

UPb.age, a fast data reduction script for LA-ICP-MS U-Pb geochronology

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ABSTRACT

Laser ablation-inductively coupled plasma mass spectrometry (LA-ICPMS) is a rapidly growing technique that allows many different types of in-situ microanalyses to be performed in geological materials. One of the most used methodologies is U-Pb isotopic dating of accessory minerals such as zircon. These analyses can be performed at the scale of tenths of micrometers, in a rapid, cost-effective way and with very good precision and accuracy. It is critical, however, to perform the data reduction in a fast, transparent and customizable way that takes into account the specific analytical procedures employed in various laboratories and the outputs of different instruments. UPb.age is a freely available data reduction script, written and developed in R, a free statistical environment. The software can read, correct and reduce U-Pb isotopic data obtained by several LA-ICPMS instruments. Its main strengths are transparency, robustness, speed, and the ability to be readily customized and adapted to specific analytical procedures used in different laboratories.

Key words: LA-ICPMS, U-Pb, geochronology, zircon, data handling.

ABSTRACT

La técnica analítica de ablación láser asociada con un espectrómetro de masas de plasma inductivamente acoplado (LA-ICPMS) es una rama de la geoquímica analítica que está en rápida expansión y ha permitido el desarrollo de diversos métodos microanalíticos aplicados a materiales geológicos. Entre estos métodos, uno de los más utilizados actualmente es la geocronología por U-Pb, por medio de la cual se pueden obtener, de manera rápida y bastante económica, fechamientos isotópicos de minerales accesorios, como el zircón, a la escala de pocas decenas de micrómetros y con una buena precisión y exactitud. Sin embargo, es crítico que los datos adquiridos durante una sesión analítica puedan ser leídos, corregidos y filtrados, para finalmente obtener relaciones isotópicas y, por ende, edades, de una manera precisa y rápida. UPb.age es un script gratuito desarrollado para este fin que fue escrito y desarrollado en R, un lenguaje de programación de distribución libre especialmente enfocado a la estadística. UPb.age es capaz de leer los archivos obtenidos con diferentes instrumentos (ICPMS) y permite realizar la reducción de esos datos de manera rápida y precisa. Tiene además la ventaja de ser fácilmente adaptable a las necesidades de diferentes laboratorios, distintas técnicas analíticas o protocolos empleados.

Palabras clave: LA-ICPMS, U-Pb, geocronología, zircón, manejo de datos.

INTRODUCTION

Microanalytical techniques are gaining a widespread use in geosciences, because they provide a fast, precise and accurate way to determine compositional variations in glasses, minerals, and rocks. LA-ICPMS (laser ablation-inductively coupled plasma mass spectrometry; *e.g.*, Kosler and Sylvester, 2003; Solari *et al.*, 2010 and references therein) has been applied to a wide variety of geological research applications, most of which grew in the last 15 years. This technique permits high mass resolution, and is particularly applied to resolve isotopic abundances of trace elements, including the rare earth elements (REE) (*e.g.*, Belousova *et al.*, 2006; Whitehouse, 2003), as well as to determine isotope ratios. For those radioisotope chains in which isotopic pairs are not affected by isobaric interferences (*e.g.*, ^{87}Rb interference on ^{87}Sr), LA-ICPMS is able to determine isotopic ratios with sufficient precision to calculate ages of minerals at a sub-micrometric scale.

The development of LA-ICPMS techniques started some 20 years ago and has progressed rapidly to the current status of instrumentation and applied methodologies (*e.g.*, Kosler and Sylvester, 2003; Sylvester, 2008; Gehrels *et al.*, 2008; Frei and Gerdes, 2009; Solari *et al.*, 2010). The main advantages of the LA-ICPMS systems are the relatively low instrumental cost, the rapid data acquisition (one analysis in less than two minutes), and the flexibility of the instrument. Besides, LA-ICPMS systems are able to obtain precise data from the analysis of target spots of 20–40 μm in diameter, and 10–30 μm depth.

Arguably the most useful isotopic system analyzed by LA-ICPMS is the U(Th)-Pb (Solari *et al.*, 2010, and references therein). Zircon is the most important mineral commonly dated by U(Th)-Pb, because of its physical and chemical resistance, its common presence as accessory mineral in many felsic and intermediate igneous rocks, as well as its ability to crystallize during high-grade metamorphism or to form overgrowths around older, xenocrystic cores.

At Laboratorio de Estudios Isotópicos (LEI), Centro de Geociencias, UNAM, a LA-ICPMS system, composed of a Resonetics M50 workstation coupled to a Thermo XSeries II quadrupole ICPMS is installed and has been running since summer 2007. The system was recently described by Solari *et al.* (2010), who introduced the methodology and precision and accuracy for U(Th)-Pb zircon analyses. This is the analytical technique currently more commonly applied and requested by internal (*i.e.*, UNAM) and external users at LEI, UNAM. In the period February-June of 2010 about 150 samples were dated, with more than 7,000 zircons ablated. Because the analytical work also requires a precise and robust way to perform the data reduction, calculate ages and elemental concentrations from the analyzed spots, it is mandatory to have a reliable and transparent, yet customizable software. This paper deals with the description of the software we developed,

the philosophy behind it, and how it compares with other similar softwares currently available.

PURPOSE AND ANALYTICAL BACKGROUND

The UPb.age software was written in order to facilitate rapid and transparent data reduction for U-Pb mineral dating by LA-ICPMS at LEI, UNAM. The instrumental setup, consists of the ICPMS tuning to reach stable conditions, in which the signal of one reference isotope (in general, ^{238}U) yields a signal of about 3000 cps/ppm. Using the NIST-SRM 612 standard glass, which contains about 38 ppm U, the user tunes the instrument to achieve 120,000–130,000 cps for ^{238}U . If correctly tuned, the $^{238}\text{U}/^{232}\text{Th}$ ratio is about 1–1.1 and oxide production, expressed as the ThO/Th ratio, must be around 0.5 % or less. The standard laser conditions used to achieve those ICPMS parameters are: energy of 120 mJ, spot size of 33 μm , demagnification of 15x, raster velocity of 0.5 mm/min and a pulse frequency of 5 Hz. Those values, together with a He carrier gas flow of 700 ml/min and a N_2 addition of 2.8 ml/min, are satisfactory conditions for U-Pb analyses (Solari *et al.*, 2010). Once the tuning conditions are met, the analytical session can start. A normal sequence consists of the analysis of a standard glass and a standard zircon, followed by the unknowns. Generally, the sequence starts with two analyses of the NIST-SRM 610 standard glass, followed by five analyses of a standard zircon (*e.g.*, Plšovice standard zircon, *ca.* 337 Ma, Sláma *et al.*, 2008), and thereafter one standard zircon each five unknowns, to end with two standard zircons and one NIST-SRM 610 standard glass. This sequence is known as standard-bracketing method (*e.g.*, Jackson *et al.*, 1992, 1996; Gehrels *et al.*, 2008; Solari *et al.*, 2010) and allows the use of the standard zircon to monitor and correct for both instrumental drift and down-hole fractionation (see below); it is well known that the best results are met when the matrix analyzed is matched (*e.g.*, Hirata and Nesbitt, 1995; Kosler and Sylvester, 2003; Jackson, 2008). It is also important to note that all analytical parameters (laser energy and pulse frequency, timing, gas flows, etc.) must be kept constant during the analytical session, in order to minimize the potential of differential fractionation and uncertainties introduced by parameter variations. Each analysis begins with 25 seconds of background acquisition with no laser firing, followed by 30 seconds of ablation. Additional 20 seconds of ablation cell washout is generally adequate for the signals to return to background levels. Normally, seventeen isotopes are scanned during each analysis, allowing for quantitative measurement of those isotopes necessary for U-Pb dating (lead, uranium and thorium isotopes), and detailed monitoring of major and trace elements such as Si, P, Ti, Zr, and REE as a check for the presence of microscopic inclusions in the zircons. These elemental concentrations are also useful for zircon petrogenesis studies (*e.g.*, Belousova *et al.*, 2002; Hoskin and Schaltegger, 2003; Allen and Barnes, 2006).

The common Pb correction is performed offline, using the algebraic methodology of Andersen (2002), because of the ^{204}Hg interference on the tiny ^{204}Pb does not allows an accurate online measurement.

Although alternative software is currently available (e.g., *Glitter*: van Ackerbergh *et al.*, 2001; Griffin *et al.*, 2008; *Iolite*: Paton *et al.*, 2010), these tools are either restricted in their input and output formats or do not provide full documentation of their calculations. UPb.age was written to allow the operator full control over the applied corrections for optimum consistency and robustness and to customize the input and output data format to any instrument.

REQUIREMENTS AND BASIC CONCEPTS

UPb.age can read the raw data of laser ablation spot analyses recorded by the Plasmalab[®] software of the Thermo X seriesII ICP-MS. With a sequence of input commands received from the user, UPb.age can rapidly apply different corrections, recalculate U-Th-Pb ratios, errors and correlation coefficients. It yields a comma-separated-value (CSV) output, which can be opened in Excel[®] to allow age calculations and visualization using the Excel[®] macro ISOPLOT of Ludwig (2008). Because each ICP-MS has its own output file format, generally related to the proprietary software that controls the mass spectrometer, a simple script is used to convert the ICP-MS output file to a uniform format that can be read by UPb.age. A script named file.trans is distributed together with UPb.age, and used to convert the Plasmalab files generated by the Thermo XSeries II mass spectrometer. However, file.trans can be easily adapted to convert files generated by other ICP-MS instruments (e.g., Agilent,

Perkin-Elmer, Elan, etc.).

UPb.age and file.trans are written in R, a free software environment for statistical computing and graphics, which can be freely downloaded from the Comprehensive R Archive Network (CRAN) available at <<http://www.r-project.org>> (R Development Core Team, 2010). The package MASS, which is part of the bundle VR, must be loaded automatically in the R environment to allow UPb.age to correctly run (Venables and Ripley, 2002). Although the R environment is available and runs on a wide variety of UNIX, Windows and MacOS platforms, the current version of UPb.age runs only on Windows[®] computers, or a Windows[®] emulation machine software on other platforms. This is because some of the functions used are not available yet for Unix and MacOS[®] platforms. UPb.age is distributed under the GNU General Public License Version 2, June 1991 and can be used free of charge. It can be downloaded from the LEI webpage (http://www.geociencias.unam.mx/~solar/index_files/LEI/Quienes_somos.html), or obtained from the authors.

Once the R software is installed, UPb.age is opened and read from inside the R-console, either by typing the terminal-like command `choose.file()` at the window prompt, or by selecting the same command from the File tab of the R console. The user is then stepwise guided through the data evaluation process (Figure 1). Interaction with the program is via the R Graphics Device.

REGRESSION MODELS

Two linear regression models are used in the UPb.Age script:

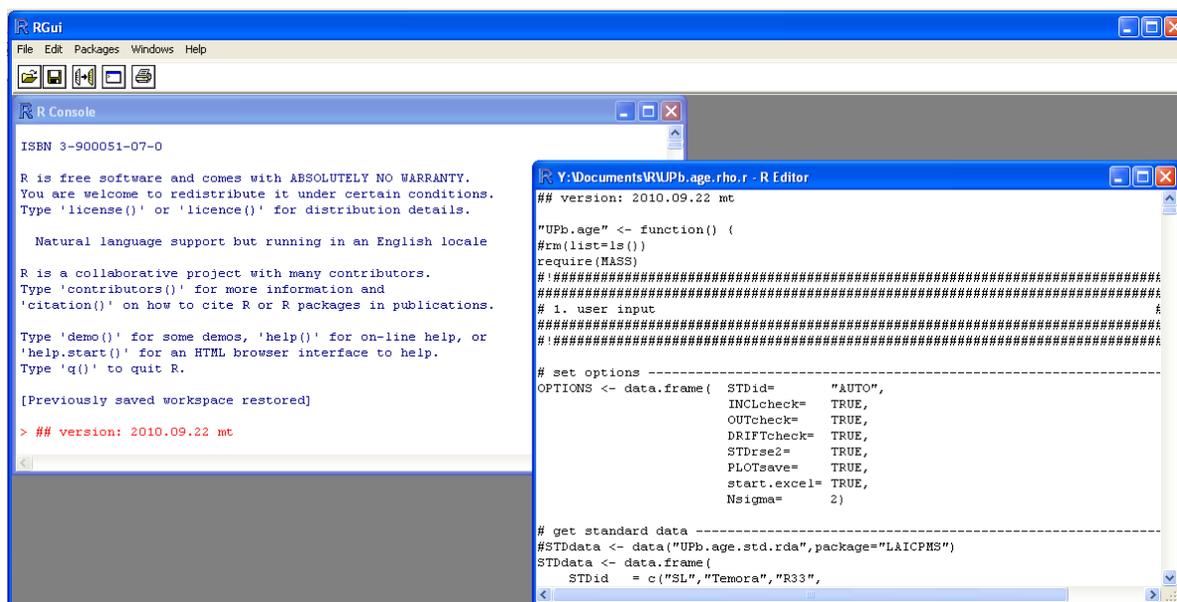


Figure 1. A screenshot of the R console, with the command line window, as well as the script window opened with part of UPb.age script visible.

a) The function *lmsreg* of the package MASS is used to check the data for inclusions and outliers. *lmsreg* is a robust regression model based on the median of the data points (for details, type `?lmsreg` into the R console). *lmsreg* is applied to an overlay of ratios of all measurements. The residuals of the regression model are used to detect outliers and inclusions or zonations. Multiples of the standard deviation (sigma) of the residuals can be set as threshold value (OPTIONS, Nsigma). If, within a measurement, three or more data points in a row are detected as outliers the measurement is presented to the user. This measurement can then be excluded, a new integration window can be set or the inclusion can be ignored.

b) The function *lm* is part of the R base package and fits a linear regression through the data points on the basis of the least mean square method. *lm* is used for drift correction and for the ‘t-zero’ method to address downhole fractionation (see below). For drift correction, a linear regression is fitted through the ratio values of the standard measurements with respect to their position in the measurements sequence.

A DATA EVALUATION SESSION

A working example will demonstrate UPb.age functionality during a reduction session. The sample is a Cenozoic natural zircon of the many analyzed every year in the LEI, UNAM.

Read raw data files

After typing “UPb.age ()” into the R console the user is prompted to choose the files containing the raw data measured by LA-ICPMS. The files must be in comma separated value (CSV) format, *i.e.*, with the data columns separated by “;”. If the file extension is .xl, it is assumed that the files are from the software of a Perkin Elmer Elan 6x00 instrument and the first line will be ignored. Such simple format is chosen because it is readily available as a common output by many ICP-MS instruments. The files chosen for data reduction must include both standard and unknown zircon analyses. A progressive number must be included in the data labels, which must be in the exact order as analyzed. This labelling is necessary because, in the standard bracketing method, the analyzed standard zircons are used to correct the data of unknown zircons for instrumental drift, and thus the order in which they are analyzed is crucial.

Integration windows

In the first step, an overlay of the ^{238}U signal for all the standard/unknown zircons, is presented to the user (Figure 2a). The user must indicate start and end of background and laser signal, collected without and with the laser firing,

respectively. It is assumed that data acquisition is triggered at the same interval for all measurements and thus the same integration windows will be applied. Background-corrected signals are calculated by subtracting the average background signal from the laser signal.

Check for inclusions and/or zonations

Suspicious measurements are evaluated for the presence of outliers or variations (in general, those points outside ± 2 sigma) in the $^{207}\text{Pb}/^{235}\text{U}$, $^{206}\text{Pb}/^{238}\text{U}$ and $^{208}\text{Pb}/^{232}\text{Th}$ ratios, first for the standard, and then for the unknown zircons (Figure 2b). The possible presence of inclusions or crystal zoning is evaluated for each individual analysis by monitoring the signal of isotopes such as ^{175}Lu , ^{163}Dy , ^{140}Ce , ^{89}Y , ^{31}P , whose variation can indicate the presence of an inclusion or a zonation which could be important to indicate an age variation (Figure 2c). If such inclusion affects the isotopic ratios of interest to calculate the U-Pb ages, then the user can act in different ways. In the case of standard measurements, the user can choose to ignore the detected inclusion/zoning or to exclude this measurement from further evaluation. In the case of sample measurements, the user has the choice to exclude the measurement, to set new integration windows or to ignore the detected inclusion/zoning. If a new window is set (*e.g.*, Figure 2c), the result for this measurement is recalculated by applying the reduced window to all measurements. In this case, those excluded analyses, or those in which the time integration was reduced, are marked in the final output file as “excluded (user)”, or “changed window”, respectively.

Check for outliers

After checking for inclusions/zonations, both standard and unknown ratios are checked again for outliers (± 2 sigma), taking into account the removed measurements and new integration windows (Figures 2d and 2e). The outliers in the standard and sample measurements (if detected) are presented to the user for decision whether to remove them or not. An important point to underline is that care must be taken when removing outliers from unknown (*i.e.*, sample) analyses in which heterogeneous zircons were measured. This is the case, for instance, of detrital zircon studies, or metamorphic samples in which inherited cores and overgrowths were analyzed (*e.g.*, Figure 2f). In this case, the removal of outliers is not possible, because a large number of analyses will fall outside ± 2 sigma and would be eliminated.

Check for instrumental drift

Isotope ratios and a linear model for the average

ratios of the standard measurements are then presented to the user (Figure 2g). UPb.age offers the ability to correct for instrumental drift using a linear model.

Other methodologies use running average (sliding window) calculations (e.g., Gehrels *et al.*, 2008), or mode

complex splines (e.g., Paton *et al.*, 2010) to address instrument drift. Although these methods may accurately fit the observed data, they require a highly detailed evaluation of instrument performance and assumptions about the causes of instrument drift. If the observed variation is not true

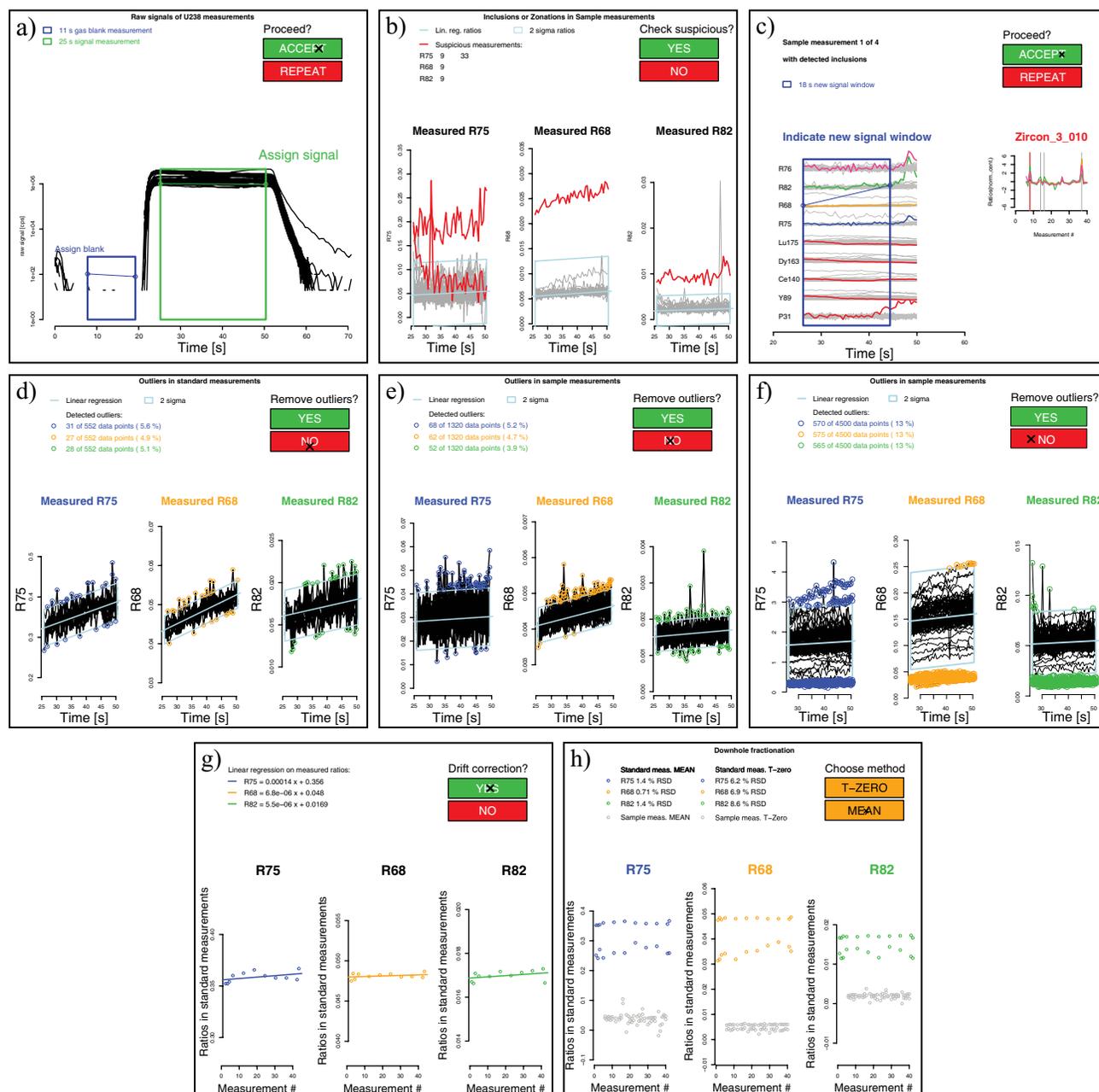


Figure 2. Screenshots of the graphic outputs from UPb.age. a: Integration window showing the ^{238}U signal used to monitor the acquired signal, and set the integration times of background and signal. b: Suspicious presence of inclusions and/or zoning for standard and unknown zircon analyses, evaluated by sudden variation of $^{207}\text{Pb}/^{235}\text{U}$, $^{206}\text{Pb}/^{238}\text{U}$ and $^{208}\text{Pb}/^{232}\text{Th}$ ratios outside ± 2 sigma. c: Further evaluation of a possible inclusion, for each suspicious analysis, by monitoring the signal variation of ^{175}Lu , ^{163}Dy , ^{140}Ce , ^{89}Y , ^{31}P isotopes. The selection of a new integration window, in blue, avoids a zoning and/or inclusion. d: Outlier (outside ± 2 sigma) values for standard zircon measurement ratios. e: Outlier (outside ± 2 sigma) values for sample zircon measurement ratios obtained for an igneous rock. f: An example of the same diagram as "e", but obtained for a metasedimentary rock with obvious spreading in Pb/U ratios, and thus in age. In this case, most data are identified as outliers, and not just a few ratios dispersed within one analysis. g: Proposed linear correction for instrumental drift, as calculated by the variation of the ratios obtained for standard zircons along the whole analytical experiment. h: Down-hole fractionation evaluation, with the two possible methods: mean or t-zero. See text for further explanations. R76: $^{207}\text{Pb}/^{206}\text{Pb}$; R75: $^{207}\text{Pb}/^{235}\text{U}$; R68: $^{206}\text{Pb}/^{238}\text{U}$; R82: $^{208}\text{Pb}/^{232}\text{Th}$.

instrument drift, but is instead caused by standard inhomogeneity or blank variation, then a correction using these more complex procedures will introduce systematic error to the corrected values of the unknowns.

Down-hole fractionation

The majority of LA-ICP MS measurements are done using single hole drilling mode, which offers the best lateral resolution. This is essential because the analyzed minerals are commonly only a few hundreds of μm . Changes in the ablation and aerosol characteristics with ongoing single hole drilling, are reflected in progressive changes in the measured element ratios. This process is known as down-hole fractionation (Eggins *et al.*, 1998; Kosler and Sylvester, 2003; Paton *et al.*, 2010). Usually, the averaged values of the ratios are then taken as a measure to evaluate the mineral age. The error due to down-hole fractionation can be minimized by using the same integration times for standards and samples. Horn *et al.* (2000) proposed to address down-hole fractionation by evaluating the initial ratio values rather than the average. This value at zero ablation time (t-zero) is evaluated in our script by applying a linear regression to the individual ratios of all measurements and taking the axis intercept as the fractionation-corrected ratio for the age determination. A plot is presented to the user showing the raw results of the evaluation obtained by both the t-zero and mean values methods, along with their relative standard deviations (RSD) (Figure 2h).

Write result files

A new folder named UPb.age.OUTPUT is generated within the folder containing the raw data files. All the graphics produced by UPb.age during the different steps of the data reduction process are automatically saved in this folder. Those output files are automatically saved with both .emf (enhanced metafile) and .pdf (portable document format) extensions, which can be readily opened and edited in both Windows[®] and/or MacOS[®] platforms. Two .csv (comma-separated value) files are also generated by the reduction process: data.csv and results.csv. Data.csv contains the background, drift and down-hole fractionation corrected mean values in counts-per-second (cps), as well as their standard errors (1sigma absolute), for all the measured isotopes (major, trace and REE elements). These data are then used to calculate the absolute element abundance in the zircon, using a spreadsheet algorithm. The file results.csv contains the corrected $^{207}\text{Pb}/^{235}\text{U}$, $^{206}\text{Pb}/^{238}\text{U}$, $^{208}\text{Pb}/^{232}\text{Th}$, and $^{207}\text{Pb}/^{206}\text{Pb}$ ratios, as well as their relative 1 sigma % standard errors. The uncertainty due to the inhomogeneity of the natural standard zircon is then propagated by quadratically adding the average 1sigma standard error of the reference zircons used as bracketing in the same experi-

ment (*e.g.*, Horstwood *et al.*, 2003). Finally, the Results.csv file also contains the error correlation (*Rho*), which is defined as the ratio of the covariance to the product of the standard deviations (in %) of the two ratios $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{235}\text{U}$, that constitute the two axes of the conventional (or normal) concordia of Wetherhill (*e.g.*, Schmitz and Schoene, 2007; Paton *et al.*, 2010). Alternatively, the error correlation between the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{235}\text{U}$ ratios is simplified by calculating the ratio of the former to the latter (*e.g.*, Horstwood, 2008; Frei and Gerdes, 2009). In the normal (Wetherhill) concordia diagram, the *Rho* varies from 0 to 0.9, being zero for those ratios that are not correlated, and 0.9 for those errors which are highly correlated. The error correlation in UPb.age is calculated after Pearson ('Pearson *Rho*') using the function *cor* of R. The values of *Rho* obtained for each analysis are quite similar to those obtained by Paton *et al.* (2010) in *Iolite*, suggesting that the calculated errors on isotope ratios measured by quadrupole ICPMS are strongly uncorrelated or that other sources dominate the error propagation (*e.g.*, Figure 3). A simple explanation of the lack of error correlation is the lack of simultaneous detection of the different isotopes due to the presence of only one collector in the quadrupole ICPMS.

FURTHER DATA MANIPULATION

One of the main advantages of UPb.age is its speed to reduce data. A normal experiment in which around 50 unknown zircons, alternately with 12-15 standard zircons, and a couple of glass standards are analyzed, can be reduced in few minutes, including the necessary screening of those analyses suspect of zoning or inclusions. Because of the reduced size of the script, it can be run on a Windows[®] computer with 1-2 Mb of RAM. The ability to automatically save pdf images of each reduction step (*e.g.*, Figure 2) allows more in-depth screening of suspect analyses, opening the possibility to reduce the data several times for instance changing the background and signal timing, eliminating bad standard analyses, and so on.

The results.csv and data.csv files can be readily imported and sorted in Excel[®]. All Excel[®] versions are able to import comma-separated values (csv) files, however only those versions prior to 2007 are able to correctly handle the Isoplot (Ludwig, 2008) plug-in used to plot concordia diagrams. Once imported, the data can be readily plotted with Isoplot for a quick data evaluation or further treated with the Andersen (2002) macros, to correct the obtained ratios for common Pb by means of an algebraic method, and then recalculate the corrected ages. Furthermore, an Excel[®] macro developed at CGEO allows the operator to automatically order, correct for common Pb, generate a publication-ready data table, as well as recalculate the major and trace-element concentrations of the analyzed zircons, and produce a chondrite-normalized REE diagram with the obtained final data.

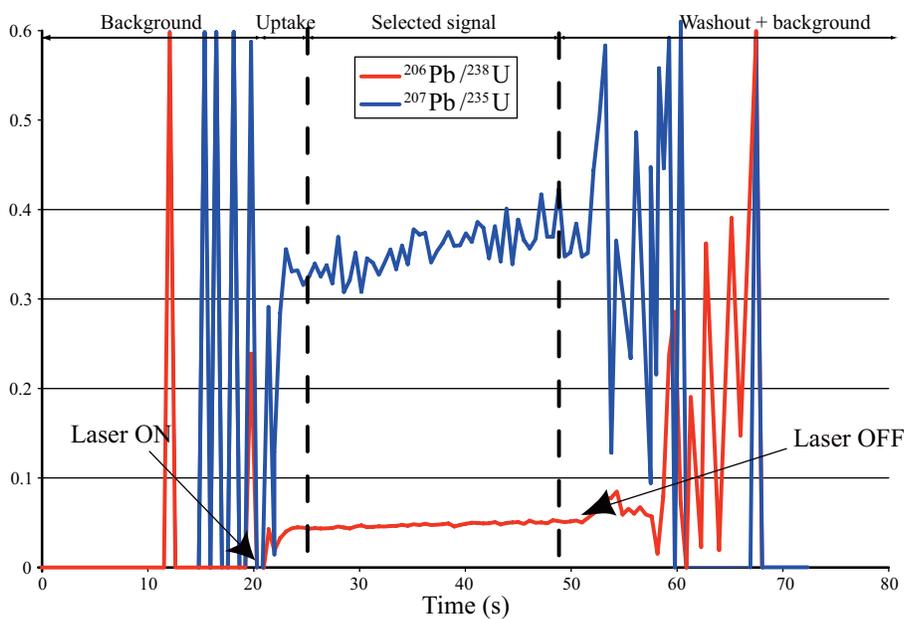


Figure 3. An example of $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{235}\text{U}$ isotope ratio signals, as measured in a standard Plešovice zircon. Uncorrected for instrumental drift, down-hole fractionation, or outliers.

COMPARISON WITH OTHER SOFTWARE

An exercise to compare data reduction employing different software was conducted by von Quadt *et al.* (2009). They concluded that the results obtained with different software for data of the same run, varied between 1–2%. Some of the common software used to reduce U-Pb data are not free, such as *Glitter* (van Achterbergh *et al.*, 2001). Other software are customized to be used only for a specific protocol employed in some laboratories, *e.g.*, *Lamdate* (Košler *et al.*, 2008), which is tuned to be used by those labs using a tracer thallium solution during LA-ICPMS analyses (*e.g.*, Košler and Sylvester, 2003). UPb.age was compared to *Iolite*, which was recently presented, at least for the U-Pb data reduction module, by Paton *et al.* (2010). This module is freely distributed, although it runs under Igor Pro, a statistical software licensed by Wavemetrics Inc. The comparison we conducted involved reducing one dataset (an Cenozoic unknown sample analyzed at LEI, UNAM, in June 2010) independently with both software packages, and choosing the software parameters as similar as possible. The two resulting U-Pb concordia diagrams are presented in Figure 4. The error ellipses obtained with *Iolite* (Figure 4a) are slightly smaller than those obtained with UPb.age (Figure 4b), however, in *Iolite* we did not propagate some uncertainties that were propagated in UPb.age.

CONCLUDING REMARKS

U-Pb zircon geochronology by LA-ICPMS is an important tool that is gaining widespread use as modern

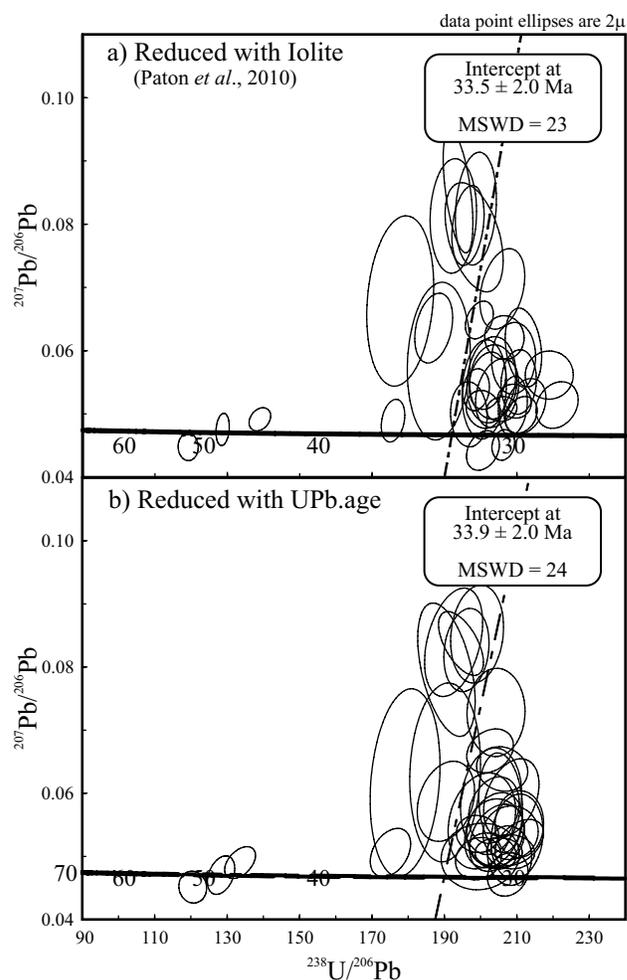


Figure 4. A data reduction comparison of an Cenozoic unknown volcanic zircon sample. a: Raw data analyzed with *Iolite* (Paton *et al.*, 2010); b: raw data analyzed with UPb.age.

analytical facilities become increasingly available, reducing prices and turnaround times. The analytical setup must be coupled with a fast, yet reliable and transparent method of data reduction. UPb.age, a script written in R, combines the robustness and completeness of other available software, with the advantages of being completely free, transparently written and customizable.

ACKNOWLEDGEMENTS

Several people contributed to this software development with their comments, criticisms, bug reports and suggestions. In particular, we want to acknowledge J.P. Bernal, A. Gómez-Tuena, and O. Pérez-Arvizu of CGEO, UNAM. C. Ortega-Obregón developed and regularly updates the Excel[®] macros able to quickly read, reduce and plot the output files of UPb.age, as well as recalculate the elemental concentrations. LAS wants to acknowledge the Conacyt grant 54559, which financed part of the script development, whereas MT acknowledges a UNAM-DGAPA postdoctoral fellowship. The journal reviewers B.V. Miller and M. Petrelli are acknowledged for their fair reviews which improved the manuscript clarity. Teresa Orozco, Technical Editor of the RMCG, is thanked for her support and editorial handling.

REFERENCES

- Allen, C.M., Barnes, C.G., 2006, Ages and some cryptic sources of Mesozoic plutonic rocks in the Klamath Mountains, California and Oregon, *in* Snoke, A.W., Barnes, C.G. (eds.), Geological studies in the Klamath Mountains province, California and Oregon: A volume in honor of William P. Irwin: Boulder, Colorado, Geological Society of America, Special Paper 410, 223-245.
- Andersen, T., 2002, Correction of common lead in U–Pb analyses that do not report ²⁰⁴Pb: *Chemical Geology*, 192(1-2), 59-79.
- Belousova, E.A., Griffin, W.L., O'Reilly, S.Y., Fisher, N.I., 2002, Igneous zircon: trace element composition as an indicator of source rock type: *Contributions to Mineralogy and Petrology*, 143(5), 602-622.
- Belousova, E.A., Griffin, W.L., O'Reilly, S.Y., 2006, Zircon crystal morphology, trace element signatures and Hf isotope composition as a tool for petrogenetic modelling: examples from Eastern Australian granitoids. *Journal of Petrology*, vol. 47, p. 329-353.
- Eggins, S.M., Kinsley, L.K., Shelley, J.M.G., 1998, Deposition and element fractionation processes occurring during atmospheric pressure laser sampling for analysis by ICPMS: *Applied Surface Science* 127-129, 278-286.
- Frei, D., Gerdes, A., 2009, Precise and accurate in situ U–Pb dating of zircon with high sample throughput by automated LA-SF-ICP-MS: *Chemical Geology*, 261(3-4), 261-270.
- Gehrels, G.E., Valencia, V.A., Ruiz, J., 2008, Enhanced precision, accuracy, efficiency, and spatial resolution of U–Pb ages by laser ablation–multicollector–inductively coupled plasma–mass spectrometry: *Geochemistry, Geophysics, Geosystems* (G³), 9(3), publicado: 20 de marzo de 2008, paper number Q03017 10.1029/2007GC001805.
- Griffin, W.L., Powell, W.J., Pearson, N.J., O'Reilly, S.Y., 2008, GLITTER: Data reduction software for laser ablation ICP-MS, *in* Sylvester, P. (ed.), *Laser Ablation ICP-MS in the Earth Sciences: Current practices and outstanding issues*: Mineralogical Association of Canada, Short Course Series, 40, p. 307-311.
- Hirata, T., Nesbitt, R.W., 1995, U–Pb isotope geochronology of zircon: evaluation of the laser probe - inductively coupled plasma mass spectrometry technique: *Geochimica and Cosmochimica Acta*, 59(12), 2491-2500.
- Horn, I., Rudnick, R.L., McDonough, W.F., 2000, Precise elemental and isotope ratio determination by simultaneous solution nebulization and laser ablation-ICP-MS: application to U–Pb geochronology: *Chemical Geology*, 164(3-4), 281-201.
- Horstwood, M.S.A., Foster, G.L., Parrish, R.R., Noble, S.R., Nowell, G.M., 2003, Common-Pb corrected in situ U–Pb accessory mineral geochronology by LA-MC-ICP-MS: *Journal of Analytical Atomic Spectrometry*, 18(8), 837-846.
- Horstwood, M.S.A., 2008, Data reduction strategies, uncertainty assessment and resolution of LA-(MC-) ICP-MS isotope data, *in* Sylvester, P. (ed.), *Laser ablation ICP-MS in the Earth Sciences: current practices and outstanding issues*: Mineralogical Association of Canada, Short Course Series, 40, 283-303.
- Hoskin, P.W.O., Schaltegger, U., 2003, The composition of zircon and igneous and metamorphic petrogenesis: *Reviews in Mineralogy and Geochemistry*, 53(1), 27-62.
- Jackson, S.E., Longrich, H.P., Dunning, R., Fryer, B.J., 1992, The application of laser-ablation microprobe-inductively coupled plasma mass spectrometry LAM-ICP-MS to *in situ* trace element determinations in minerals: *Canadian Mineralogist*, 30, 1049-1064.
- Jackson, S.E., Longrich, H.P., Horn, I., Dunning, R., 1996, The application of laser ablation microprobe (LAM)-ICP-MS to *in situ* U–Pb zircon geochronology, *in* Sixth V.M. Goldschmidt Conference, Heidelberg: *Journal of Conference Abstracts*, 1, 283.
- Jackson, S.E., 2008, Calibration strategies for elemental analyses by LA-ICP-MS, *in* Sylvester, P. (ed.), *Laser ablation ICP-MS in the Earth Sciences: current practices and outstanding issues*: Canada, Mineralogical Association of Canada, Short Course Series, 40, 169-188.
- Košler, J., Sylvester, P.J., 2003, Present Trends and the Future of Zircon in Geochronology: *Laser Ablation ICPMS: Reviews in Mineralogy and Geochemistry*, 53(1), 243-275.
- Košler, J., Forst, L., Sláma, J., 2008, Lamdate and lamtool: spreadsheet-based data reduction for laser ablation ICP-MS, *in* Sylvester, P. (ed.), *Laser ablation ICP-MS in the Earth Sciences: current practices and outstanding issues*: Canada, Mineralogical Association of Canada, Short Course Series, 40, 315-317.
- Ludwig, K.R., 2008, *Manual for Isoplot 3.7*: Berkeley Geochronology Center, Special Publication No. 4, rev. August 26, 2008, 77 pp.
- Paton, C., Woodhead, J.D., Hellstrom, J.C., Hergt, J.M., Greig, A., Maas, R., 2010, Improved laser ablation U–Pb zircon geochronology through robust downhole fractionation correction: *Geochemistry Geophysics Geosystems* (G³), 11, paper number Q0AA06, doi: 10.1029/2009GC002618
- R Development Core Team, 2010, R: A language and environment for statistical computing: Vienna, Austria, R Foundation for Statistical Computing, ISBN 3-900051-07-0, URL <http://www.r-project.org>.
- Schmitz, M.D., Schoene, B., 2007, Derivation of isotope ratios, errors and error correlations for U–Pb geochronology using ²⁰⁵Pb–²³⁵U–(²³³U)-spiked isotope dilution thermal ionization mass spectrometric data: *Geochemistry, Geophysics, Geosystems*, v. 8, doi:10.1029/2006GC001492.
- Sláma, J., Košler, J., Condon, D.J., Crowley, J.L., Gerdes, A., Hancher, J.M., Horstwood, M.S.A., Morris, G.A., Nasdala, L., Norberg, N., Schaltegger, U., Schoene, B., Tubrett, M.N., Whitehouse, M.J., 2008, Plešovice zircon -A new natural reference material for U–Pb and Hf isotopic microanalysis: *Chemical Geology*, 249(1-2), 1-35.
- Solari, L.A., Gómez-Tuena, A., Bernal, J.P., Pérez-Arvizu, O., Tanner, M., 2010, U–Pb zircon geochronology by an integrated LA-ICPMS microanalytical workstation: achievements in precision and accuracy: *Geostandards and Geoanalytical Research*, 34(1), 5-18.

- Sylvester, P. (ed.), 2008, Laser Ablation ICP-MS in the Earth Sciences: Current practices and outstanding issues: Mineralogical Association of Canada, Short Course, 40, 356 pp.
- Van Achterbergh, E., Ryan, C.G., Jackson, S.E., Griffin, W.L., 2001, Data reduction software for LA-ICP-MS, *in* Sylvester P.J. (ed.), Laser ablation-ICP-mass spectrometry in the Earth Sciences: Principles and applications: Ottawa, Ontario, Mineralogical Association of Canada, Short Course Series, 29, 239-243.
- Venables, W.N., Ripley, B.D., 2002, Modern Applied Statistics with S: New York, Springer, Fourth Edition, 503 pp.
- Von Quadt, A., Guillong, M., Peytcheva, I., 2009, Uncertainties of LA-ICPMS U-Pb zircon ages caused by the use of different data reduction software: *Geochimica and Cosmochimica Acta*, Abstract Supplement, 73(13), A1396.
- Whitehouse, M.J., 2003, Rare earth elements in zircon: a review of applications and case studies from the Outer Hebridean Lewisian Complex, NW Scotland: London, Geological Society, Special Publications, 220(1), 49-64.

Manuscript received: September 26, 2010

Corrected manuscript received: November 26, 2010

Manuscript accepted: December 1, 2010