirectory of the ADO directory. This can be found by typing in the STATA command window: **personal** [return].

The procedure for installing SHRIMPTOOLS is as follows:

1. Download the Shrimptools_date.zip archive from this link (www.ugr.es/~fbea)
2. Unzip the archive and open the resulting folder.
3. Move all files to the corresponding /ado/personal directory. To find where it is, just type: **personal** [return] in Stata's com-

mand window. Do not place the Shrimptools_date folder itself inside the /ado/personal directory, just the .*ado* files. **Tip: be sure your user has write and read permissions on theado folder. Otherwise you will have problems to write new standard files**

4. Download and unzip the folder Auxilary_files. This contains two table templates, one in Apple Numbers and the other in Microsoft Excel mentioned before, plus two .pd files for training: the_nice_file.pd, and the_silly_file.pd. The latter is corrupted so that the users can learn how to deal with such problems.

6. Future developments and updates

We shall try to keep SHRIMPTOOLS up to date with the development of the SHRIMP. We are also developing routines for multicollector work, namely, Pb and O isotopes. However, given that Peter Lanc's POXY software covers this subject well, we are not in a hurry to develop our own routines.

SHRIMPTOOLS is updated frequently. Updates and new versions will be posted at the link mentioned before.

7. How to mention SHRIMPTOOLS

Bea, F. Shrimptools, a platform-independent software for U-Th-Pb SHRIMP data reduction and analysis. Computers and Geosciences (submitted).

8. Reporting bugs and suggestions

Bugs and suggestions can be reported to:

- fbea@ugr.es
- pmontero@ugr.es
- ibersims@ugr.es

STATA basics

1. STATA, to begin with

STATA is a complicated program that requires training to use it efficiently. We strongly recommend that ISOTOOLS users to spend some time learning STATA basics using the excellent documentation provided with the program. Here we outline the STATA features and commands that are essential to work with ISOTOOLS. In no way can this replace STATA's Getting Started manual

STATA is both menu-driven and command-line driven. When you open STATA, the following multi-window screen appears:

Figure 1.1. Main STATA window

The screen is composed of four windows:

results window: Where all results appear

variables window: Where the names of your variables appear (note that no variable appears in Fig. 1.1 because no dataset is open). This window has two columns: name and label. Name is how STATA refers the variable. Label explains what the variable is. See Section 4 item 1.7

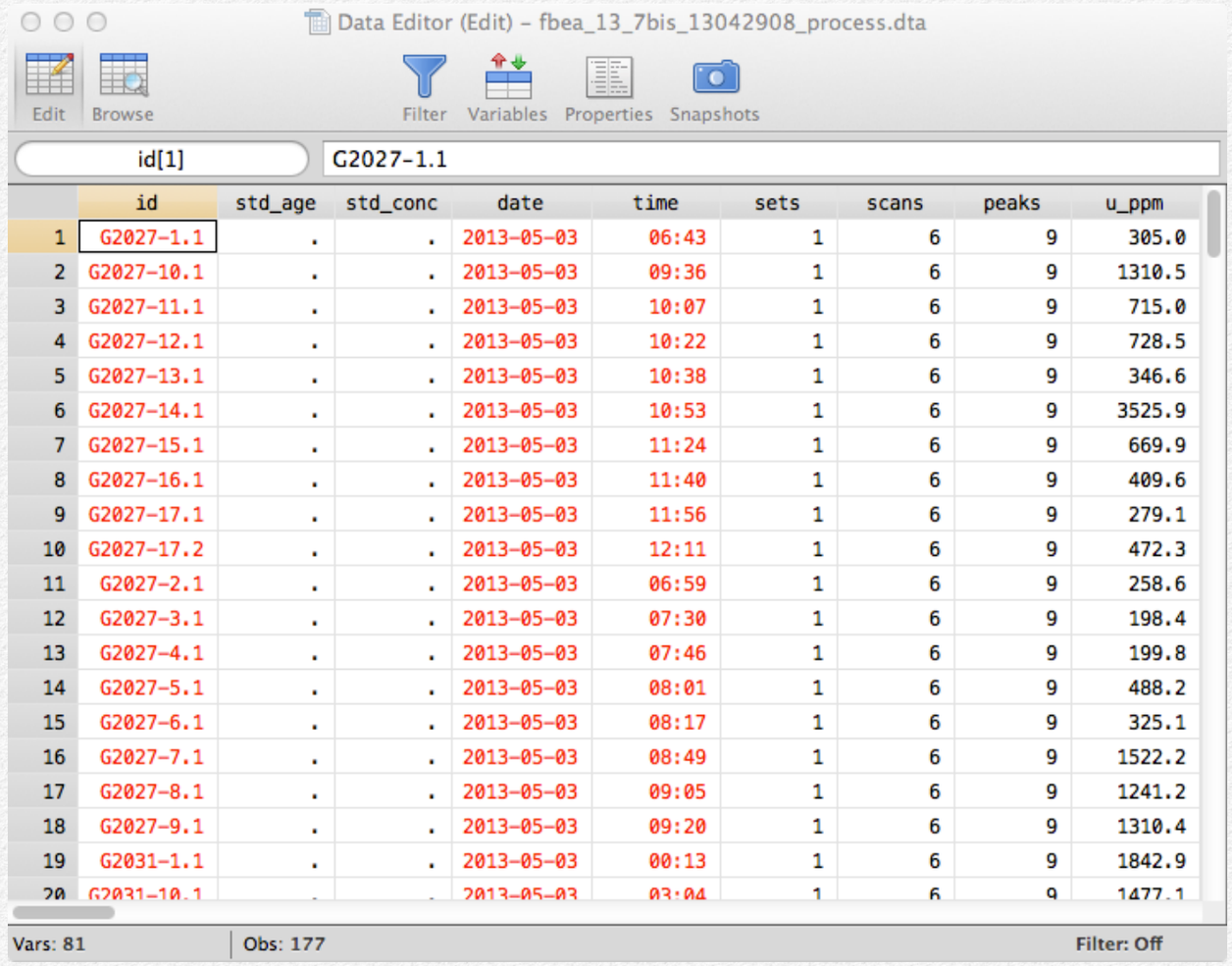
command window: Where the user enter commands using the keyboard

already-done command window: Where all commands written since STATA was opened are recorded. The user can save this window and reuse all the commands.

The look of the results window may be different from that shown in Figure 1.1. It can be changed in the STATA General Preferences window. Go to the *window screen,* select ***results window,*** and change ***Color scheme*** to ***classic.*** We found this color scheme visually pleasant and the least tiring after a long STATA session.

The easiest way to place a variable name in the command window is by clicking on it in the command window.

The easiest way to reuse a command is by clicking on it in the already done command window.



	id	std_age	std_conc	date	time	sets	scans	peaks	u_ppm
1	G2027-1.1	.	.	2013-05-03	06:43	1	6	9	305.0
2	G2027-10.1	.	.	2013-05-03	09:36	1	6	9	1310.5
3	G2027-11.1	.	.	2013-05-03	10:07	1	6	9	715.0
4	G2027-12.1	.	.	2013-05-03	10:22	1	6	9	728.5
5	G2027-13.1	.	.	2013-05-03	10:38	1	6	9	346.6
6	G2027-14.1	.	.	2013-05-03	10:53	1	6	9	3525.9
7	G2027-15.1	.	.	2013-05-03	11:24	1	6	9	669.9
8	G2027-16.1	.	.	2013-05-03	11:40	1	6	9	409.6
9	G2027-17.1	.	.	2013-05-03	11:56	1	6	9	279.1
10	G2027-17.2	.	.	2013-05-03	12:11	1	6	9	472.3
11	G2027-2.1	.	.	2013-05-03	06:59	1	6	9	258.6
12	G2027-3.1	.	.	2013-05-03	07:30	1	6	9	198.4
13	G2027-4.1	.	.	2013-05-03	07:46	1	6	9	199.8
14	G2027-5.1	.	.	2013-05-03	08:01	1	6	9	488.2
15	G2027-6.1	.	.	2013-05-03	08:17	1	6	9	325.1
16	G2027-7.1	.	.	2013-05-03	08:49	1	6	9	1522.2
17	G2027-8.1	.	.	2013-05-03	09:05	1	6	9	1241.2
18	G2027-9.1	.	.	2013-05-03	09:20	1	6	9	1310.4
19	G2031-1.1	.	.	2013-05-03	00:13	1	6	9	1842.9
20	G2031-10.1	.	.	2013-05-03	03:04	1	6	9	1477.1

Figure 1.2. STATA editor window

1. The first time you open STATA it is a good idea to type the following command in the command window:

2. **set more off, permanently** [return]

3. This ensures that output will be uninterruptedly displayed in the results window.

2. STATA data files

STATA data files have the extension .dat. STATA can only open one file at time, however the file may be really large. Even the simplest STATA flavor (see www.stata.com) can handle files much larger than required by SHRIMPTOOLS.

The file content can be seen and accessed at any time by clicking the Data Editor or the Data Browser buttons in top of the main window toolbar. This opens a new window displaying a spreadsheet-like editor (Fig. 1.2).

There is an important difference between the Data Editor and the Data Browser. Whereas in the former we can modify the data, in second we cannot, just look at them.

The Data Editor and Data Browse can be invoked through the command window by typing:

edit [return] or **browse** [return]

The user can specify which variables should be shown in the editor/browser and in which order they will appear. For example typing:

edit id u_ppm th_ppm [return] will show the variables id, u_ppm, and th_ppm in the editor.

3. Variable types and empty values

STATA uses different variable types which, for the sake of simplicity, can be grouped in two categories, numeric variables and string variables. The Editor represents numeric variables in black and string variables in red.

If a numeric variable in a given observation is empty, STATA places a dot (.) in it. It is important to remember that STATA understand the dot (.) as the largest possible numerical value so that the boolean condition **. > any number** is always true. If a string variable is empty, STATA puts an empty string in it.

4. A few useful STATA commands

A user with no experience with STATA still can run SHRIMPTOOLS, but he needs to understand the following commands.

list (can be abbreviated as **l,** for example **l** id [return] lists all ids in the file). If no variables are mentioned, the whole dataset would be listed. If some variables are written after list, only those would be listed. For example: **list** u_ppm **(**or **l** u_ppm**)** lists only the variable with the concentration of Uranium in ppm. The output appears in the results window.

generate variable_name (can be abbreviated **gen** variable_name). Creates a new variable "variable_name". For example, **gen** sum**=** a **+** b, creates the variable sum by adding the variables a and b

To create a new numeric variable with no values type: **gen** variable_name**=.** (note the dot).

To create a new string variable with no values type: **gen** variable_name**=**”” (note the double quote).

replace variable_name (cannot be abbreviated). Changes the value of the variable_name. For example, replace sum= sum*3 changes the value of sum by three times its value; replace sum = other_variable changes the value of sum by that of other-variable.

Caution: replace string_variable= “pepa” is not the same as replace string_variable=pepa. In the first case all values of the string_variable are changed to the string “pepa”. In the second case string_variable is replace by another string variable called pepa.

Tip: **generate** and **replace** accept the conditional **if**. For example, **generate** sum = a + b **if** es==1, creates the variable sum, storing in it a + b only in those observations for which the variable es is equal to 1. If for a given observation the condition es==1 is not fulfilled, the variable remains empty for that observation. Note that the boolean condition of equality is written with double =, that is ==.

drop variable_name drops the variable variable_name

drop in 3 drops the observation nº 3

drop in 3/35 drops the observations nº 3 to nº 35

drop if variable_name==*any_value* drops all observations for which variable_name has the value *any_value*

summarize variable_name1 variable_name2 etc... (can be abbreviated **sum** variable_name1 variable_name2 etc...) displays (results window) the summary statistics for variable_name1 variable_name2 etc...

ci variable_name1 variable_name2 etc... displays (results window) the mean, standard errors, and confidence intervals for variable_name1 variable_name2 etc...

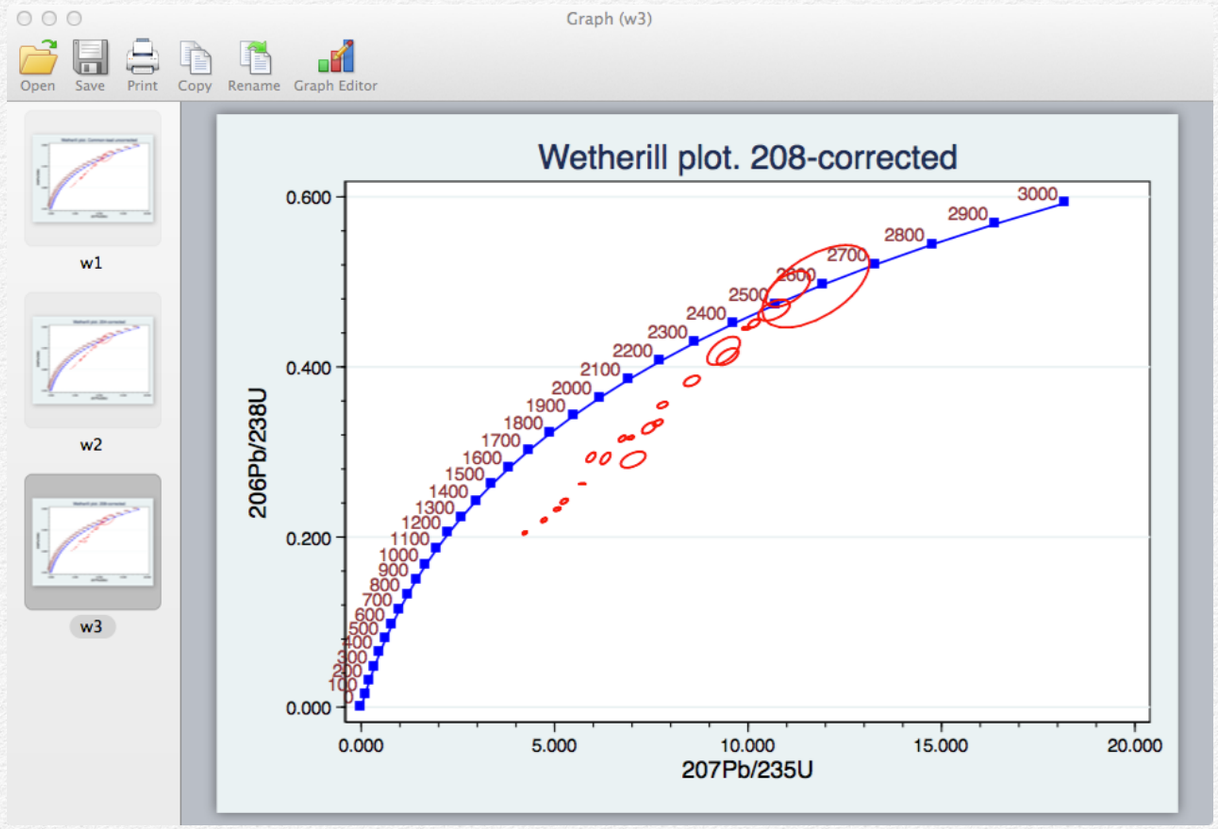


Figure 1.3. STATA tabbed graph window

Summarize and **ci** also accept the conditional if. For example: **summarize** variable_name1 **if** es==1 calculates the summary statistics for variable_name1 in those observations that have the control variable es set equal to 1.

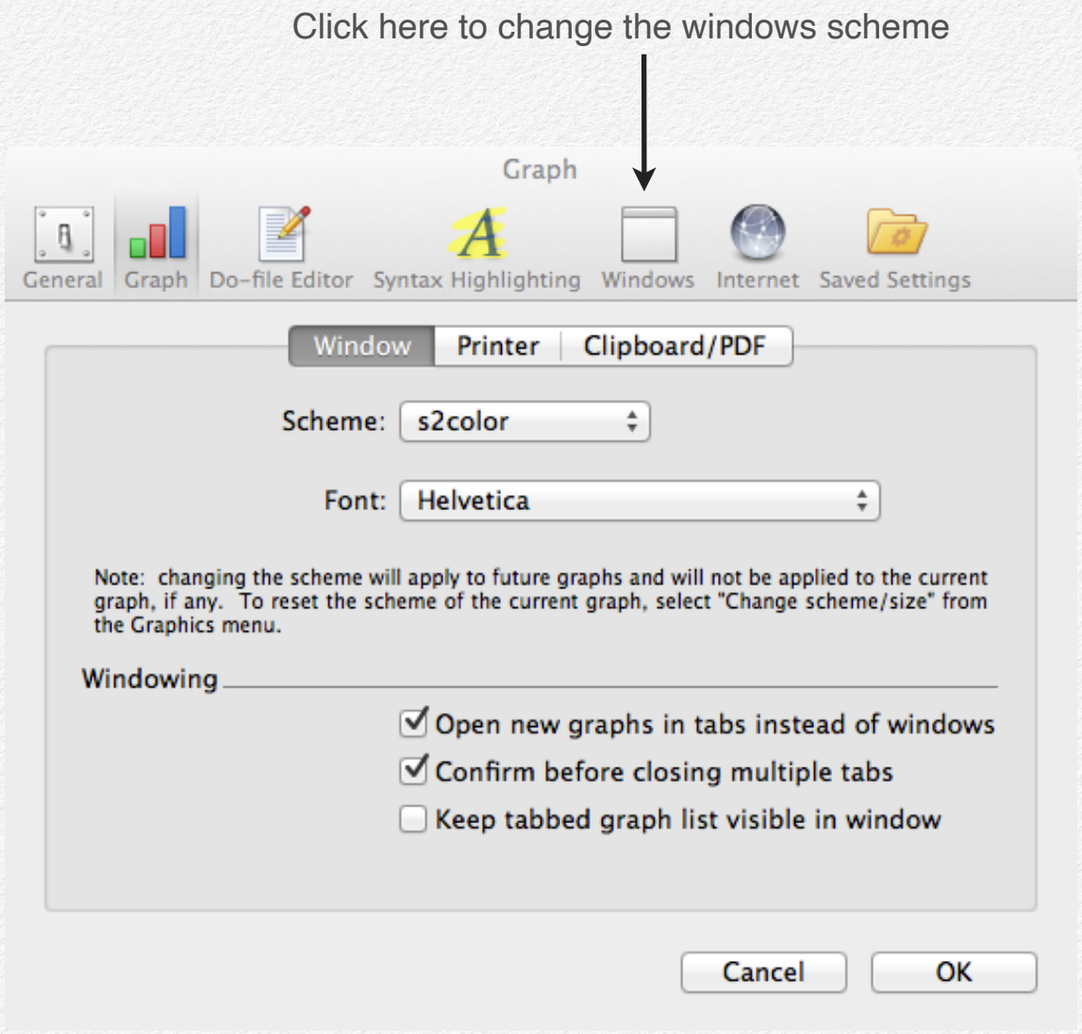
5. The graphics window

STATA can display many graphs simultaneously. This can be done either in a tabbed single graphic window (Fig. 3) or as multiple floating windows. This option should be selected in STATA graph preferences screen, as shown in Figure 1.4.

Working with SHRIMPTOOL we found it advantageous to keep the windows tabbed.

Graphs can be kept displayed as long as they are not replaced by new graphs with the same name. If we want to keep a graph, we must rename it using the command: **graph rename** new_name.

Tip: STATA takes a while to make the first graph after opening the program. This is due to the way STATA handles code. Subsequent graphs appear more quickly.



Fgure 1.4. Stata preferences screen.

Running SHRIMPTOOLS

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Invoking SHRIMPTOOLS

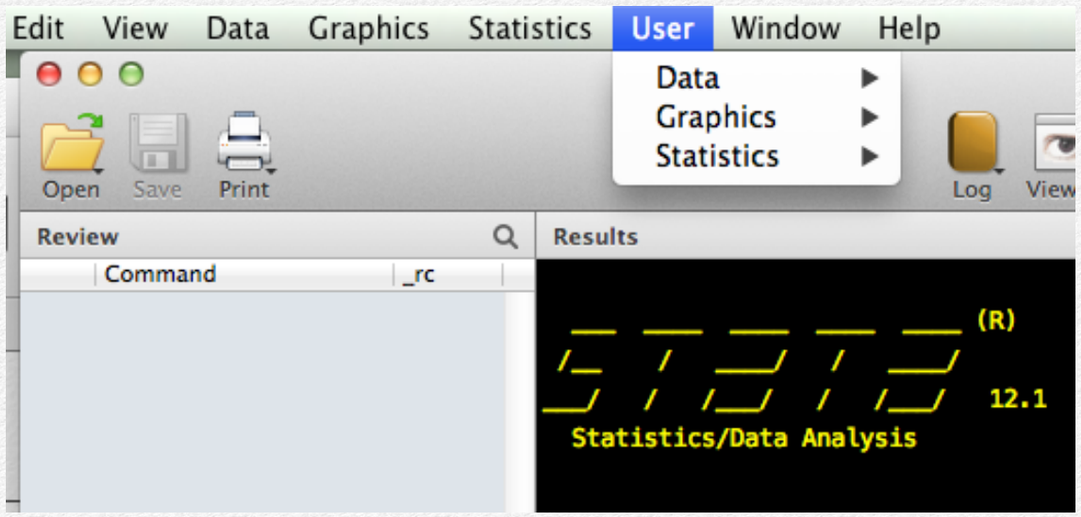

Figure 2.1. STATA User menu before activating SHRIMPTOOLS

1. Starting SHRIMPTOOLS

Before activating SHRIMPTOOLS, and only for training purposes, go to the STATA User menu and pull it down. Three options appear: ***Data***, ***Graphics***, and ***Statistics*** (Fig. 2.1).

Then, in the command window type: **shrimptools** [return]

At this point two things should happen:

1. The user menu changes to incorporate a new item **SHRIMPTOOLS** (Figure 2.2)
2. The results screen displays a message like that shown in Figure 2.3

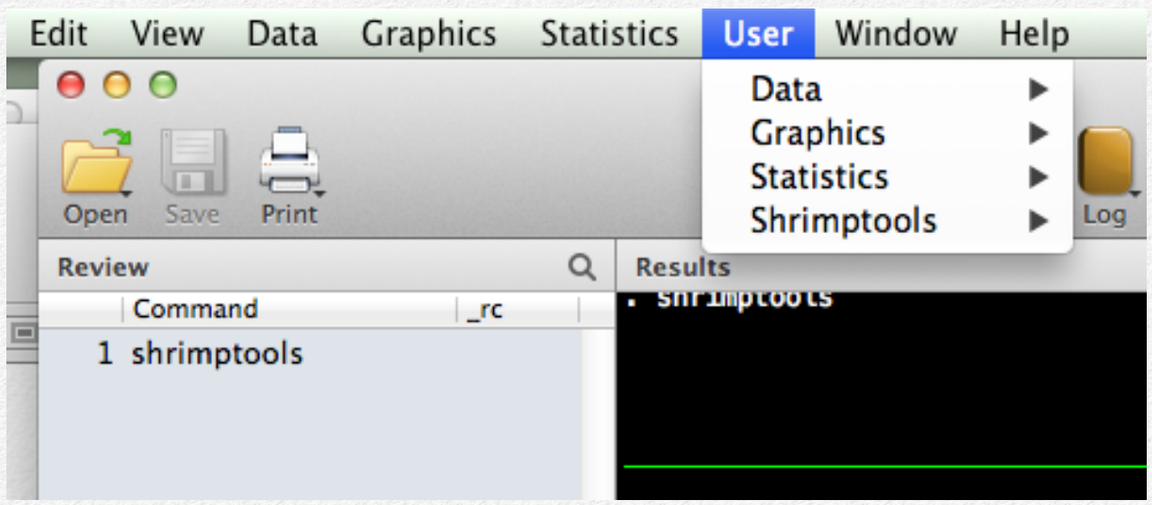

Figure 2.2. STATA user menu after activating SHRIMPTOOLS. Note the appearance of a fourth item: **Shrimptools.** Compare with Fig. 2.1.

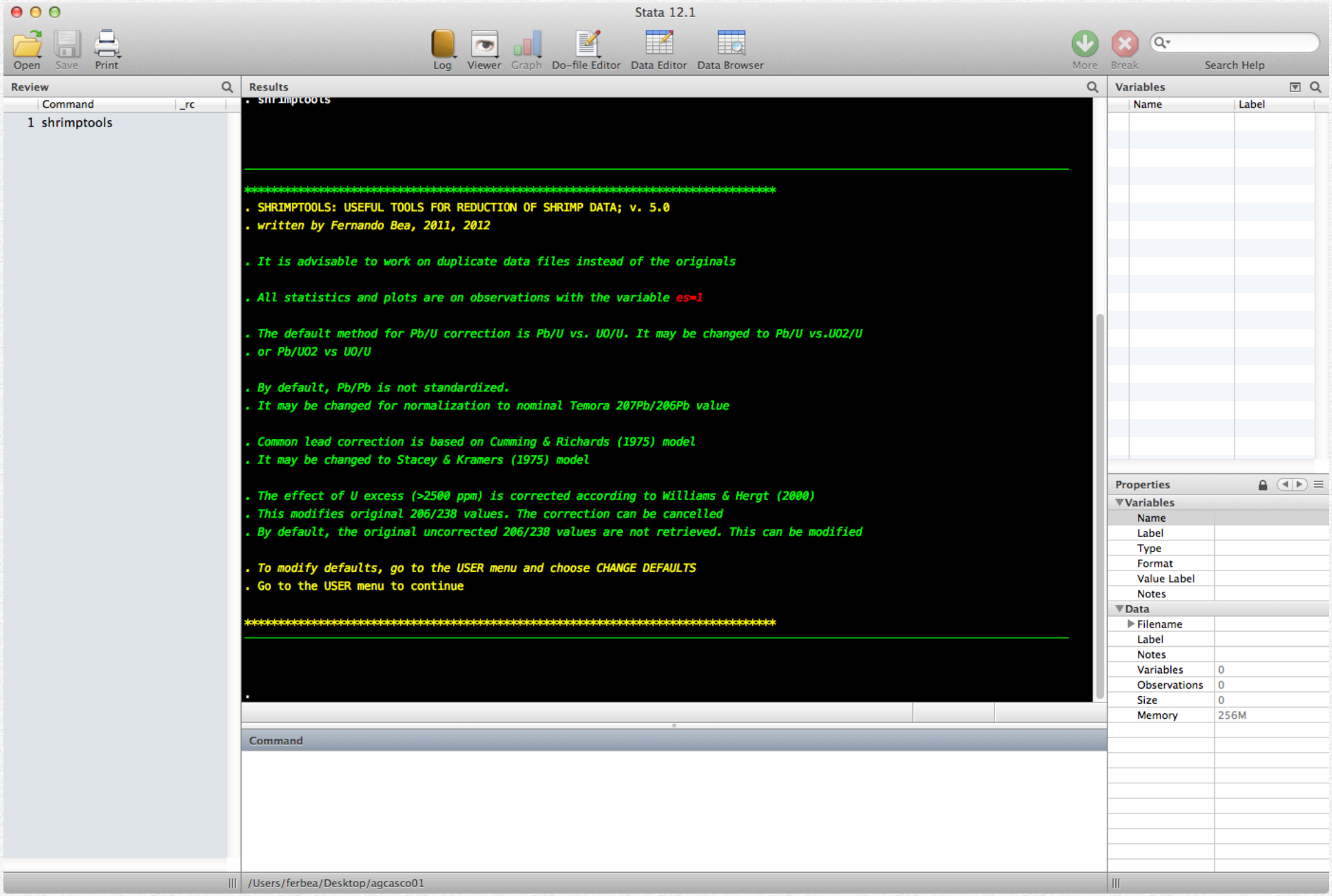

Figure 2.3. Results window displaying SHRIMPTOOLS starting message. Note in the upper left corner the command issued to invoke it. If this screen appears, SHRIMPTOOLS was launched successfully.

2. Troubleshooting invoking SHRIMPTOOLS

If none of the above happens or you get an error message, there are only two possible reasons:

1. **shrimptools** [return] was mistyped in the command window. Note it must be written in lower case and entered with the return key

2. the ado files are not in the correct location (see Chapter 1).

Beginning with SHRIMPTOOLS

1. Before beginning

Please, read the starting message displayed when you type **shrimptools** [return] ver carefully. It gives some instructions about how to run the software. The normal workflow for dealing with geochronological data is:

1. Reduce a SHRIMP .pd data file
2. Work with that file to group the spots, calculate the ages and plot them in concordia diagrams
3. Study the occurrence of outliers and calculate averages for each group
4. Transfer the results to a publication-ready table

All these task can be done with SHRIMPTOOLS. You can also transfer the reduced isotope ratios to ISOPLOT. You can practice with the file the_nice_file.pd provided with the software.

Reducing a SHRIMP .pd data file creates a STATA file with all the relevant isotope ratios and element concentrations. Two versions of this file are automatically saved within the .pd file directory. One is a STATA .dat (binary) file; it would be used in STATA . The other is a plain text (.txt) file containing exactly the same information; it can be used in any other program for example ISOPLOT. These files are named after the .pd file. For exam-

ple, the_nice_file.pd after being reduced creates the files the_nice_file_process.dat and the_nice_file_process.txt.

All age calculations, concordia plots, statistics, etc… are done once my_file_process.dat is created. SHRIMPTOOLS can also process isotope data reduced by other programs, but the user must create a .dat file with the same conventions and variable naming. This is quite tiresome and time consuming; it is better to begin from scratch using the .pd file.

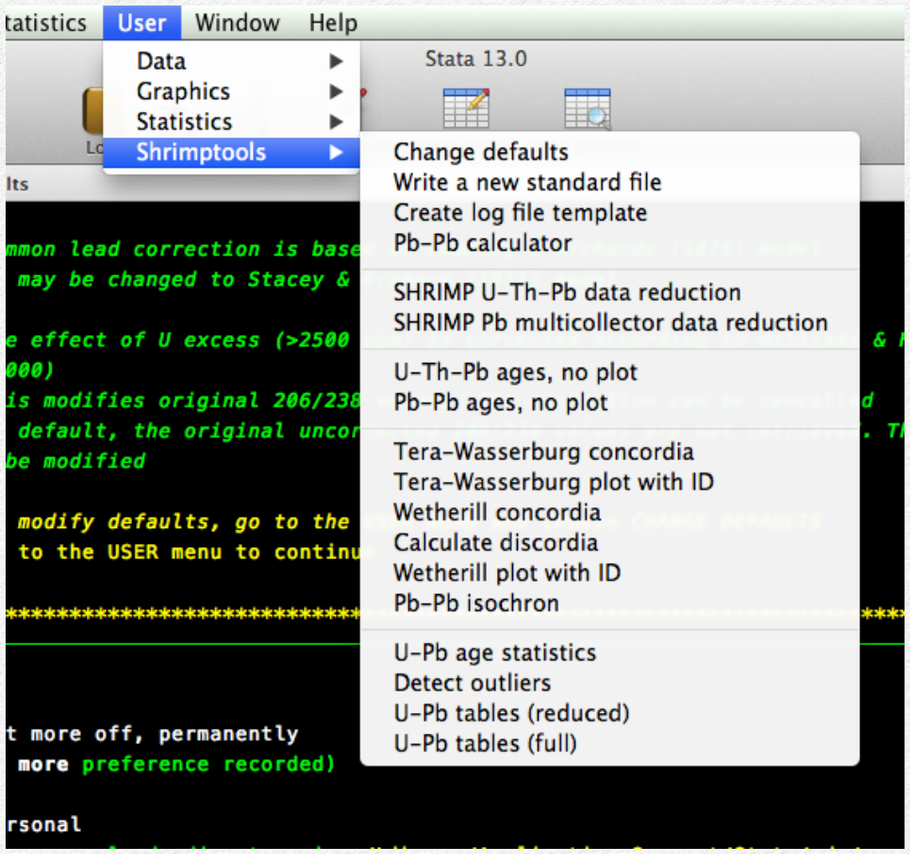

Figure 2.4. The SHRIMPTOOLS menu.

2. The SHRIMPTOOLS menu (Fig. 2.4)

Most task done by SHRIMPTOOLS are called from the ***User > Shrimptools*** menu. This is split in five blocks:

Block 1 (handy things you do not often use)

- Change defaults
- Write a new standard file
- Create log file template
- Pb-Pb calculator

Block 2 (data reduction)

- SHRIMP U-Th-Pb data reduction
- SHRIMP Pb multicollector data reduction

Block 3 (age calculations with no plots)

- U-Th-Pb ages, no plot
- Pb-Pb ages, no plot

Block 4 (plots, discordia, and Pb-Pb isochron)

- Tera-Wasserburg concordia
- Tera-Wasserburg plot with ID
- Wetherill concordia
- Calculate discordia
- Wetheril plot with ID
- Pb-Pb isochron

Block 5 (statistics and tables)

- U-Pb age statistics
- Detect outliers
- U-Pb tables (reduced)
- U-Pb tables (full)

The next sections explain, in detail, the meaning of each command.

Block 1: handy things you do not often use

1. **Change defaults**
2. **Write a new standard file**
3. **Create log file template**
4. **Pb-Pb calculator**

1. Change defaults

By default SHRIMPTOOLS chooses what we consider to be the best options for data reduction and age calculation, but many of these default options can be changed in ***User > Shrimptools > Change defaults***. You can modify:

1. How $^{206}Pb/^{238}U$ is calculated: $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$?, $^{206}Pb/^{238}U$ vs. $^{260}UO_2/UO$?, or $^{206}Pb/^{260}UO_2$ vs. UO/U?, the default is $^{254}UO/^{238}U$. If you want to use the others options, make sure that $^{260}UO_2$ has been measured

2. $^{207}Pb/^{206}Pb$ standard normalization. The default is NO. Option YES is only advisable when the unknowns are younger than the standard

3. U-excess correction. This corrects $^{206}Pb/^{238}U$ when the U concentration is higher than 2500 ppm; it follows the procedure of Williams & Hergt (2000). The default is YES

4. Retrieve original $^{206}Pb/^{238}U$. This retains the original value before the U-excess correction. The default is NO

5. Which Pb isotope model to assume for common lead correction: Stacey & Kramers (1975) or Cummings & Richard (1985). The default is Cummings & Richard (1985)

6. The percentage of discordia above of which the ID spots are shown in either the ***Tera-Wasserburg plot with IDs*** or the ***Wetherill concordia plot with IDs***. The default is 5%

7. Which kind of f206 (fraction of non radiogenic ^{206}Pb) is displayed in the reduced tables: f206 based on ^{204}Pb (the default) or f206 based on ^{208}Pb?. The full tables option gives both calculations

Changes made are maintained as long as you do not close STATA or do not invoke SHRIMPTOOLS again. However, the changes are NOT permanently recorded. To restore the defaults run the same routine or just enter **shrimptools** [return] again.

2. Write a new standard file

SHRIMPTOOLS has a database of standards. Using this option you can add new ones, just follow the on-screen instructions.

3. Create log file template

This routine creates a .dat file template suitable for storing the isotope ratios and ages of each sample during a SHRIMP run. It is useful for having a quick look at provisional results during an analytical session, but of o use if you are not running the SHRIMP. Data transfer from the SHRIMP to an external computer needs some additional routines that are not included in SHRIMPTOOLS.

4. Pb-Pb calculator

This is a simple calculator for $^{207}Pb/^{206}Pb$ ages, a legacy of the old good times when we did lead-evaporation analyses. To exit the calculator key a 9 as the entry for the $^{207}Pb/^{206}Pb$ ratio.

Block 2: data reduction

Data reduction is the primary task for which SHRIMPTOOLS was designed. The mathematics involved, including error calculation, are explained in Chapter 3.

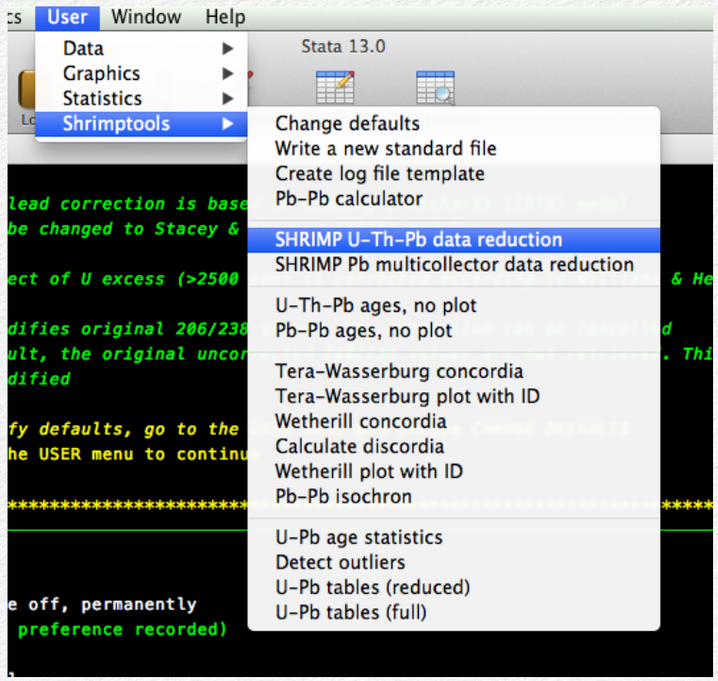

Figure 2.5. Calling SHRIMP U-Th-Pb data reduction.

1. SHRIMP U-Th-Pb data reduction

SHRIMPTOOLS processes SHRIMP .pd files. It does not process .op files, because they contain less information. Neither does it processes .xlm files because, at the moment, we found no advantage in doing so. Nonetheless, this may change in the future.

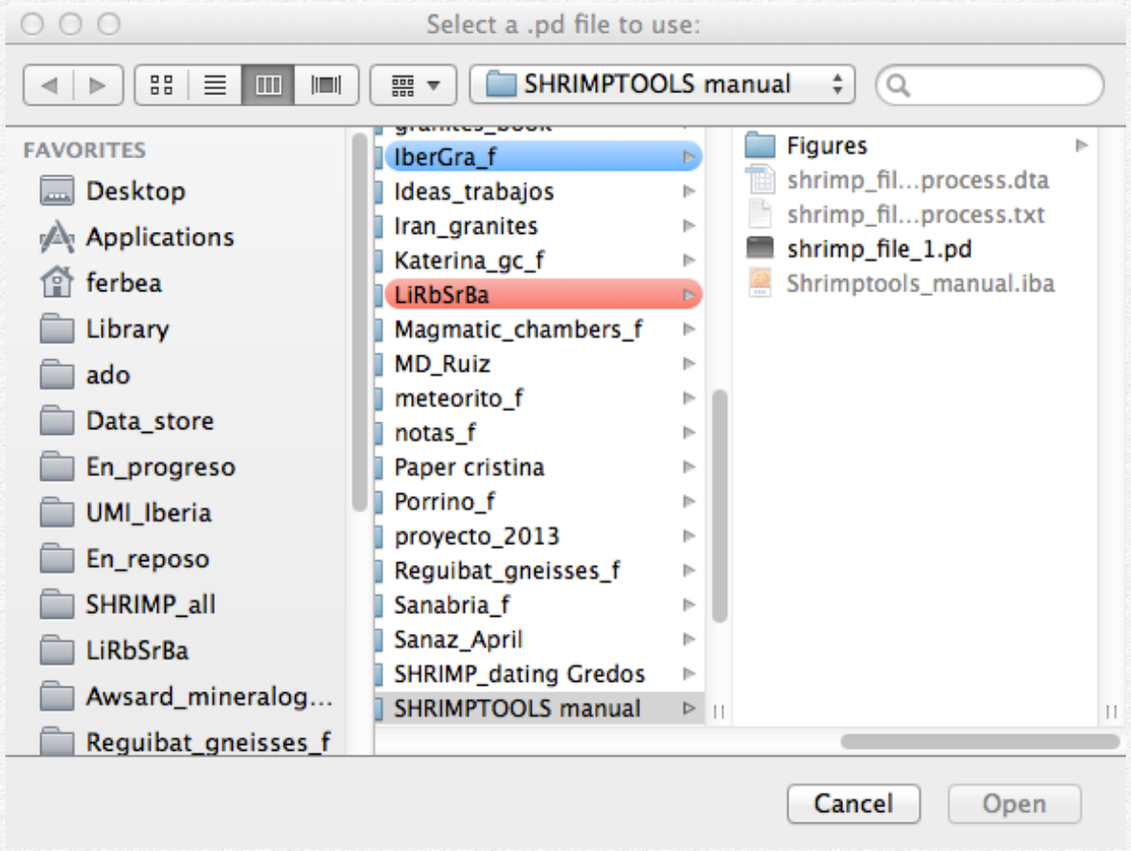

Figure 2.6. The open file dialog. Note that only the .pd file is enabled

The file must have been acquired measuring the following masses: $^{196}Zr_2O$, ^{204}Pb, $^{204.1}$background, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{238}U, ^{248}ThO, ^{254}UO, and (optional) $^{260}UO_2$

To process a .pd file, go to ***User > Shrimptools > SHRIMP U-Th-Pb data reduction*** (Fig. 2.5). Once you call the routine a self-explanatory red line appears in the results window:

This routine will destroy all data currently in memory. Do you want me to continue? (y/n).

If you enter YES, an open dialog appears (Fig. 2.6). Otherwise you get the message:

SHRIMP_DECO program aborted by the user.

The open dialog looks for the .pd file on the desktop, but you can go to any other directory. Note that only .pd files are enabled.

```
This routine will destroy all data currently in memory. Do you want me to continue? (y/n). y
User chose /Users/ferbea/En_progreso/SHRIMPTOOLS manual/shrimp_file_1.pd as the filename


SHRIMP SW v3.12 SHR 2 ACQUISITION PRAWN DATA FILE
analyst fbea, mount 13_7bis,
fbea_13_7bis_13042908.52.pd, 29/04/2013, 8:52 AM
Reading analysed spot 1; Spot ID = SL13
Reading analysed spot 2; Spot ID = TEM-7.1
Reading analysed spot 3; Spot ID = REG47-22.1
Reading analysed spot 4; Spot ID = REG47-23.1
Reading analysed spot 5; Spot ID = REG47-24.1
Reading analysed spot 6; Spot ID = TEM-8.1
Reading analysed spot 7; Spot ID = REG47-25.1
Reading analysed spot 8; Spot ID = REG47-26.1
Reading analysed spot 9; Spot ID = REG47-27.1
```

Fig 2.7. Reading a .pd file

Figure 2.7. Results window displayed during the file readout.

Once the .pd file is open you will see messages in the result windows displaying (1) the heading of the .pd file, and (2) the number and ID of each spot read (Fig. 2.7). After finishing it displays the total number of spots in the .pd file and a list of the standards currently in the SHRIMPTOOLS database. Before going any further, we must discuss some conventions regarding how to name and use the standards.

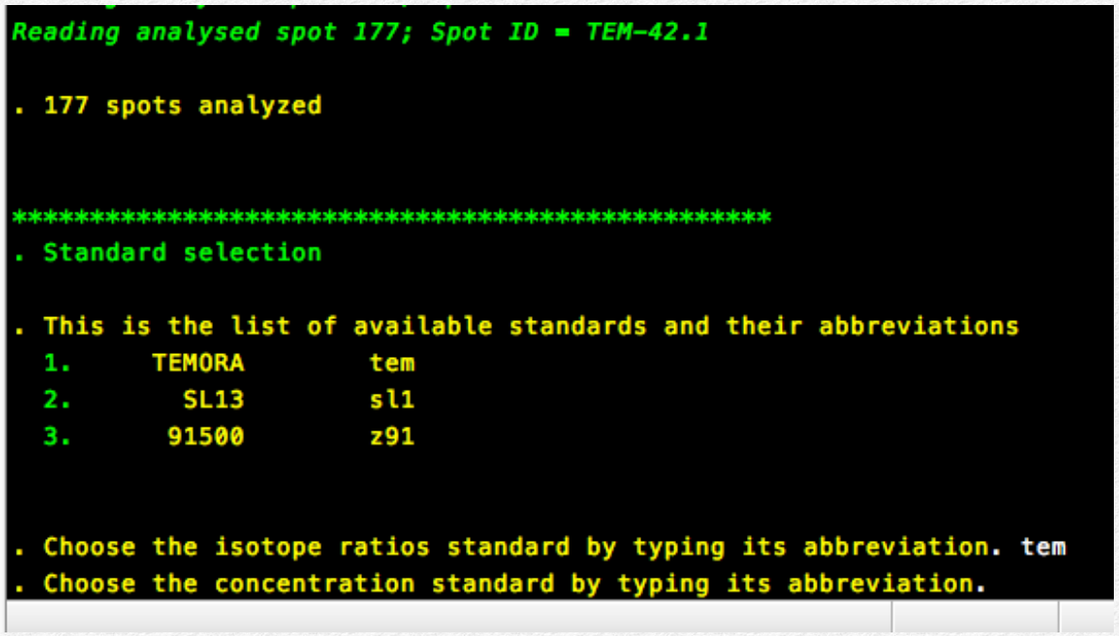

Fig 2.8. Asking for the name of standards to be used in data reduction.

1.1. Conventions using and naming standards

SHRIMPTOOLS accepts any standard, which can be easily added to its database with the routine called by ***User > Shrimptools > Write a new standard file.*** In principle we use two types of standards, one for age and the other for concentration. The standard for age is usually analysed every four unknowns (see Fig. 2.7) whereas the standard for concentration is analysed just once at the beginning of a session. The isotope ratios standard (also named as the age standard) can be used as concentration standards if you so specify it.

One measurement of the concentration standard is always required; otherwise the element concentrations will not be calculated. It there is more that one measurement of the concentration standard, the software uses the average.

For SHRIMPTOOLS to recognize that a spot belongs to a given standard you must name it accordingly during the analytical session. The software trims the spot IDs to the first three characters, which must match the standard abbreviation (upper case or lower case does not matter). For example, the TEMORA standard should be named as TEM-1, TEM-2, ...TEM-XX. Other formats such as TEMORA-1, TEMORA-2, etc… are acceptable as well, but T-1, T-2,... or TE-1, TE-2 are not. The standard SL13 must be named SL13, or SL13-1, etc. The best way is using the standard abbreviations (lower case or upper case) displayed by the program (Fig. 2.8).

If you have an old file with these standards named in a different way, your best option is to use a text editor such as TextWrangle and edit them using find/replace.

1.2. Troubles reading .pd files

If SHRIMPTOOLS issues an error reading a .pd file, the reason is almost certainly the bad structure of the file. It normally happens when the SHRIMP was aborted analysing one spot and the data for such these incomplete spot were incorporated in the .pd file.

To fix this problem, you must identify the spot at which the file reading was aborted. You can do this by just looking at the last

id	206Pb/238U	date	time	nº
TEM-7.1	.1289768	2013-04-29	09:48	2
TEM-8.1	.1156097	2013-04-29	10:52	6
TEM-9.1	.1270468	2013-04-29	12:10	11
TEM-9.1	.1300172	2013-04-29	13:59	15
TEM-10.1	.125127	2013-04-29	14:31	17
TEM-11.1	.1237751	2013-04-29	16:09	22
TEM-12.1	.1330292	2013-04-29	17:27	27
TEM-13.1	.1296668	2013-04-29	18:45	32
TEM-14.1	.1291519	2013-04-29	20:03	37
TEM-15.1	.1208684	2013-04-29	21:21	42

Figure 2.9. List of standards.

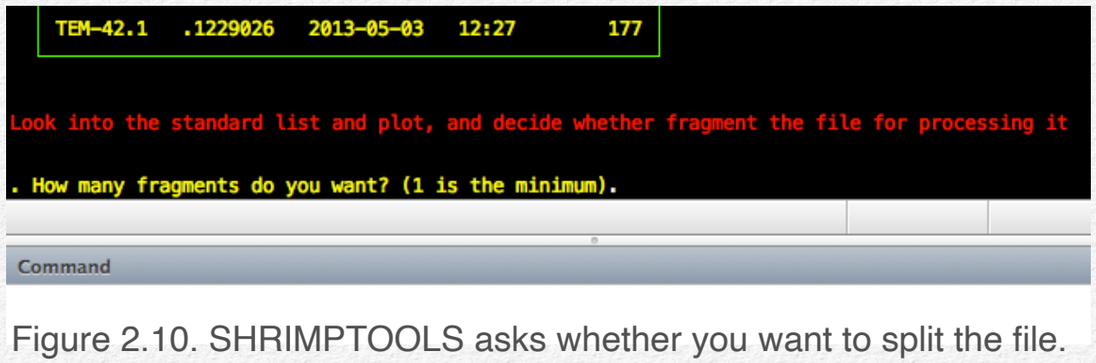

Figure 2.10. SHRIMPTOOLS asks whether you want to split the file.

spot ID displayed in the results window. Once the rogue sample is identified, open the .pd file with a text processor, find the sample and delete it from the file. An example is given in the troubleshooting chapter at the end of the manual.

1.3. Splitting the file

Once you enter the concentration standard, SHRIMPTOOLS (1) displays a sequential list of the analysed spots of the isotope ratios standard, including its measured $^{206}Pb/^{238}U$, the date and the time at which they were measured and the standard number (Figs. 2.9 and 2.10) (2) displays a $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$ plot (Fig. 2.11) and (3) ***asks you whether you want to split the file***. This can be decided easily by looking at the table and the $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$ plot.

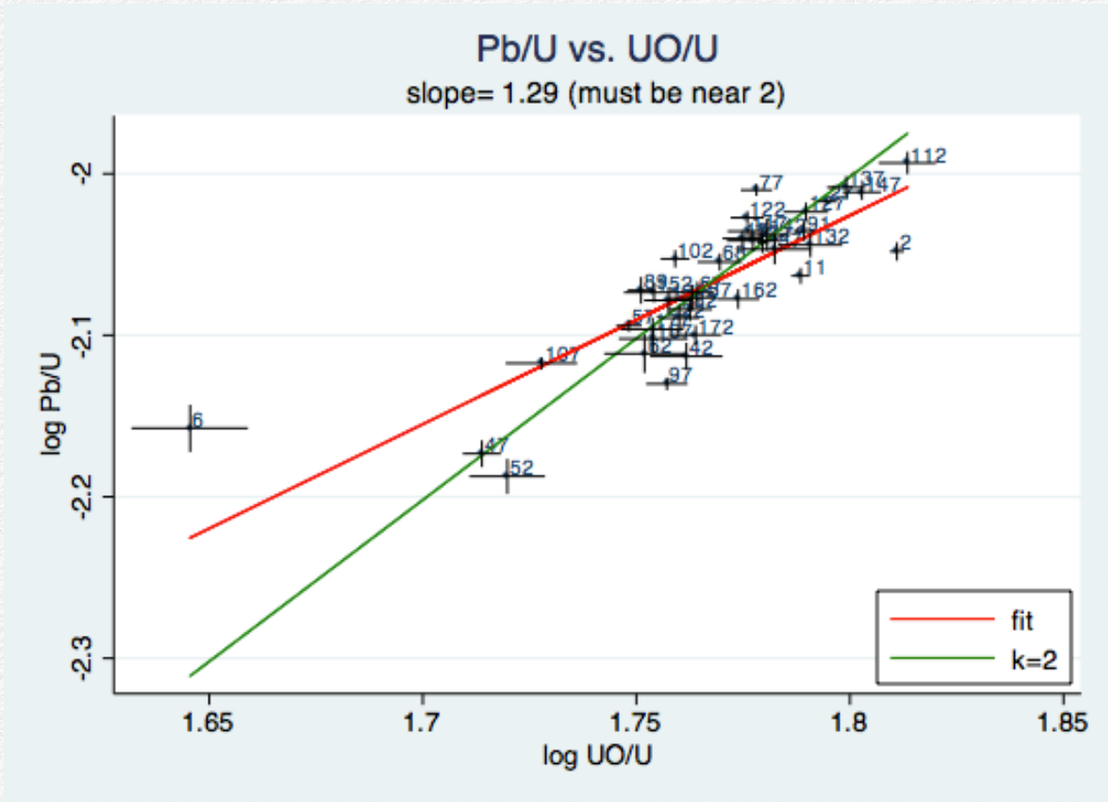

Figure 2.11. $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$ plot. This is useful for deciding whether the file should be split and which bad standards should be deleted. See text.

When a file does require splitting? Splitting files is not often done. It is useful if the SHRIMP instrumental conditions

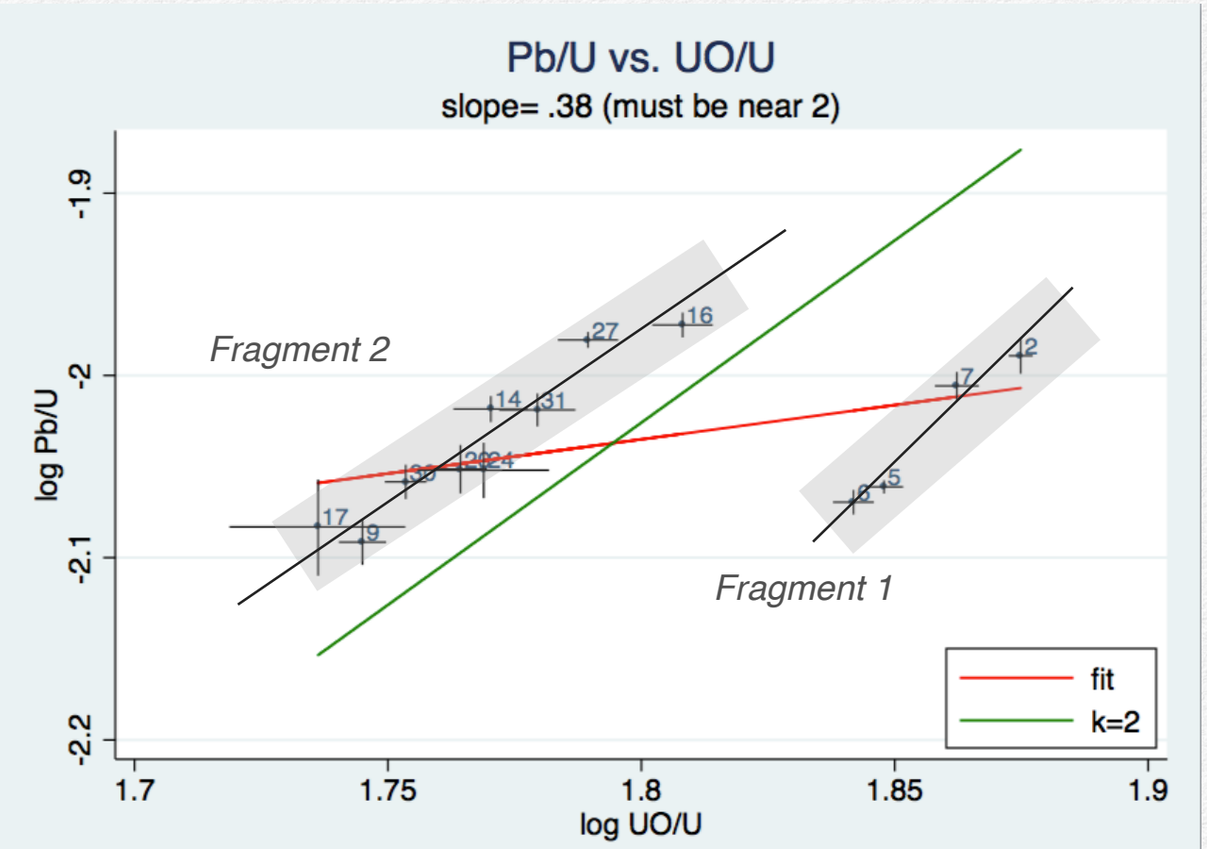

Figure 2.12. $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$ plot showing a file that must be split because of changing duo. Note de difference between the theoretical and the fixed regression line. Splitting the file causes each fragment to be reduced following their individual regression line.

changed dramatically during a run, for example because of the duo was changed, or if you have assembled a single .pd file with data from different sessions. The fragments must be sequential. The example shown in Figure 2.11 does nor require splitting (it however requires standard deletion, see below). By contrast, the example shown in Figure 2.12 does require splitting.

If you do not want to split the file, you must enter 1 when prompted:

. How many fragments do you want? (1 is the minimum)

If you specify 2 or more fragments, you are prompted to enter the number of the standards that are at the beginning and end of each fragment. In the case shown in Fig. 2.12, the first fragment would comprise the analyses between standards 2 and 7, and the second fragment those between 8 and 31.

Once the fragments are specified, the whole data reduction process is looped independently on each fragment. At the end, however, all the data are combined in the same file. In short, it does not matter how many fragments you specify; for each raw .pd file you only have one reduced .dat file that contains all your data.

1.4. Deleting standards and choosing the slope in the $^{206}Pb/^{238}U$ correction

After specifying the number of fragments SHRIMPTOOLS asks you whether you want to use all the standards displayed in the $^{206}Pb/^{238}U$ *vs.* $^{254}UO/^{238}U$ plot, or you want to delete some of them. For example, in Figure 2.11 it would be a good idea to delete standard nº 6. To do this simply enter the number of the

standard to be eliminated. Every time one standard is deleted the $^{206}Pb/^{238}U$ vs. $^{254}UO/^{238}U$ plot is redrawn and you may eliminate another standard if required. The process ends when you

```
The drift function is either a quadratic or a cubic curve, whichever yields lower residuals
207Pb/206Pb adjusted to a quadratic curve
207Pb/206Pb adjusted to a quadratic curve

Manual elimination of 207/206 and 206/238 outliers
. Shall we eliminate outliers? (y/n).
```

Figure 2.13. Drift corrections

enter 0 (zero) as the number of the next standard to be eliminated.

After deleting unwanted standard spots, the software asks you which slope should be used for the oxide correction. The theoretical value is 2, but you can choose the slope of the regression line. If the standards fit well, this would probably be the most sensible option.

1.5. Correcting for drift

After choosing the slope, SHRIMPTOOLS corrects for drift in both $^{207}Pb/^{206}Pb$ and $^{206}Pb/^{238}U$.

The software calculates two types of correction, quadratic or cubic. It then calculates the residuals for each correction type and automatically chooses the best option (Fig. 2.13) plotting the standard measurements *vs.* analysis number (analysis time, in fact). In the plot generated (Fig. 2. 14) the vertical bars indi-

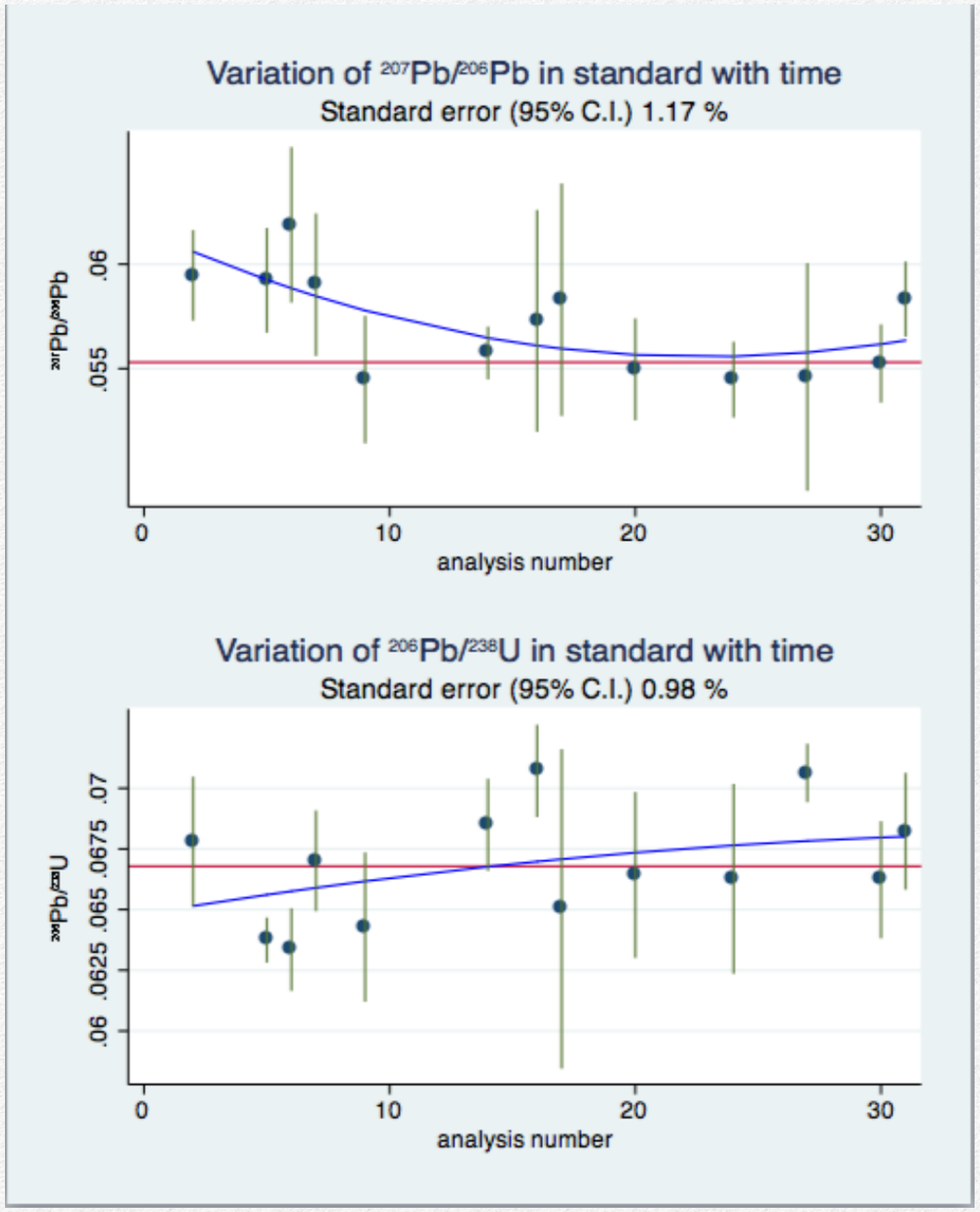

Figure 2.14. Standards vs. time. The vertical bar is the error of each measurement. The horizontal red line is the average of each measurement. The blue line is the drift function. The errors in the heading are the point-to-point error.

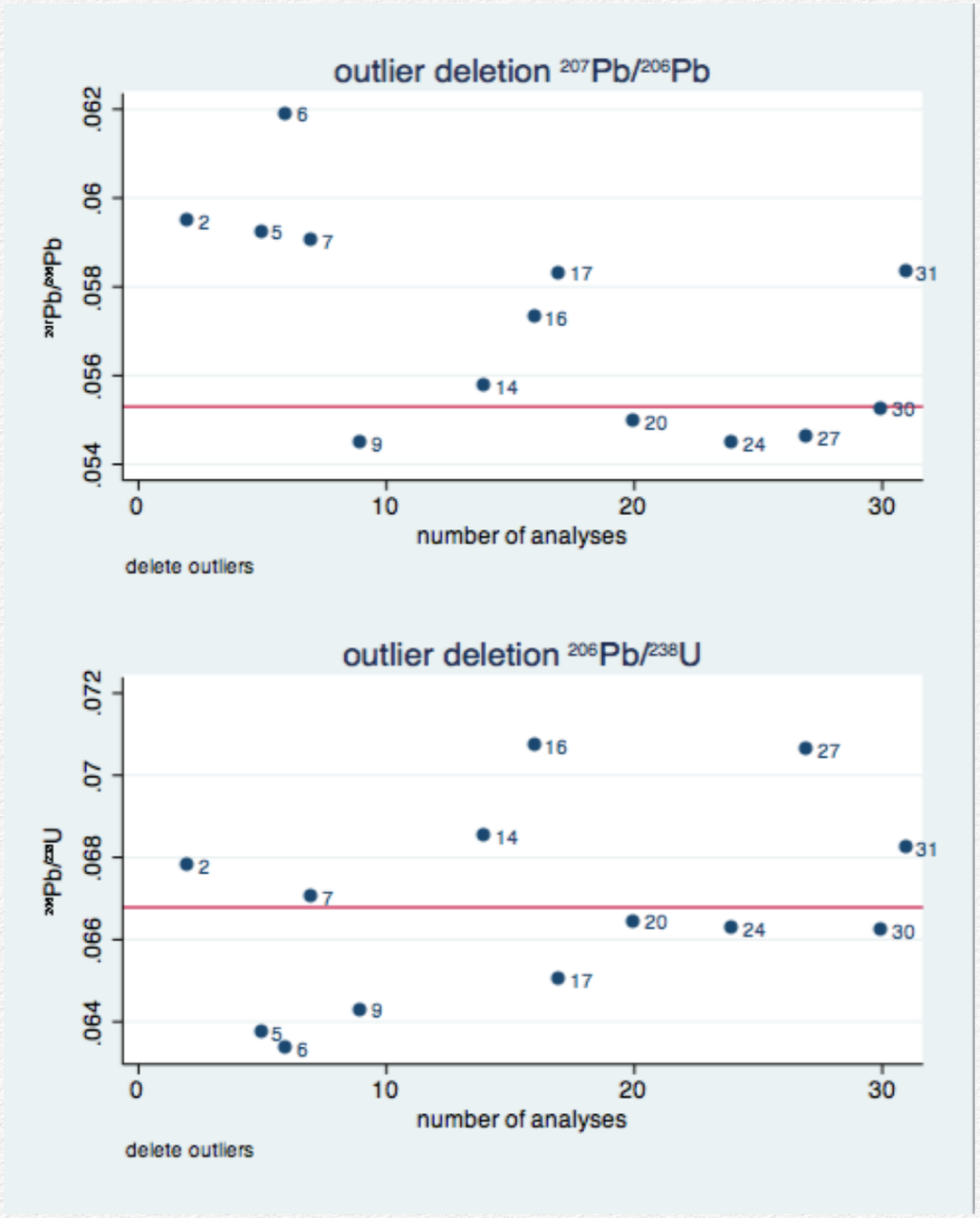

Figure 2.15. Outlier elimination window.

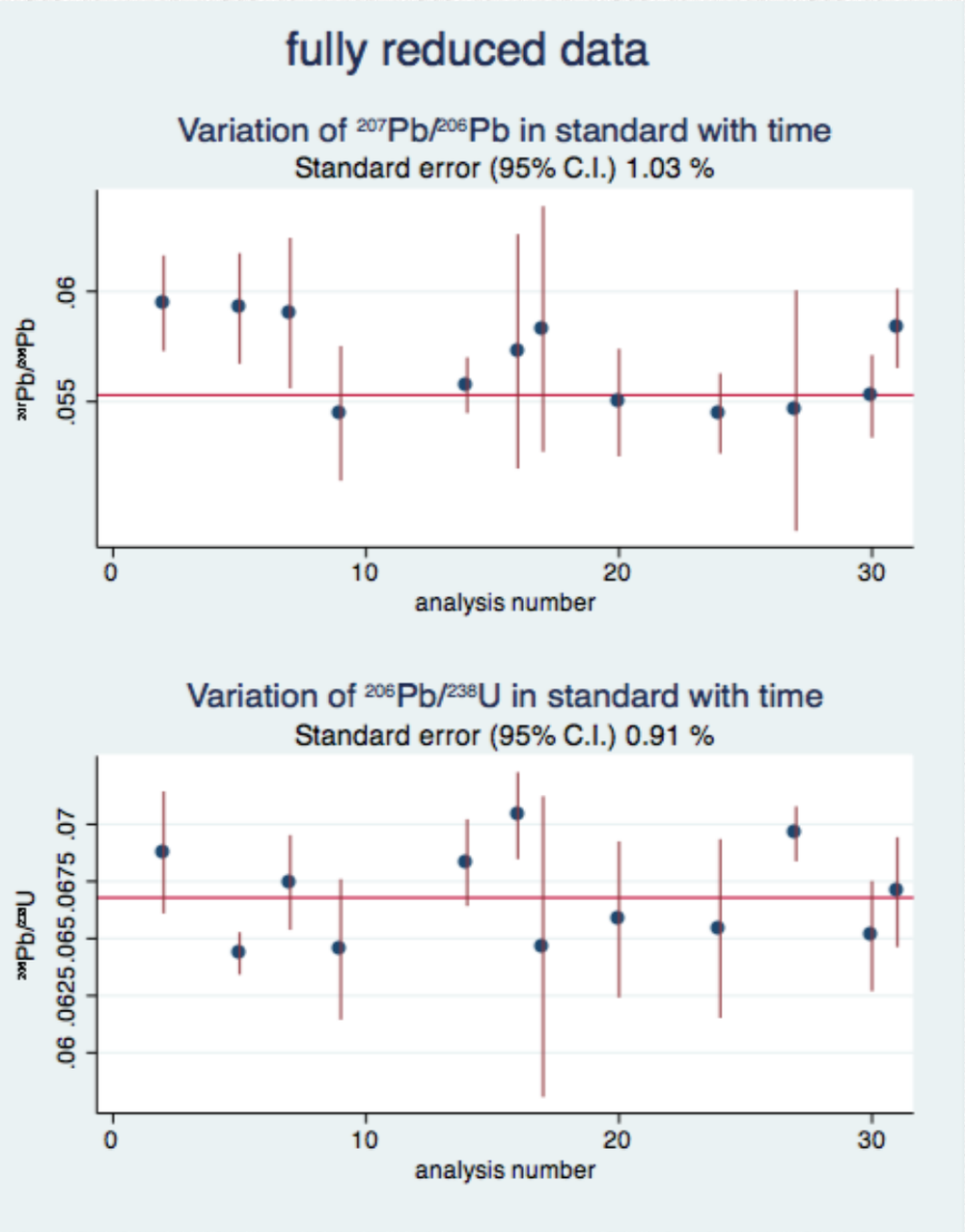

Figure 2.16. Final screen once data are fully reduced.

cates the error of each standard, the red horizontal line is the standards average, the blue line represents the drift function and the heading gives the point-to-point error.

Once the standard measurements are plotted, the software prompts you if you want to delete any standard from the drift correction. If you say YES, a new screen appears with the same plot but with no error bars, no drift function, and the vertical scale fully expanded to cover the variation range of the standards (Fig. 2.15; before being fooled by the dispersion, check the vertical scale range). Once you have finished eliminating outliers, the software recalculates the drift functions and asks whether to apply them to the unknowns. The query is:

Drift correction:
Shall we leave it uncorrected (1) correct 206/238 (2) or correct also 207/206 (3)

Option (1) means that no correction is applied. Option (2) corrects $^{206}Pb/^{238}U$. Option (3) corrects $^{206}Pb/^{238}U$ and $^{206}Pb/^{207}Pb$. There is no point in correcting $^{206}Pb/^{207}Pb$ and not correcting $^{206}Pb/^{238}U$.

1.6. Saving the fully reduced data

After cleaning up the data file, the standards with error bars and point-to-point errors are plotted anew (Fig. 2.16). Two files with the same name but different extension (one .dat and other .txt) are simultaneously automatically saved to the same directory in which the .pd file is located. The following message is displayed:

The file /Users/ferbea/Desktop/pmontero_13-3cinco_13061712_process.dta has been created in the same folder as the .pd file

The file /Users/ferbea/Desktop/pmontero_13-3cinco_13061712_process.txt has been created in the same folder as the .pd file

. Done SHRIMP_DECO.

These two files are named after the .pd file. For example, after reducing my_file.pd the two files created are my_file_process.dat and my_file_process.txt. One is a STATA .dat file would be used in STATA . The plain text (.txt) file contains exactly the same information and can be used in any other program for example ISOPLOT.

1.7. Structure and variable naming in the resulting STATA file

The file created by STATA is a rectangular array. The columns are the variables, that is, the spot names, isotope ratios, ages, etc. The rows are the observations, that is, one row for each spot measured.

The names assigned to the variables created by SHRIMP-TOOLS attempt to be self-explanatory and compliant with STATA conventions, but they might be rather dense. Therefore, we assigned labels to these variables which are more similar to

Table 2.1. Variables created during data reduction

variable	label	description (if necessary)
id	Spot identifier	The spot identifier as entered in the SHRIMP during analysis
std_age	Age standard identifier	1 means the spot is an age standard, empty (.) is not an age standard; 0 is a rejected age standard
std_conc	Concentration standard identifier	If contains 1, the spot corresponds to the age standard
date	Date of measurement	
time	Time of measurement	
sets	Number of sets	The software can reduce in the same .pd file measurements with different number of sets
scans	Number of scans	The software can reduce in the same .pd file measurements with different number of scans
peaks	Number of measured masses	The mass peaks measured may be 9 or 10, depending on whether the mass 260 (UO_2) is measured
u_ppm	U_ppm	The concentration of U in ppm
th_ppm	Th_ppm	The concentration of Th in ppm
pb_ppm	Pb_ppm	The concentration of ^{206}Pb in ppm
pb4_pb6	204Pb/206Pb	
err_pb4_pb6	± s 204Pb/206Pb	Error in $^{204}Pb/^{206}Pb$, calculated at 95% confidence level
f206	204-based f206%	fraction of non-radiogenic ^{206}Pb calculated from ^{204}Pb
pb7_pb6	207Pb/206Pb	
err_pb7_pb6	± s 207Pb/206Pb	Error in $^{207}Pb/^{206}Pb$, calculated at 95% confidence level
pb8_pb6	208Pb/206Pb	
err_pb8_pb6	± s 208Pb/206Pb	Error in $^{208}Pb/^{206}Pb$, calculated at 95% confidence level

Table 2.1. Continuation

variable	label	description (if necessary)
pb6_u8	206Pb/238U	
err_pb6_u8	± s 206Pb/238U	Error in $^{206}Pb/^{238}U$, calculated at 95% confidence level
pb7_u5	207Pb/235U	
err_pb7_u5	± s 207Pb/235U	Error in $^{207}Pb/^{235}Pb$, calculated from the errors in $^{207}Pb/^{206}Pb$ and $^{206}Pb/^{238}U$
pb8_th	208Pb/232Th	
err_pb8_th	± s 208Pb/232Th	Error in $^{208}Pb/^{232}Th$, calculated at 95% confidence level
th_u	232Th/238U	
err_th_u	± s 232Th/238U	Error in $^{232}Th/^{238}U$, calculated at 95% confidence level
comment	Comments	This variable indicates whether the spot was a bad standard or close to a bad standard
pbu_err_in_std	Point-to-point 206/238 error	This is the same for all spots, calculated from the measurements of the standard age
pbpb_err_in_std	Point-to-point 206/207 error	This is the same for all spots, calculated from the measurements of the standard age
es	Control variable for plotting	This is a dummy variable used for grouping samples, controlling which samples plot, etc… You will learn how to use it in the next sections

real names. Variable names and labels appear in the variable window. If during the process you see variables named as _000C, ignore them, they are temporary variables created by STATA, that are automatically deleted at the end of the process.

Typing **describe** [return] (or **d**[return]) in the command window will display all variable names, types, and labels plus information about the file size.

Users must not change variable names, because this would cause software malfunctions. They, however, can change variable labels at their pleasure. To change the label of the variable new_variable, simply type in the command window:

label var variable_name “new label” [return]

Table 2.1 shows a comprehensive description of the variables created during data reduction.Note that the file does not contain variables with ages. These are created after data reduction.
See next section

2. SHRIMP Pb multicollector data reduction

These routines are being tested. At the moment, it is better not to fiddle with them.

Block 3: age calculations with no plots

1. U-Th-Pb ages, no plot

This is the first task the user must do after data reduction. It does not plot concordias, it calculates the following:

1. ^{204}Pb common-lead corrected isotope ratios
2. ^{207}Pb common-lead corrected isotope ratios
3. ^{208}Pb common-lead corrected isotope ratios
4. the ages after uncorrected isotope ratios and their concordance
5. the ages after 204-corrected isotope ratios and their concordance
6. the ages after 207-corrected isotope ratios and their concordance
7. the ages after 208-corrected isotope ratios and their concordance
8. f206 from ^{204}Pb (if not calculated during data reduction)
9. f206 from ^{208}Pb

These results must be saved by the user into the .pd file using STATA's **File > Save menu**. They can be recalculated in a snap at any moment.

Table 2.2. Variables created during age calculations

variable	label
flag_uexcesscor	(no label, see note on next page)
pb6_u8_7cor	207-corrected 206Pb/238U
err_pb6_u8_7cor	±s 207-corrected 206Pb/238U
pb8_th_7cor	207-corrected 208Pb/232Th
err_pb8_th_7cor	±s 207-corrected 208Pb/232Th
pb7_pb6_4cor	204-corrected 207Pb/206Pb
err_pb7_pb6_4cor	±s 204-corrected 207Pb/206Pb
pb8_pb6_4cor	204-corrected 208Pb/206Pb
err_pb8_pb6_4cor	±s 204-corrected 208Pb/206Pb
pb6_u8_4cor	204-corrected 206Pb/238U
pb6_u8_4cor	204-corrected 206Pb/238U
err_pb6_u8_4cor	±s 204-correction 206Pb/238U
pb7_u5_4cor	204-corrected 207Pb/235U
err_pb7_u5_4cor	±s 204-corrected 207Pb/235U
pb8_th_4cor	204-corrected 208Pb/232Th
err_pb8_th_4cor	±s 204-corrected 208Pb/232Th
pb7_pb6_8cor	208-corrected 207Pb/206Pb
err_pb7_pb6_8cor	±s 208-corrected 207Pb/206Pb
pb6_u8_8cor	208-corrected 206Pb/238U

variable	label
err_pb6_u8_8cor	±s 208_corrected 206Pb/238U
pb7_u5_8cor	208-corrected 207Pb/235U
err_pb7_u5_8cor	±s 208-corrected 207Pb/235U
t_pb7_pb6	207Pb/206Pb age (Ma)
err_t_pb7_pb6	±s 207Pb/206Pb age (Ma)
t_pb6_u8	206Pb/238U age (Ma)
err_t_pb6_u8	±s 206Pb/238U age (Ma)
t_pb7_u5	207Pb/235U age (Ma)
err_t_pb7_u5	±s 207Pb/235U age (Ma)
t_pb8_th	208Pb/232Th age (Ma)
err_t_pb8_th	±s 208Pb/232Th age (Ma)
discor	% discordance of uncorrected ages
t_pb6_u8_7cor	207-corrected 206Pb/238U age (Ma)
err_t_pb6_~7cor	±s 207-corrected 206Pb/238U age (Ma)
t_pb8_th_7cor	207-corrected 208Pb/232Th age (Ma)
err_t_pb8_th_7cor	±s 207-corrected 208Pb/232Th age (Ma)
t_pb7_pb6_4cor	204-corrected 207Pb/206Pb age (Ma)
err_t_pb~6_4cor	±s 204-corrected 207Pb/206Pb age (Ma)
t_pb6_u8_4cor	204-corrected 206/Pb238U age (Ma)

Table 2.2. Continuation

variable	label
err_t_pb6_u8_4cor	±s 204-corrected 206/Pb238U age (Ma)
t_pb7_u5_4cor	204-corrected 207Pb/238U age (Ma)
err_t_pb~5_4cor	±s 204-corrected 207Pb/238U age (Ma)
t_pb8_th_4cor	204-corrected 208Pb/232Th age (Ma)
err_t_pb8_th_4cor	±s 204-corrected 208Pb/232Th age (Ma)
discor_4cor	% discordance of 204-corrected ages
t_pb7_pb6_8cor	208-corrected 207Pb/206Pb age (Ma)
err_t_pb7_pb6_8cor	±s 208-corrected 207Pb/206Pb age (Ma)
t_pb6_u8_8cor	208-corrected 206Pb/238U age (Ma)
err_t_pb6_u8_8cor	±s 208-corrected 206Pb/238U age (Ma)
t_pb7_u5_8cor	208-corrected 207Pb/235U age (Ma)
err_t_pb7_u5_8cor	±s 208-corrected 207Pb/235U age (Ma)
discor_8cor	% discordance of 208-corrected ages
f206_8	208-based f206Pb (%)

1.1 Naming conventions

The age calculations create new variables, named as shown in Table 2.2. Note that the variable flag_uexcesscor is used by the program to control whether the U-excess correction has been applied, and so avoid to applying it again.

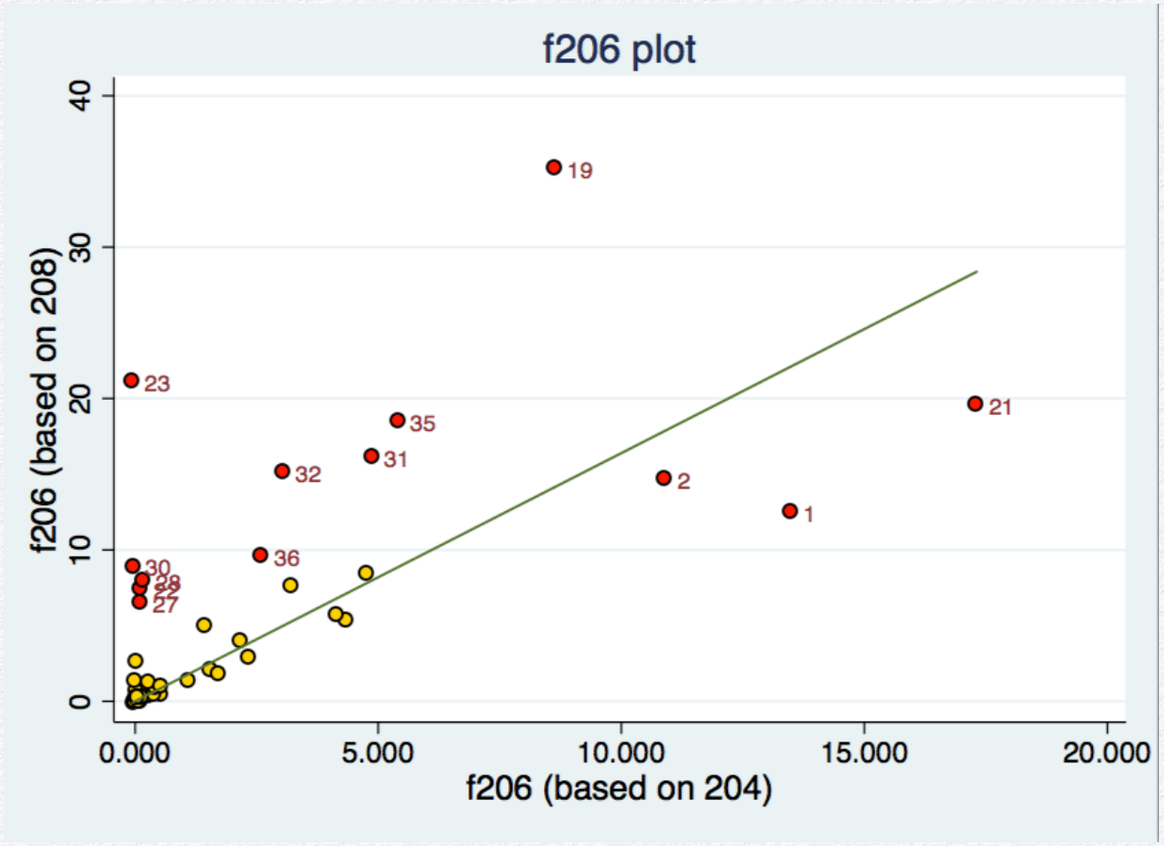

Figure 2.17. ^{208}Pb-based f(206) vs ^{204}Pb-based f(206). This plot is useful for understanding the consistency of the Th-Pb vs U-Pb isotope systems.

1.2 The f206 plot

The routine **U-Th-Pb ages, no plot** does not plot concordias, hence the name. But it does plot the 204-based f206 versus 208-based f206. Red dots represent spots with significant differences between the two parameters; the numbers are the ordinals in the STATA file. This plot is useful to check the consistency of the Th-Pb vs U-Pb isotope systems.

2. Pb-Pb ages, no plot

This routine only calculates the $^{207}Pb/^{206}Pb$ ages. It is useful for multicollector Pb isotopes, but not for normal U-Th-Pb geochron work.

Block 4: age plots

1. **Tera-Wasserburg concordia**
2. **Tera-Wasserburg plot with ID**
3. **Wetherill concordia**
4. **Calculate discordia**
5. **Wetherill plot with ID**
6. **Pb-Pb isochron**

In contrast to the routines described in the previous section,which work on ALL observations (spots) in the file, the routines described in this section ONLY work on those observations (spots) which have the control variable es set to 1. This is useful for selecting groups, including or excluding samples, etc. To change the value assigned to es, you must use the STATA commands **list**, and **replace**. A detailed example is given in Chapter 3.

Before running any of the following routines, the **U-Th-Pb ages** routine (Chapter 2, Section 5.1) must have been executed.

1. Tera-Wasserburg concordia

When this menu item is selected, the software displays a list of the U-Th-Pb ages of the samples with es == 1, and prompts for the limits of the concordia:

```
. INPUT OF AGE LIMITS FOR CONCORDIA PLOT
. Lower Limit? .
. Upper Limit? .
. Labels to plot are multiple of? .
. Shall I plot points (1), points plus error bars (2), or error ellipses (3)?.
```

Then, it plots three Tera-Wasserburg concordias, one for common-lead uncorrected data, another for 204-corrected data and the last for 208-corrected data. To select the concordia limits look at the table displayed in the results window. If the ages

are outside the limits set by the user, STATA automatically expands the plot.

2. Tera-Wasserburg plot with ID

This routine simply plots dots in $^{207}Pb/^{206}Pb$ *vs.* $^{238}U/^{206}Pb$ coordinates, with no concordia line. Points corresponding to spots with less than 5% discordance appear in yellow. Points with discordance greater than 5% appear in red marked with their ordinal number so that they can be easily identify in STATA editor.

The discordance level at which points are plot in red can be changed in the ***User > Change defaults menu***.

3. Wetherill concordia

Works in exactly the smame order as the TW concordia. The only difference is that spots can be plotted either as dots or as error ellipses, but not as points with error bars.

4. Calculate discordia

This routine calculates the best fit discordia line on a Wetherill concordia, and displays the upper and lower intercept values with errors and MSWD. The software prompts the user to specify for which data the discordia should be calculated: common lead uncorrected, 204-corrected or 208-corrected data.

There are many ways to calculate discordias, and some of them produce unreasonable low errors. The approach followed in SHRIMPTOOLS is a robust regression weighted inversely proportional to the percent of discordance and the distance to concordia, with the errors being the intercepts of the 95% confidence interval of the regression line on the concordia line. When points fit a straight line well, all algorithms yield the same results. But if the scatter around the discordia line is high, different algorithms may produce different results. In this latter case case, one must cast doubts about whether the results are of any significance.

5. Wetherill plot with ID

This routine simply plots dots in $^{206}Pb/^{238}U$ *vs.* $^{207}U/^{235}U$ coordinates, with no concordia line. Points corresponding to spots with less than 5% discordance appear in yellow. Points with discordance greater than 5% appear in red marked with their ordinal number so that they can be easily identify in STATA editor.

The discordance level at which points are plot in red and their IDs shown can be changed in the ***User > Change defaults menu***.

6. $^{207}Pb/^{206}Pb$ isochron

This routine is useful for zircons with elevated common Pb.

Block 5: statistics and tables

1. U-Th-Pb age statistics

This routine calculates the mean, standard errors, confidence intervals and MSWD of spots with the variable es ==1.

2. Detect outliers

This is a very useful routine for detecting outliers for each calculated age. It ONLY works on spots with the variable es ==1. The routine first makes a quantile plot. Then, it applies the letter-value display algorithm and defines two boundaries for outlier exclusion called ***inner fence*** and ***outer fence***.

The ***inner fence*** includes all observations comprised between the 25% quartile minus 1.5 times the 25% to 75% quartile spread, and the 75% quartile plus 1.5 times the 25% to 75% quartile spread.

The ***outer fence*** includes all observations comprised between the 25% quartile minus 3 times the 25% to 75% quartile spread, and the 75% quartile plus 3 times the 25% to 75% quartile spread.

Lastly, the software makes three kernel density plots (gaussian), one for samples inside the inner fence, another for samples inside the outer fence, and the last for all samples.

3. U-Th-Pb tables (reduced)

This routine creates a tabulated text file, that can be imported into any spreadsheet, containing the Th, U, Pb concentrations, the common-lead uncorrected and 204-corrected U-Th-Pb isotope ratios, and the common-lead uncorrected and 204-corrected U-Th-Pb ages; it only includes those spots with es set to 1.

4. U-Th-Pb tables (full)

These are similar to the reduced tables, but also include 208-corrected isotope ratios and ages, and prompts whether to include all spots in the .dat file or just those with the grouping variable es==1. It is probably the best option for tables. The resulting .txt file can be imported to Apple NUMBERS or Microsoft EXCEL templates (downloadable with SHRIMPTOOLS) to produce publication-ready tables.

Workflow and maths involved

3

Data reduction workflow

1. The data structure of single collector SHRIMP measurements

SHRIMP U-Th-Pb geochronology is currently performed in single collector mode. The resulting data structure is schematically represented in Figure 3.1.

Every spot analysis consists of one or more sets (one in most cases).

Every set consists of 4 (minimum) to 8 (maximum) scans. Increasing the number of scans increases the counting precision, but also increases the time per spot. In most cases 6 scans is precise enough for geochron and 4 scans is precise enough for provenance studies of detrital zircons.

Every scan consists of 9 or 10 mass-peak measurements: $^{196}Zr_2O$, ^{204}Pb, $^{204.1}$background, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{238}U, ^{248}ThO, ^{254}UO, and (optional) $^{260}UO_2$.

Every mass-peak is measured 10 times during a prefixed interval, frequently between 2 s, for $^{96}Zr_2O$ and ^{254}UO, up to 20 s for ^{207}Pb. The system takes another 10 measurements of the Secondary Beam (SB) total intensity simultaneously with the 10 readings of the mass-peak measurement.

Every set is reduced individually. If more than one set is measured, the final result is the grand total of all the sets.

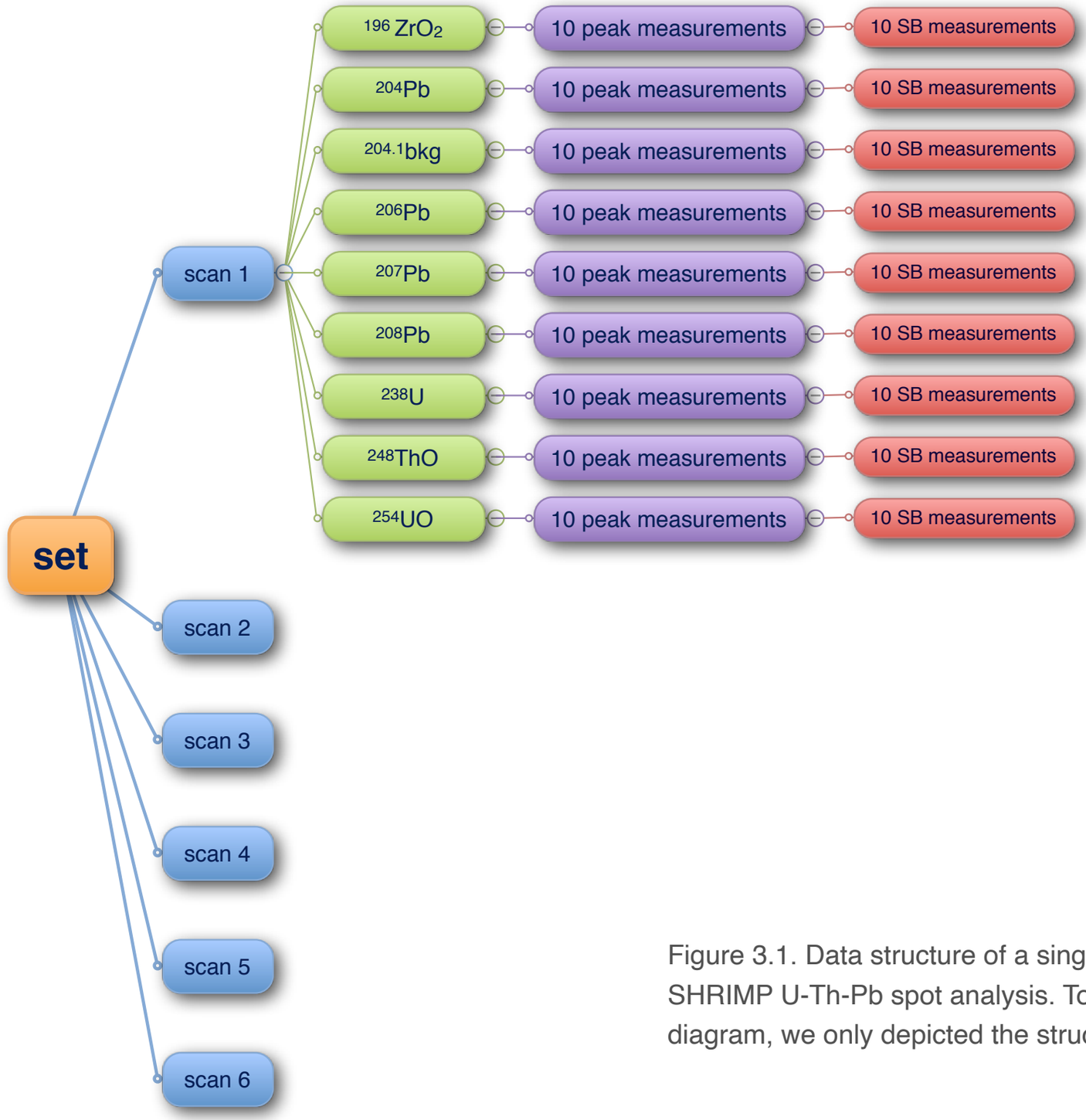

Figure 3.1. Data structure of a single collector geochron SHRIMP U-Th-Pb spot analysis. To avoid crowding the diagram, we only depicted the structure of one scan.

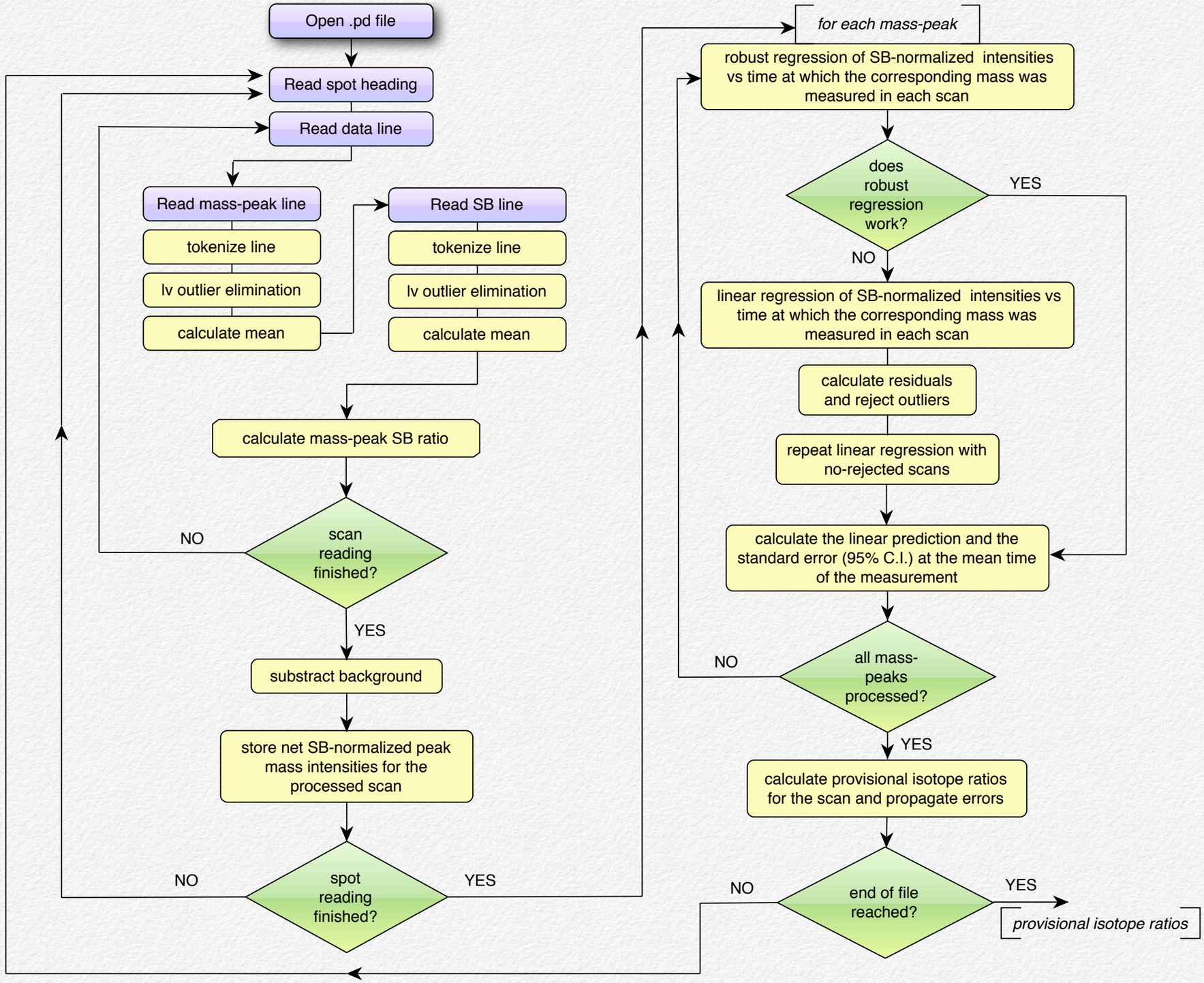

Figure 3.2. Workflow of data reduction while reading the .pd file.

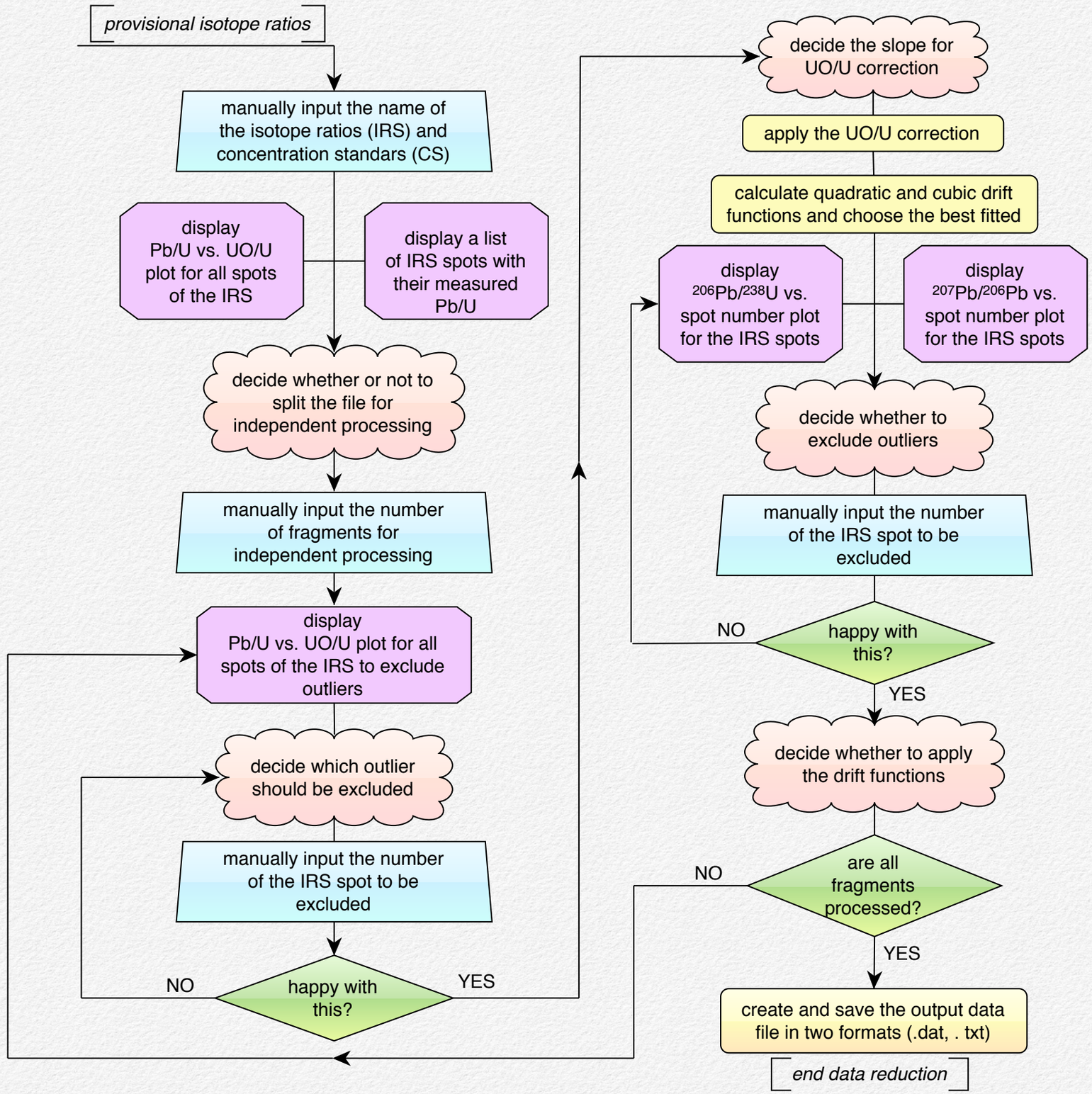

Figure 3.3. Workflow of data reduction after reading the .pd file. The cloud-like globes represent interactive contributions of the user

2. Workflow

Figures 3.2 and 3.3 show the workflow of data reduction from opening the .pd file to creating the .pd and .txt files.

3. Outlier exclusion and data averaging

The software works as follows:

It first read and tokenizes the text line containing the 10 measurements for the first mass. Then, using the letter-display value algorithm (see STATA documentation) it excludes outliers, if any, from these 10 measurements and calculates the arithmetic mean of the non-outlier mass-peak measurements.

Following this, it reads and tokenizes the text line containing the 10 measurements of the secondary beam (SB) acquired simultaneously with this particular mass peak. As before, it excludes outliers and calculates the arithmetic mean of the non-outlier SB measurements. After that, it divides the average mass-peak measurements by the average SB measurements, and stores the result. The process is repeated for each mass peak of the scan. Once finished, the SB-normalized background (measured at the mass 204.1) is subtracted from the rest of mass peaks measured in the same scan.

The process is repeated for all scans. After reading the last scan of the set, the software retains in memory one averaged and SB-normalized measurement of each mass per scan. That is, 6 measurements of each $^{96}Zr_2O$, ^{204}Pb, $^{204.1}$background, ^{206}Pb, ^{207}Pb, ^{208}Pb, ^{238}U, ^{248}ThO, ^{254}UO if the set consisted of 6 scans.

Next, to reduce the 6 values of each mass-peak to a single value, the software regress them against the time at which they were acquired (Fig. 3.4). Note that the acquisition times are different for each mass-peak.

The regression is done first using the robust regression method -**rreg**- implemented in STATA. This method is excellent for excluding outliers, but cannot be applied to measurements with many observations having identical values. This is likely to be the case in the measurements of $^{204.1}$background and ^{204}Pb, but it is highly unlike to occur in any other measurement.

If the robust regression is not possible (as mentioned above, this only happens for ^{204}Pb and $^{204.1}$background measurements), the software performs an ordinary lineal regression, calculates the residuals, eliminates the scan of the highest residual, and repeats the regression.

The differences between ordinary linear regression and robust linear regression are shown in Figure 3.4. We have found this procedure especially useful when the spot contains elevated ^{204}Pb. In this case, the first scan of ^{204}Pb tends to be much lower than the others, similar to what is illustrated in Figure 3.4.

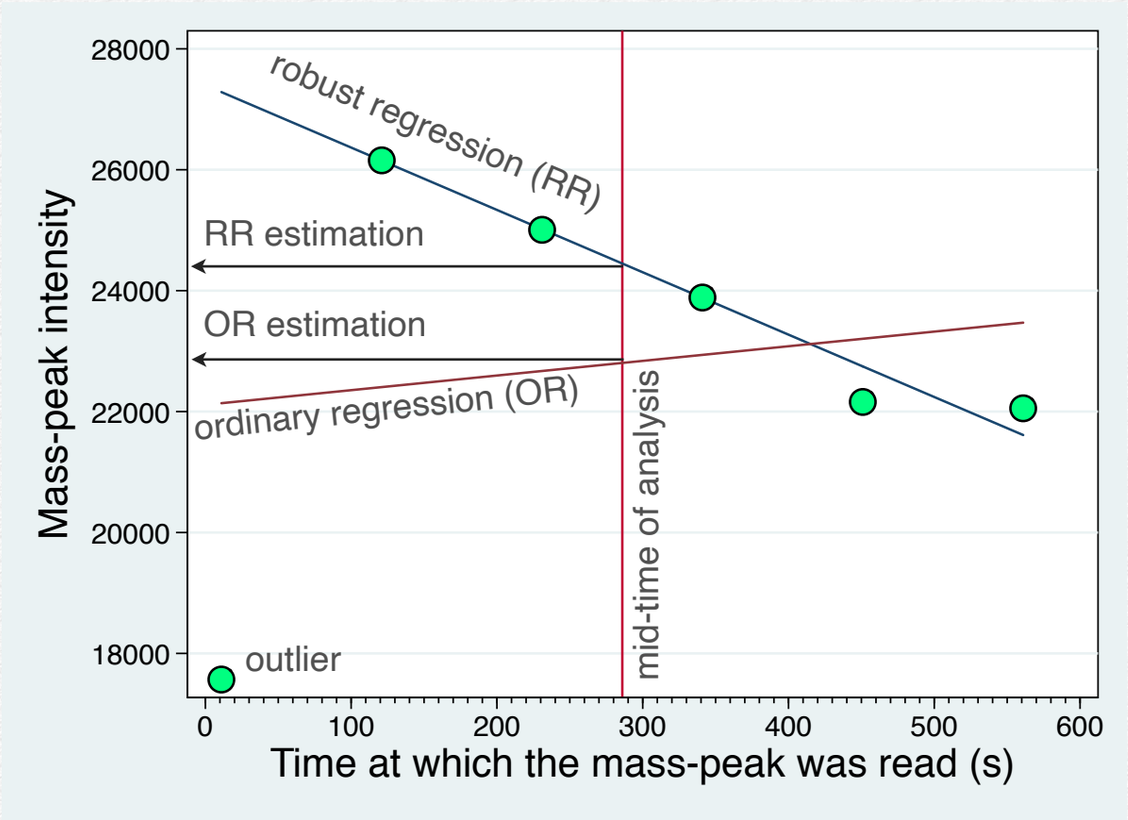

Figure 3.4. Graphic illustration of the differences between robust regression and ordinary regression when dealing with outliers. Note how the effects of these are insignificant on the robust regression method.

Once the regression, either robust or ordinary, is performed, the software calculates the scan average and associated error as the linear prediction and the standard error of the linear prediction at the mid-time of the measurement (Fig. 3.4). All errors are calculated at 95% confidence interval.

The last procedure is to calculate the required isotope ratios and propagate the errors accordingly.

4. Standard points selection

Once the scans are averaged and the errors calculated, it is still necessary (1) correct $^{206}Pb/^{238}U$ as a function of U oxidation, (2) correct for instrumental drift during (note that a SHRIMP session usually lasts for several days).

During these procedures, the software asks, twice, for deletion of the isotope ratio standard spots measured every 4-5 unknowns.

First time the prompt for deletion occurs before calculating the $\log(^{206}Pb/^{238}U)$ *vs.* $\log(^{254}UO/^{238}U)$ regression line. Even if you accept the recommended slope of 2, still is important to delete points which are clear outliers, because this would affect the position of the centroid.

The second delete prompt occurs before standard normalization, when the software displays $^{207}Pb/^{206}Pb$ and $^{206}Pb/^{238}U$ of the analysed standard spots. If one of these spots is an obvious outlier, it is better to delete it.

Age calculations

1. Calculating ages

Once the .pd and .txt files are saved, SHRIMPTOOLS has finished the data reduction. From this point onwards, you can calculate ages, etc... using ISOPLOT on the .txt file, or continue using SHRIMPTOOLS on the .pd file.

In the latter case, the first thing that must be done is to calculate all common-lead corrected isotope ratios and ages with the routine ***User > Shrimptools > U-Th-Pb ages, no plot***.

2. Grouping spots

The second thing to be done is grouping the analyses you want to work with. To understand how this works, proceed as follows:

1. Type (in the command window) **shrimptools** [return]
2. Go to the menu ***User > Shrimptools > U-Th-Pb data reduction***
3. Answer yes to the question: This routine will destroy all data currently in memory. Do you want me to continue? (y/n)
4. Once the open dialog appears, navigate to the directory containing the_nice_file.pd and open it. This will display the spots IDs as they are being read.

5. When the software displays the list of standards input **tem** (TEMORA) as isotope ratios standard and **sl1** (SL13) as concentration standard.

6. At the prompt: "How many fragments do you want?" input 1

7. At the prompt: "Manual elimination of outliers in U oxide calibration. Shall we eliminate outliers? (y/n)" input "n"

8. At the prompt: "Which slope do we use, the calculated (1) or the theoretical (2)?" input 1

9. At the prompt: "Manual elimination of 207/206 and 206/238 outliers. Shall we eliminate outliers? (y/n)" input "n"

10. At the prompt: "Drift correction: Shall we leave it uncorrected (1) correct 206/238 (2) or correct also 207/206 (3)?" input 3

11. Check that the files the_nice_file_process.dat and the_nice_file_process.txt have been created in the same directory. Check also that you are now working on the saved the_nice_file_process.dat.

12. Go to the menu ***User > Shrimptools > U-Th-Pb age calculations, no plot***

13. Type (command window) **list id es** [return]. The windows result displays a list with all analyzed spots. The variable es has a value of 1 for all samples except for the standards which have es = .

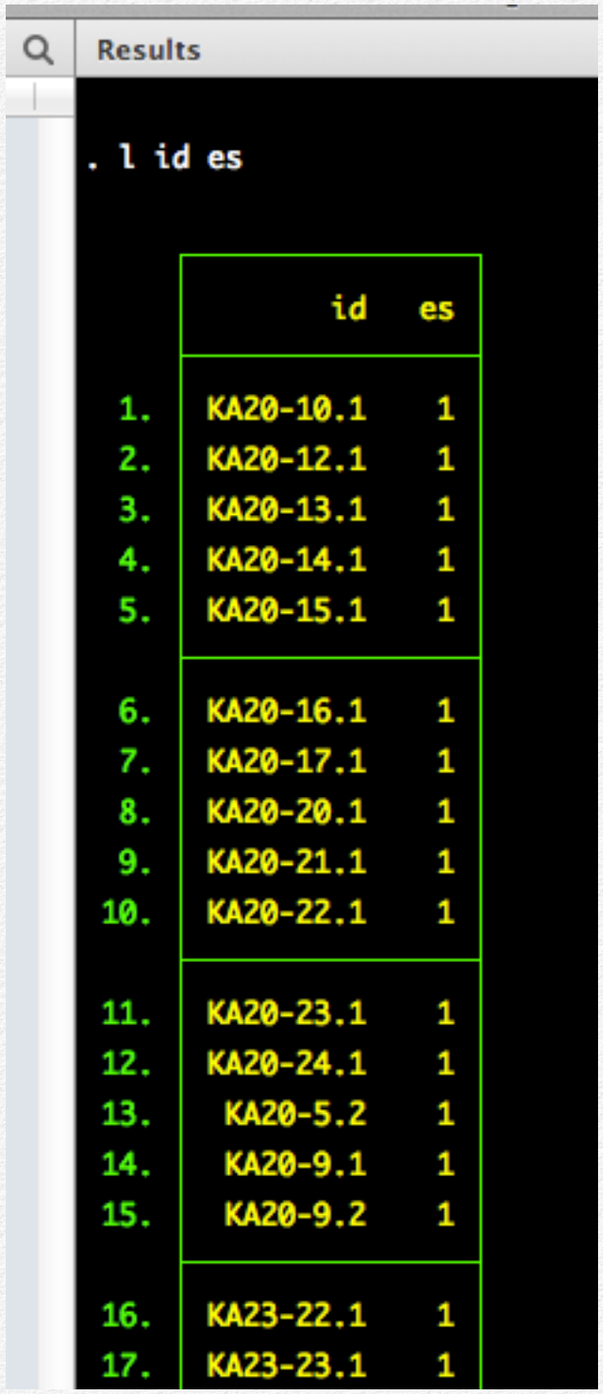

Figure 3.5. Output of **list id es**

14. Type **sort id** [return] and then **list id es** [return] (Fig. 3.5). Check how now all spots are alphabetically ordered.

15. Type **replace es=0** [return] and then **list id es** [return]. Check that all values of es are set to zero.

16. Type **replace es=1 in 1/15** [return] and then type **list id es** [return]. Check that all spots belonging to Sample KA20, and only these, have es=1

17. Type **generate es_KA20=es** [return]. This creates a new variable containing the current values of es. Now type **list id es es_KA20** [return] and

check that the two variables are equal.

18. Type **replace es=0** [return] and then type **replace es=1 in 16/29** [return]. Check that all spots belonging to Sample 1, and only these, have es=1.

19. Type generate **es_KA23=es** [return]. This creates a new variable containing the current values of es. Now type **list id es es_KA23** [return] and check that the two variables are equal.

20. Repeat the procedure for all samples in the file, selecting the ordinal numbers in the list displayed after the command **list id ...**

21. Once all groups are made, type **replace es=0** [return] and then type replace **es=es_K20** [return].

22. Now try different concordia plots and age statistics using the Shrimptools menu. Check that only the spots corresponding to the selected sample are considered.

23. Now type **replace es=0** [return] and try the same plots and statistics. They are empty.

24. Type **replace es=es_KA20 + es_KA23** [return] and try the same plots and statistics. These will include the spots corresponding to samples 1 and 2.

25. You may want to save your grouping. If so, use the ***File > Save*** menu.

26. If you want to get rid of any grouping variable, for example es_KA20, just type **drop es_KA20** [return], etc...

Therefore, combining **sort id** [return, **list id es** [return] to check whether es is enabled, **replace es=0** [return] to disable es in the whole data set, and **replace es=1 in x/y** [return] to enable es in the desired samples is a fast and easy way to select the samples we want to project. If these are not correlative, it is possible to replace es=1 in different x/y, or change es manually in the editor. Simply type **edit id es [return]**.

If you find a combination of es values that defines a particular group you want to work with in the future, you can create as many new variable es_my_group as desired and save them in the .pd file as illustrated in the example above.

Once grouping samples is done you have at your fingers the enormous statistical power of STATA to work with your data.

3. Finding and deleting outliers

a) Identifying discordant spots

Once you have selected all points belonging to a given sample, it may be that some of them are markedly discordant and you want to identify them. For this task, go to ***Users > Shrimptools > Wetherill plot with ID*** (or ***Tera-Wasserburg with ID***). In this

plot all samples with discordance greater than 5% appear in red and the points are identified with their ordinal number. Type **edit id** [return] or **list id** [return] to check the spots to which they correspond. If you want to narrow the discordance percentage at which points are identified, go to ***Users > Shrimptools > Change defaults*** and proceed accordingly.

If you want to delete *permanently* one spot, type **delete in x**, where x is the ordinal number. If you want to delete *permanently* several spots, type **delete in x/y,** where **x** to **y** is the range of ordinal numbers. See the STATA manual and Chapter 1, Section 2.

b) Identifying concordant points with elevated dispersion from the mean

The procedure described above is meant to identify discordant points. The procedure described below is intended to identify concordant points that have ages very that are very different to the cluster around the mean. For this, go to ***Users > Shrimptools > Detect outliers***. See the description about how this routine works in Chapter 2, Section 7.

4. Calculating statistics and creating tables

Once you have defined which spots should be used for calculating the mean ages (that is, all with es set to one, the rest with es set to any other value), you can calculate all the mean ages, errors, and MSWDs with ***Users > Shrimptools > U-Th-Pb statistics.***

Please, note that the errors calculated here reflect just the dispersion around the mean value. These must be expanded with the point-to-point error of the standards which was calculated during data reduction. The user must do this manually, adding up the value stored in the variables pbu_err_in_std and pbpb_err_in_std to the error of the mean for each age.

After this, the most probable action is to create publication-ready tables for each group. For this task SHRIMPTOOLS provides two options:
(1) ***Users > Shrimptools > U-Th-Pb tables (reduced)***
(2) ***Users > Shrimptools > U-Th-Pb tables (full)***

The first option creates a text file that is directly readable by any spreadsheet. It contains al thel isotope ratios and ages, except those 208-corrected, for the spots with es set to 1.

The second option creates a text file that is directly readable by any spreadsheet. It contains all the isotope ratios and ages and the user can choose which spots are included, either all or just those with es set to 1. Templates to import the .txt files created with this utility into Apple NUMBERS and Microsoft EXCEL are also provided.

What if?

1. **SHRIMPTOOLS cannot be invoked**
2. **The version is higher than the STATA version**
3. **A .pd file stops reading**
4. **After saving the .pd and .txt files the routine *U-Th-Pb ages, no plot* gives an error**
5. **Trying a concordia plot or age statistics gives an error**
6. **The error message "the variable variable is already defined"**
7. **You cannot create a new standard file**

1. What if SHRIMPTOOLS cannot be invoked?

Download the latest version of the software. Check it is properly installed in the ADO/PERSONAL directory of your computer (see Chapter 2, Section 1). Check the spelling typed in the command window, it must be **shrimptools** [return].

2. What if the version is higher than the STATA version?

All SHRIMPTOOLS routines are set to version 11 or 12. If you try to run these with any STATA version before 11, you will see the error message

this is version 10.0 of Stata; it cannot run version 11.0 programs
You can purchase the latest version of Stata by visiting
http://www.stata.com.

The version in STATA ado files permits continued use of old ADOs in newer STATA versions. If you see the above error message you can (i) upgrade STATA, (ii) open the offending ADO file with a text processor and manually change the version number. It is in the second line of the program as shown below:

program define shrimp_tables_full
version 11
etc...

If you manually change *version 11* to *version 10*, the ADO will work with STATA v. 10. Save the file with the same format and extension.

If you want to run the modified ADO file, either quit STATA and begin anew, or in the command window type:

program drop “ADO name” [return].

3. What if a .pd file stops reading?

This is usually caused by an incomplete spot analysis. It happens when the SHRIMP was aborted during a measurement and the data were incorporated in the .pd file.

For example, try to reduce the_silly_file.pd provided with the software. It will display readings until you get:

Reading analysed spot 11; Spot ID = KA29-23.2
in not found.

The red sentence is an error message that occurred reading the spot labeled SAMPLE4-6.1. Despite this error, you still can reduce the data file as follows:

1. *Open the .pd file with a text processor*
2. *Find the offending spot. In this case KA29-23.2*
3. *Delete all lines corresponding to that sample*
4. *Save the .pd file with the same format and extensionReduce the resulting file*

4. After saving the .pd and .txt files the routine U-Th-Pb ages, no plot gives an error?

The cause is that any essential concentration or isotope ratio was not calculated during data reduction. Open the editor and check it. The most common situation is that the U, Th and Pb concentrations were not calculated because the concentration standard was not measured at the beginning of the session. If so, there are two possible corrections:

1. *Open the .pd file with a text processor and paste the readings of the concentration standard from another .pd file*
2. *Use the age standard also as concentration standard*

None of these solutions is optimal. If the CL images of the age standard grains do not show excessive contrast, the second would probably be the most reasonable. If, on the other hand, the standard age grains are heterogeneous and there is a recent .pd file created under the same instrumental conditions, the first option is probably more advisable.

5. Trying a concordia plot or age statistics gives an error?

This occurs when the routine ***U-Th-Pb ages, no plot*** has not been executed previously. Run it and try again

6. The error message “the variable variable is already defined”?

This may occur when a routine has been aborted and the software has not cleaned up all temporary variables. If so, check the names in the variables window. You can delete all undesired variables after es by typing **delete var1-var2** [return]. After this run the routine ***U-Th-Pb ages, no plot.***

7. An error message saying that you cannot create or modify an standard file?

This occurs because the ado folder has no write permission for the current user. Change it.