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A review of detrital zircon data treatment, and launch of a new tool 'Dezirteer' along with the suggested universal workflow

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ABSTRACT

Overwhelming numbers of detrital zircon (dZr) U—Pb ages have been acquired all over the globe in the last few decades, opening new horizons for employing big data approaches. However, several impediments such as frequent publication of heavily filtered data tables with omitted analyses, failure to cite the logic on "best age" computation, and generally the lack of uniformity among data treatment approaches delay the employment of this growing volume of data to the full extent. We have developed Dezirteer software to address some of the impediments. The program runs on any OS as a Python package and can be installed in Windows via an executable installer. Dezirteer imports U-Th-Pb LA-ICPMS geochronology data (either as .csv files from Iolite or Glitter, or from a manually-filled template). First, it allows the user to define and apply filters (by elevated discordance, analytical uncertainty, and U concentration). Next, the user defines computations (discordance calculation, type of Pb-correction, choosing "best age"), and Dezirteer applies them on dZr datasets. Finally, Dezirteer exports data and manipulations on them, unequivocally separated. Dezirteer permits to quickly assess the results of filters and computations visually (concordia, probability density curves, kernel density estimates, histograms, and cumulative diagrams) and numerically (Kolmogoroff — Smirnov statistics, Likeness, and Similarity coefficients, peaks locations). Thus, our program can be used as a substitute for several existing software packages and provides some unique functionality. We propose several guidelines for publishing U-Th-Pb dZr data to increase the data's trustworthiness and usability and improve the transparency of manipulations on these data. Most importantly, dZr data must be published before extensive filtering and interpretation, while all further filtering and computational aspects should be described. Such an approach will significantly simplify the use of global dZr data by the scientific community and step forward towards employing big data approaches in dZr studies.

1. Introduction: problem of big data approaches to detrital zircon U—Pb geochronology

Detrital zircon (dZr) U—Pb geochronology is a quickly developing field within geosciences. The number of publications supported by dZr data is growing each year exponentially. The numbers of dZr analyses per publication also grew substantially in the mid-nineties due to the introduction of laser ablation with inductively coupled plasma mass spectrometry (LA-ICPMS), yielding a 7–10 times increase in productivity compared to secondary ionization mass spectrometry (SIMS) and even a steeper increase compared to thermal ionization mass spectrometry (TIMS). While most labs currently operate at 100 or fewer analyses per hour, (Sundell et al., 2021) suggest faster sample throughput by LA-ICMPS, up to 1200 analyses per hour, increasing the gap in productivity even further.

The large and quickly growing number of published analyses (the most extensive compilation by Voice, Kowalewski, and Eriksson (2011) contains >200,000 dZr dates) allows the use of big data approaches. In one example of employing big data, (Puetz, Ganade, Zimmermann, and Borchardt, 2018) analyzed seven of the largest geochronologic databases, revealing what appear to be harmonic geological cycles of 93.5 and ~ 187 Ma that have persisted throughout terrestrial history. In another example by Voice, Kowalewski, and Eriksson (2011), a compilation of ~200,000 worldwide detrital zircon analyses revealed the presence of six prominent statistically significant age peaks at 3.2–3.0, 2.7–2.5, 2.0–1.7, 1.2–1.0, 0.7–0.5, and 0.3–0.1 Ga. Such studies, backed

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by big data, greatly enhance our understanding of Earth's history and processes.

The main impediment of using the growing volume of data is a place to lodge information that is open to the curious. Currently, the available big databases (e.g., the National 79 Geochronological Database in the United States [Sloan, Henry, Hopkins, & Ludington, 2003], the Canadian 80 Geochronology Knowledgebase [http://gdr.nrcan.gc.ca/geochron/index_e.php], the Brazilian 81 National Geochronological Database [Silva, Rodrigues, Silveira, & Pimentel, 2003]) are broken up on a provincial or national scale.

A second impediment involves data presentation and the challenges in extracting data from pdf files. In this case, encouragement of supplementary files in a consistent format will be helpful.

The subjectivity in data processing approaches is another challenge. As noted in Horstwood et al. (2016), "unlike for other isotopic systems or methods <...> the LA-ICP-MS U-(Th-)Pb community has not published recommended guidelines and standards for handling and reporting of data in the scientific literature". Indeed, unlike many other fields of science, raw dZr data (files containing time slices with either counts per second values from isotopic counters or volt measurements from Faraday cups) are rarely reported. In addition, any further data manipulations are often described too sparingly. In many cases, published data tables contain only variably filtered data, with less reliable analyses omitted, while not always clearly citing the reasons for deletion or describing the computation and filtering algorithms used. Filtering out data points inevitably introduces bias. The absence of a uniform approach for filtering makes the data comparison from different samples and stratigraphic units challenging (Nemchin and Cawood, 2005) and often meaningless. To compare data from various sources, they need to be brought to common denominators: data must be published separated from subsequent manipulations, allowing others to re-use just the data without the interpretational layer. Filters and computations must be comprehensively reported so that they are understood by others and can be replicated.

Another obstacle to the analysis of large dZr data sets is the inefficiency of existing computational tools in applying filtering and computational algorithms to hundreds, thousands, and tens of thousands of analyses.

Our new tool 'Dezirteer' solves some of the impediments above: it permits a rapid way to batch-process and analyze large amounts (10^2–10^5) of dZr analyses; prepares publication-ready tables and images; promotes data separated from any manipulation on them.

2. Practical aspects of data filtering, calculation, visualization, and interpretation

2.1. Workflow for producing geochronology data

The commonly used workflow for producing geochronology data of detrital zircons (dZr) on LA-ICPMS includes the following steps:

- Rock processing, followed by zircon separation and mounting.
- Imaging of mounted zircons by microscopy (optical or electron microscope; cathodoluminescence investigation).
- LA-ICPMS measuring session. Zircons of unknown age are interspersed with standard zircons of known age (U—Pb ratio standards) and commonly with concentration standards (NIST glasses). Detector readings (in volts or counts or cps, depending on the detector type) are recorded continuously during a session and saved to data files.
- Data files with recorded detector readings are imported into data reduction software. By far, the two most used programs are Iolite (Paton, Hellstrom, Paul, Woodhead, and Hergt, 2011) and Glitter (Griffin, 2008). Time series data (detector readings vs. session time) are baseline-corrected, manually analyzed for irregularities (e.g., non-zircons, drill-throughs), and mathematically corrected for instrument drift and downhole fractionation. Resulting isotopic ratios are exported as tables.
- In a typical case, reduced data files are opened in spreadsheet software, such as MS Excel. Then, a set of filters is applied either manually (by scrolling through data and crossing out unfit analyses by eye), semi-automatically (by applying formulas and logic in the spreadsheet software), or automatically (usually by using spreadsheet macros). Some researchers are using self-written scripts, often in R-programming language. Filtered data are grouped in tables; diagrams are plotted ;statistical tests (e.g., Kolmogoroff-Smirnov, Likeness, Similarity) are conducted.

The first four steps are described in numerous publications and are out of the scope of this study. The last step — data filtering and visualization — is the topic of this contribution. Dezirteer software is designed to import data either from Iolite/Glitter-produced files or from a template; apply user-defined computations and filters; visualize them as concordia-discordia, kernel density estimates/probability density, histograms and cumulative diagrams; export the data tables and plots.

2.2. Filters

Several filtering algorithms are used in various combinations in order to break dZr analyses down into 'good' and 'bad' pools:

2.2.1. By elevated discordance

Discordance is generally interpreted as being caused by loss of radiogenic lead, gain of excess U after primary crystallization, incorporation of common lead, and intermediate daughter product disequilibrium (Schoene, 2013; Andersen, Elburg, and Magwaza, 2019). Some degree of filtering out highly discordant analyses is a common practice, with usual cutoffs at +5–30% positive and 5–10% negative (e.g., Voice, Kowalewski, and Eriksson, 2011). The level of discordant filter is greatly dependent on the nature of the study: if within a mix of Archean and Proterozoic grains, relative proportions of these ages are essential, a generous cutoff might be employed; on the other hand, if studying a specific age, a tight discordance filter might be more appropriate to achieve the best age resolution (Gehrels, 2011).

2.2.2. By individual analysis error

Filtering out analyses with large uncertainties is used in literature, although less often than filtering out discordant analyses. This filter is particularly important for younger Phanerozoic grains, where error ellipses are often located close to and parallel to the concordia curve (Nemchin and Cawood, 2005), resulting in potential misinterpretations of discordant analyses as concordant. Usually, 5–10% cutoff values are used.

2.2.3. By uranium concentration

Elevated levels of radiogenic elements, such as U, are known to have a destroying effect on the crystalline lattice of zircons, increasing the U—Pb isotopic discordance (e.g., Nasdala, Pidgeon, Wolf, and Irmer, 1998), making them invalid for dating purposes. Nevertheless, analyses with higher U concentrations might be more accurate and should not be mindlessly discarded. Such phenomena was demonstrated in (Allen & Campbell, 2012) and was attributed to a better match between the matrix and the primary standard. Overall, U concentration by itself should probably not be considered solid filtering criteria. Zircon grains with higher U concentrations are not necessarily metamict, depending on the duration a grain existed below annealing temperature (Herrmann et al., 2021).

2.2.4. Filtering of 'contaminant' grains

Some contamination levels are not uncommon at all stages of mineral separation, leading to sample contamination by foreign zircons and other minerals. Quite often, a variety of analyses are blamed on contamination and omitted from publications. We are advising against it and strongly propose that all zircon analyses should be published.

2.3. Computations

Analyses that were not filtered out and landed in the "good" pool require further mathematical manipulations before the 'best age' can be reported.

2.3.1. Calculating the 'best age': which isotopic system to use?

This topic has been discussed in many publications (e.g., Nemchin and Cawood, 2005; Gehrels, 2011). Out of four measured isotopic pairs ($^{207}Pb/^{206}Pb$, $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, $^{208}Pb/^{232}Th$), only the former two are used regularly for the 'best age' calculations.

$^{207}Pb/^{235}U$ isotopic ratio is not used due to very low counts of ^{207}Pb resulting in low precision. ^{235}U is rarely measured, but instead, it is calculated from the fixed $^{238}U/^{235}U$ ratio (137.88: Steiger and Jager, 1977; 137.817: Livermore, Connelly, Moynier, and Bizzarro, 2018; 137.818: Hiess, Condon, McLean, and Noble, 2012).

Th/Pb age is rarely used for zircons in practical applications. The half-life of ^{232}Th is formally known with a precision of ~1% (Steiger and Jager, 1977), which is almost an order of magnitude larger than the stated precision for ^{238}U and ^{235}U half-lives (Jaffey, Flynn, Glendenin, Bentley, & Essling, 1971). $^{208}Pb/^{232}Th$ age is disadvantageous for precise dating by ID-TIMS. Nevertheless, the $^{208}Pb/^{232}Th$ age can be used for testing close versus open system behavior of dated dZr.

The $^{206}Pb/^{238}U$ ratio is *de facto* the default system for younger zircons, and $^{207}Pb/^{206}Pb$ for the older ones, with a cutoff between 600 and 1500 Ma. Many publications use a cutoff at 1 billion years (e.g., Veevers, Saeed, Belousova, and Griffin, 2005; Sevastjanova et al., 2011), or 1.4 billion years (e.g., Bradley et al., 2007), usually without substantiation). The physical reason for the cutoff is the balance of analytical errors of both measurements. Young zircons have low counts of ^{207}Pb, yielding in poor $^{207}Pb/^{206}Pb$ uncertainties. Precision of $^{206}Pb/^{238}U$ does not necessarily correlate with age, but is dependent on zircon's uranium content. —

A higher uranium concentration results in quicker accumulation of Pb in the crystalline lattice, therefore shifting the ideal crosspoint to the younger part of the age spectra. Vice versa, low uranium concentration shifts the ideal cross point to the older part of an age spectrum. Powerman, Shatsillo, Chumakov, Kapitonov, and Hourigan (2015) used a simple model to estimate the influence of uranium concentrations on the ideal crosspoint. To have reasonable approximations for the cutoff values, the expected $^{207}Pb/^{206}Pb$ age uncertainties were forward-modeled for a series of ages. The cutoff value was defined as age, at which the error in $^{207}Pb/^{206}Pb$ age became less than 1%, assumed to be a typical value for $^{206}Pb/^{238}U$ age error. Crosspoint age varied hyperbolically from ~1400 Ma (at 80 ppm U) to ~800 Ma at 1000 ppm U (Fig. 1).

2.3.2. How to assess concordance?

Several different methods are routinely used to assess the degree of discordance. Two of the most common methods involve calculating relative difference between either $^{206}Pb/^{238}U$ and $^{207}Pb/^{235}U$, or $^{207}Pb/^{206}Pb$ and $^{206}Pb/^{238}U$ (Gehrels, 2011) age estimates. However, the former pair is usually limited to younger zircons, where $^{207}Pb/^{206}Pb$ ages can be less precise than $^{207}Pb/^{235}U$ ones.

In another method, Puetz, Ganade, Zimmermann, and Borchardt (2018) define discordance in terms of absolute age differences. Alternatively, Spencer, Kirkland, and Taylor (2016) propose to define discordance in terms of U—Pb compositions rather than ages.

(Vermeesch, 2020) suggests an alternative method of assessing discordance by measuring the Euclidean distance between ln ($^{207}Pb/^{206}Pb$) and ln($^{238}U/^{206}Pb$) ratios and presents two options of doing so. In the first option, the distance along a perpendicular line to the concordia curve is measured. However, this option does not take the analytical precision of the isotopic measurements into account; to overcome this issue, (Vermeesch, 2020) proposes another option: measuring the line connecting the measured log ratio and the maximum likelihood composition on the concordia line. The latter method is considered superior to alternatives by Vermeesch (ibid.), resulting in the tightening of subpopulations without changing their position or relative size.

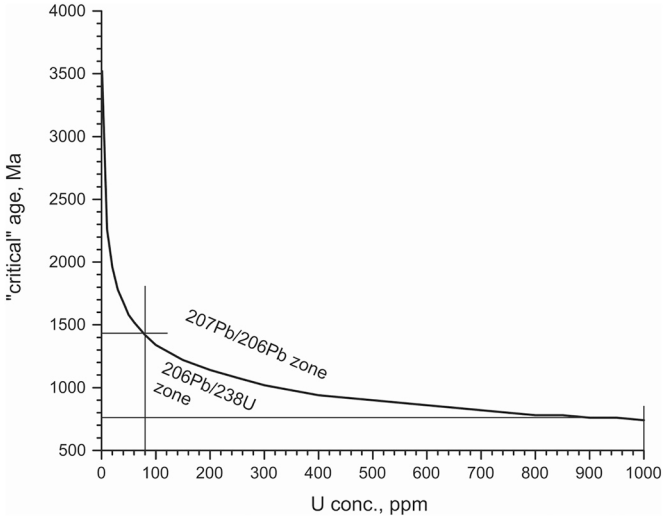

Fig. 1. Diagram, modified from Powerman, Shatsillo, Chumakov, Kapitonov, and Hourigan (2015), demonstrating the forward-modeled relationship between uranium concentration of a zircon and the age at which uncertainty in $^{207}Pb/^{206}Pb$ age becomes less than 0.01. The following input parameters were used: (1) uranium concentration; (2) volume of ablated material that were similar to common amounts of zircon material removed from ablation crater; (3) instrumental sensitivities. For each age, the amounts of ^{206}Pb and ^{207}Pb were calculated, in ions and in cps. The errors were derived from the counting statistics.

2.3.3. Common Pb correction

Geochronology age calculations require radiogenic ratios. Several mathematical corrections can be employed to account for non-radiogenic Pb. Four types of common Pb corrections are more or less commonly used in detrital zircon studies: (1) correction by ^{204}Pb, (2) by ^{207}Pbc, (3) by ^{208}Pbc, and (4) "Andersen-type". All corrections depend on the common Pb model of crustal evolution. In the overwhelming majority of detrital zircon papers, the model by Stacey and Kramers (1975) is used. In igneous geochronology, Pb-bearing cogenetic minerals (e.g., feldspars or sulfides) may be used to assess common Pb composition (e.g. Marfin et al., 2020); however, this method is not applicable to detrital zircon studies.

The ^{204}Pb correction (Ireland and Williams, 2003) employs the fact that the ^{204}Pb isotope is strictly non-radiogenic and can be used as an estimate of common Pb in zircon. This correction can be applied to all four ratios ($^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, $^{208}Pb/^{232}Th$, $^{207}Pb/^{206}Pb$) and results in four different corrected ages. While this seems to be an ideal solution (since there is no need to assume concordance or time of Pb loss), there are limitations. The ^{204}Pb correction can only be applied to datasets with accurately measured ^{204}Pb isotope; in ICPMS applications this can only be accomplished on instruments with electronic multipliers. It is equally important for the instrument to measure ^{202}Hg accurately in order so correct for Hg interference at the 204 mass. Many ICPMS instruments lack the sensitivity in detecting Hg interferences, and/or get Hg contamination from the helium gas, used to transfer ablated material from lasers. Challenges above limit the ability to apply the ^{204}Pb correction. In fact, this problem is not limited to LA-ICPMS: even SHRIMP age measurements that employ a ^{204}Pb correction often do not achieve concordance and then a ^{207}Pb correction is invoked (sometimes without adequately identifying the reason in the text).

The ^{207}Pb and ^{208}Pb methods require making an important assumption that initially concordant U—Pb and U-Th-Pb isotope systems, correspondingly, were disturbed just by the contamination of

common Pb.

The ^{208}Pb method assumes that a zircon grain is initially concordant in $^{238}U/^{206}Pb$ and $^{208}Pb/^{232}Th$, while potentially discordant in $^{207}Pb/^{235}U$ and $^{206}Pb/^{238}U$ ratios. Such scenario is unrealistic; radiogenic Pb, which is not concordant in all three ratios, will result in erratic ages when this correction is applied (Andersen, Elburg, and Magwaza, 2019).

The ^{207}Pb method is based on the assumption that the observed Pb composition is a true binary mixture of concordant radiogenic Pb and common Pb; the initial concordance is assumed. Zircons that have experienced Pb loss at any time will yield 207-corrected ages that are too young. Only those zircons unaffected by Pb loss at any point in their history will yield true ages when 207-corrected (Andersen, Elburg, and Magwaza, 2019). This method is applicable primarily to relatively young zircons where the discordance cannot be detected within the limits of analytical uncertainty. Although Ireland and Williams (2003) recommend limiting this method to Phanerozoic, there are numerous examples where Phanerozoic grains demonstrate excessive lead loss.

Another method, usually referred to as the 'Andersen correction', uses an assumption that observed $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, and $^{208}Pb/^{232}Th$ ratios of a discordant zircon can be accounted for by a combination of Pb loss at a defined time, and the presence of common Pb (Andersen, 2002). There is a *caveat*: this correction requires an assumption that the time of Pb loss is known, which is not a common case, and certainly not so for dZr applications.

In our opinion, common Pb correction should rarely (if ever) be used in dZr studies. Each correction requires crucial assumptions (such as initial Pb composition, time of Pb loss, concordance), which can be hard to substantiate for complex multi-source geological systems. Furthermore, concealed ancient Pb loss and overcorrection result in bias towards younger ages, while remaining within the acceptable discordance limits (Andersen, Elburg, and Magwaza, 2019). Therefore, in our opinion, analyses with elevated ^{204}Pb levels should be discarded (but still reported as such) either at data reduction stage (in Iolite), or in other instruments. The rest should be reported uncorrected.

2.4. Visualization aspects

Three major types of diagrams are generally used to visualize dZr ages distributions:

(1) concordia-discordia diagrams are extensively used in geochronology for reconstructing crystallization and Pb loss history of igneous and metamorphic rocks. Still, they are substantially less helpful for that purpose in multi-sourced detrital samples, comprised of zircons with dissimilar (and often radically different) geological journeys. Concordia diagrams in dZr studies are mainly used for a quick visual assessment of analyses in terms of their discordance degree. The two most popular concordance diagrams are the conventional Wetherill diagram ($^{206}Pb/^{238}U$ is plotted against $^{207}Pb/^{235}U$) and the Tera-Wasserburg diagram ($^{207}Pb/^{206}Pb$ is plotted against $^{238}U/^{206}Pb$). And while it is considered good practice to plot data comprehensively, discordant grains are often omitted from graphs.
(2) Data distribution plots include probability density plots, kernel density estimates and binned frequency diagrams.

Binned frequency diagrams (i.e., histograms) are commonly used for displaying age data to show a potentially representative sampling of the timing of when zircons crystallized in the source rocks. Histograms are somewhat useful in demonstrating the general durations of magmatic pulses in a region. However, the spread in data in a dZr spectra is affected by data reproducibility and internal analytical precision and not an accurate representation of the duration of specific events affecting a single rock volume.

Probability density plots (PDP) and Kernel Density Estimates (KDE) are continuous curves that are easy to interpret and compare. PDPs are calculated by summing Gaussian distributions, with their means and standard deviations corresponding to the individual ages and their respective analytical uncertainties. Vermeesch (2012) argues that PDPs can produce counter-intuitive results when data quantity and /or quality are high and proposes a more robust approach, kernel density estimates (KDE), which also involve summing Gaussian distributions, but without considering analytical uncertainties. KDE calculations require a kernel and a bandwidth to be chosen. There are a few approaches to calculate optimum bandwidths, described by Vermeesch (ibid.).

(3) Cumulative probability plots are constructed by integrating the respective probability plots (PDP or KDE). Cumulative plots are used for statistical testing (e.g., Kolmogoroff-Smirnov statistics: Kolmogoroff, 1941; Lovera, Grove, Cina, and Kimbrough, 2008), providing opportunities for testing various geological hypotheses based on (dis-)similarities of datasets.

2.5. Existing software packages and their limitations

Several software packages are used to analyze and visualize U—Pb dZr data. They fall into two categories: (1) data reduction software, intended to convert time series data from ICPMS instruments into tables with isotopic ratios and elemental concentrations; (2) software for visualizing reduced data and applying calculations to assess, evaluate and interpret data.

2.5.1. Data reduction software currently available and commonly used

Software of the first category include Glitter , Iolite and LADR.

Glitter (Griffin, 2008, http://www.glitter-gemoc.com) software provides "real-time, on-line and user-friendly treatment of quantitative chemical data produced during an analysis of solid micro-samples by laser ablation microprobe–inductively coupled plasma–mass spectrometry (LAM–ICP–MS)" (ibid.). Glitter is compatible with raw data files exported at least ten different mass-spectrometers. It graphs the pixel maps of time-resolved signals and isotopic ratios; allows interactive and automated selection of optimal signal time intervals; calculates elemental concentrations using external calibration standards, corrects for mass-dependent instrumental drift; calculates $^{207}Pb/^{206}Pb$, $^{206}Pb/^{238}U$, and $^{207}Pb/^{235}U$ ages and uncertainties; generates interactive U/Pb concordia plots; exports results in spreadsheet format. One of Glitter's notable features is its ability to calculate dates in real-time (i.e., during ICPMS measuring session). However, in our view, Glitter's most significant limitation is the inability to correct data for downhole fractionation, known phenomena during prolonged drilling of zircons by a laser beam.

Iolite (Paton, Hellstrom, Paul, Woodhead, and Hergt, 2011) is the alternative software that "handles everything from basic trace element experiments, right through to imaging, geochronology and isotopic systems (e.g., Sr, Hf isotopes), with the ability to fully (or partially) automate the entire process" (www.iolite.xyz). It imports raw data files produced by at least eight models of mass spectrometers (Rittner and Müller, 2012).

Similar to Glitter, Iolite imports ICPMS-produced data files, applies baseline and instrument drift corrections, calculates $^{207}Pb/^{206}Pb$, $^{206}Pb/^{238}U$, and $^{207}Pb/^{235}U$ ratios, ages, and uncertainties. Unlike Glitter, Iolite lacks the possibility of conducting real-time analysis during mass spectrometry sessions. Strong points of Iolite include correction of data for downhole fractionation, imaging capabilities, multi-session data storage for long-term reproducibility, and uncertainty propagation.

LADR (Laser Ablation Data Reduction) is another data reduction software recently released by Norris, Danyushevsky, Olin, and West, 2021(https://norsci.com). The program can model and correct for downhole fractionation and instument drift; employ secondary standards to correct for matrix effects; apply a robust error propagation from all sources of uncertainty.

Data reduction is an essential prerequisite step for further data analysis in ***Dezirteer***.

2.5.2. Post-data reduction software

Isoplot (Ludwig, 2003) is a popular software for the visualization of geochronology data (including dZr applications). Isoplot, an MS Excel add-on, is aimed to interpret a variety of isotopic data. —For dZr geochronology, Isoplot constructs UPb concordia plots and calculates ages using conventional concordia intercepts; extracts reliable ages and errors from complex suites of single-zircon dates; deconvolutes mixtures of components (such as dZr ages) having Gaussian error-distributions using the Sambridge and Compston (1994) approach; calculates and constructs plots for either error-weighted or robust averages of a single variable. Graphs are plotted in MS Excel and are importab;e to vector graphing software suites (e.g., Adobe Illustrator and CorelDraw).

IsoplotR (Vermeesch, 2018) is similar to Isoplot in functionality. Unlike its predecessor, it is no longer an add-on to Excel. IsoplotR exists in three versions: online, offline (runs in R language), and command-line interface. IsoplotR includes functions for U—Pb, Pb—Pb, $^{40}Ar/^{39}Ar$, Rb—Sr, Sm—Nd, Lu—Hf, *Re*—Os, U-Th-He, fission track and U-series disequilibrium dating (Vermeesch, 2018). In the light of dZr analysis, IsoplotR provides all calculations and plotting available in Isoplot and features some additions, such as implementing different methods to correct for the presence of common Pb and corrections for four isotopic disequilibria.

Neither of the two programs addresses all aspects previously discussed in this chapter in their current versions (although IsoplotR seems to be rapidly evolving).They were designed to solve a broad range of isotopic problems and are not solely devoted to dZr data manipulations. Both lack the ability to filter out analyses; define rules that govern how 'best age' and discordance are calculated.

Topsoil software (Bowring and PI CIRDLES.org Open Source Development Team, 2016) is another alternative for Isoplot. Topsoil is based on Java and requires to be somewhat knowledgeable in the information technology industry; a user must know how to clone a repository from GitHub, be familiar with CLI or NetBean IDE. To our knowledge, the current version of Topsoil does not address the filtering and computational issues.

UPbplot.py is a free Python (3.6.x) script developed by Atsushi Noda (2016, 2017) and the Geological Survey of Japan. —The program is aimed at the calculation and visualization of U—Pb age data. It permits plotting scattered data with error ellipses on conventional ($^{207}Pb/^{235}U$-$^{206}Pb/^{238}U$) and Tera-Wasserburg ($^{238}U/^{206}Pb$-$^{207}Pb/^{206}Pb$) concordia diagrams, and calculation of one- or two-dimensional weighted mean, concordia, and concordia-intercept ages with errors on both concordia diagrams. This program does not address the filtering and computational issues.

Density plotter (Vermeesch, 2012) is a Java-based software that plots Kernel Density Estimates (KDE). KDEs are calculated by summing a set of Gaussian distributions without taking analytical uncertainties into account and are presented as a more robust alternative to the PDP (probability density plots). PDPs, per Vermeesch (2012), produce counter-intuitive results when data quantify and/or quality is high. Density Plotter does not address data filtering and computation.

Excel-based tools by the LaserChron (University of Arizona) are available at the center's website (http://laserchron.org/laserchron/). ——These Excel-based macros include: a routine for calculating normalized and cumulative age probability plots: a routine for evaluating whether U—Pb analyses have experienced Pb loss, and/or overgrowth/recrystallization of metamorphic zircon; an instrument for calculating degrees of Overlap (whether two samples contain the same set of ages, irrespective of their relative abundances), and Similarity (relative abundances of similar ages); Kolmogoroff-Smirnov (K—S) test. These tools do not address data filtering and computation aspects.

DetritalPy is an open-source Python-based tool by Sharman, Sharman, and Sylvester (2018). This software can import data tables; plot sample locations on an interactive, zoomable map and export them to Google Earth; allows rapid identification of geographically related samples; calculating and visualizing maximum depositional ages; multidimensional scaling; calculation of similarity and dissimilarity metrics (e.g. similarity, likeness, K—S statistic); plotting dZr distributions in comparison to another variable (e.g., Th/U); exporting U—Pb age and error data and age distributions as CSV files. DetritalPy does not permit the user to define algorithms for filtering data and to produce "best ages". Instead, it requires the imported tables to include the "best Age" column.

DZstats, a MATLAB-based application by Saylor and Sundell (2016) allows user to plot dZr sets and apply a variety of statistical tests. The five metrics commonly used as quantitative descriptors of sample similarity in dZr are provided to the user: K—S and Kuiper tests, Cross-correlation, Likeness and Similarity coefficients of probability density plots, kernel density estimates, and locally adaptive, variable-bandwidth KDEs (LA-KDEs).

3. Treatment of data in Dezirteer

Data filtering is labor-intensive and prone to human errors when done manually. Going through hundreds or thousands of analyses requires the use of more robust automatic approaches, minimizing the human factor problem and decreasing any bias. Another important aspect of analyzing reduced data is the ability to quickly visualize them and compare them to other samples.

We have developed ***Dezirteer*** (an acronym for 'DEtrital ZIRcons'; 'TE' is reserved for trace elements functionality planned in subsequent releases), — a program to conduct rapid analysis and filtering of Glitter- or Iolite-reduced data. We believe that it answers some of the challenges as mentioned earlier.

Dezirteer is supplied as an MS-Windows executable installation file or as a Python package to be run on any Python (version>3.4) interpreter irrespective of the operating system. ***Dezirteer*** graphic user interface (GUI) is shown in Fig. 2.

The workflow of ***Dezirteer*** (Fig. 3) consists of the following general stages: data ingestion; data scrubbing; tables and graphics export.

NB: It is necessary to note that any software is constantly evolving; therefore, some of the following descriptions might become outdated in a few months and even weeks following the publication. Readers are advised to visit www.dezirteer.com for the latest ***Dezirteer*** release and documentation.

3.1. Data import

The first step in U—Pb analysis with ***Dezirteer*** involves importing data tables produced by data reduction software, Iolite or Glitter. Data can also be imported via the template included in the installation package so that any published dZr results can be analyzed, including cases with only limited available information. ***Dezirteer*** permits multiple data files to be imported; any of the three supported formats (Iolite, Glitter, and template) can be mixed, allowing data from different sources to be easily compared.

In order to import Glitter, Iolite, or template data to Dezirteer, the user must ensure their correct format, including the presence of required channels. This information is listed in Appendix A.

After the file or files are imported, the analysis table and the sample list are automatically filled. Then, ***Dezirteer*** is ready for data scrubbing.

3.2. Data scrubbing

Data scrubbing is a cycle that can be divided into two general parts: parameter tuning and data analysis.

3.2.1. Parameter tuning

During parameter tuning, a user provides instructions on calculating

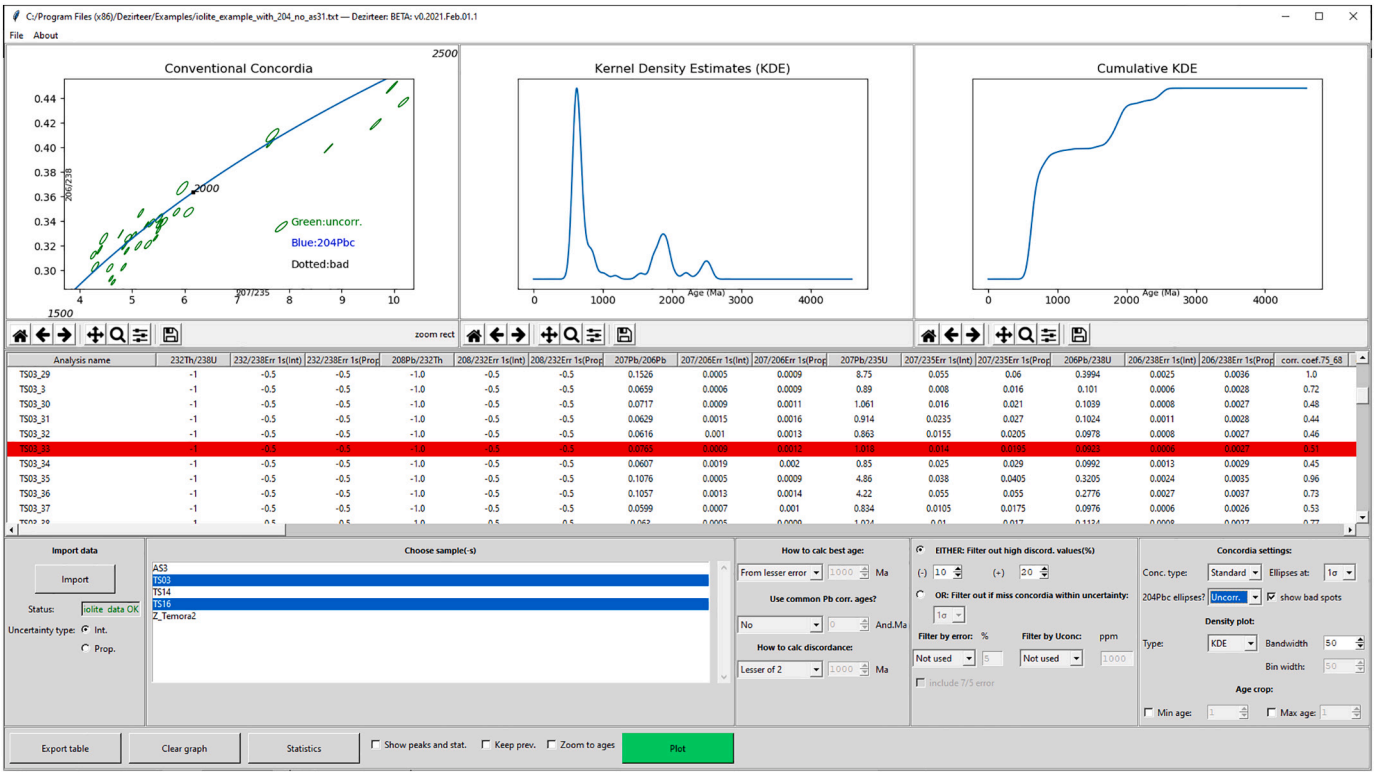

Fig. 2. Graphical user interface of ***Dezirteer***.

the degree of discordance, employing common Pb correction, choosing the isotopic system, separating analyses into 'good' and 'bad' pools by applying filters, plotting data.

Choosing the type of uncertainties (Iolite only). Iolite provides an option to export both internal and propagated uncertainties. Dezirteer can process either one, given that appropriate Iolite channels exist in the imported file.

Applying filters. The goal of filtering is to divide all analyses into 'good' and 'bad' sets. Analyses from the 'good' set are included into calculations, used for plots and subsequent geological interpretations. Analyses from the 'bad' pool are not employed in calculations; they do not contribute to the probability plots (however, if the user desires, can still appear on concordia-discordia diagrams, distinctively marked); they are still exported as tables, clearly marked as invalid. Users can define the following filters:

- Filter by Uconc (uranium concentration in ppm) is available for data files containing correspondent channels (Appendix A).
- Filter by analytical % error, either only in $^{206}Pb/^{238}U$ isotopic ratio, or by that and in $^{207}Pb/^{235}U$ ratio as well.
- Filter by discordance. There are two ways Dezirteer filters out discordant grains. In the first one, the user sets thresholds on positive and negative discordance values (e.g., +20%, −10%). Dezirteer then applies user-set computations to calculate discordance and filters out analyses that do not pass the filter. In the second one, Dezirteer uses uncertainty bars to judge whether a measurement is concordant or not. The user sets the interval from 1σ to 10σ; if analysis intersects the concordia line along both axes, it is considered concordant.

'Best age' computation. There are five options for calculating the 'best age':

- From the lesser error: ***Dezirteer*** uses the isotopic system ($^{206}Pb/^{238}U$ or $^{207}Pb/^{206}Pb$) with the least % error for each analysis.
- Fixed age limit: user defines the age limit of the threshold; if $^{206}Pb/^{238}U$ age is younger than the threshold, it is be used for the 'best age'; otherwise the $^{207}Pb/^{206}Pb$ age is employed.
- $^{207}Pb/^{206}Pb$ option restricts best ages to the Pb—Pb system.
- Similarly, in the last case, only the $^{206}Pb/^{238}U$ is used for all analyses.
- Finally, 'best' age can be computed by applying one of the common Pb corrections that assume concordance.

Common Pb correction. There are five options in Dezirteer: no common Pb correction (recommended for most cases), ^{204}Pb-corr.; ^{207}Pb-corr., ^{208}Pb-corr.; and Andersen's correction.

In its current version, Dezirteer employs the common lead model by Stacey and Kramers (1975) only.

It is important to note that while Dezirteer applies Pb correction to the whole suite of analyses, it is still possible to import previously corrected data via template and mix it with uncorrected data. This situation must be avoided.

Computation of discordance. Currently, there are four ways to calculate discordance:

- Compare two discordance values ($^{207}Pb/^{206}Pb$)—($^{206}Pb/^{238}U$) and ($^{207}Pb/^{235}U$)—($^{206}Pb/^{238}U$) and automatically choose one with the lesser absolute value. This option accounts for large discordance values, caused by low isotopic counts and large analytical errors.
- Switch between ($^{207}Pb/^{206}Pb$)—($^{206}Pb/^{238}U$) and ($^{207}Pb/^{235}U$)—($^{206}Pb/^{238}U$) systems in terms of discordance calculation at the user-set $^{206}Pb/^{238}U$ age threshold.
- Always use one of the two systems for discordance calculation, either ($^{207}Pb/^{206}Pb$)— ($^{206}Pb/^{238}U$) or ($^{207}Pb/^{235}U$)—($^{206}Pb/^{238}U$).

In the subsequent Dezirteer releases we will implement another way to assess discordance: by measuring the Euclidean distance between ln (207Pb/206Pb) and ln(238U/206Pb) ratios, as suggested in (Vermeesch, 2020).

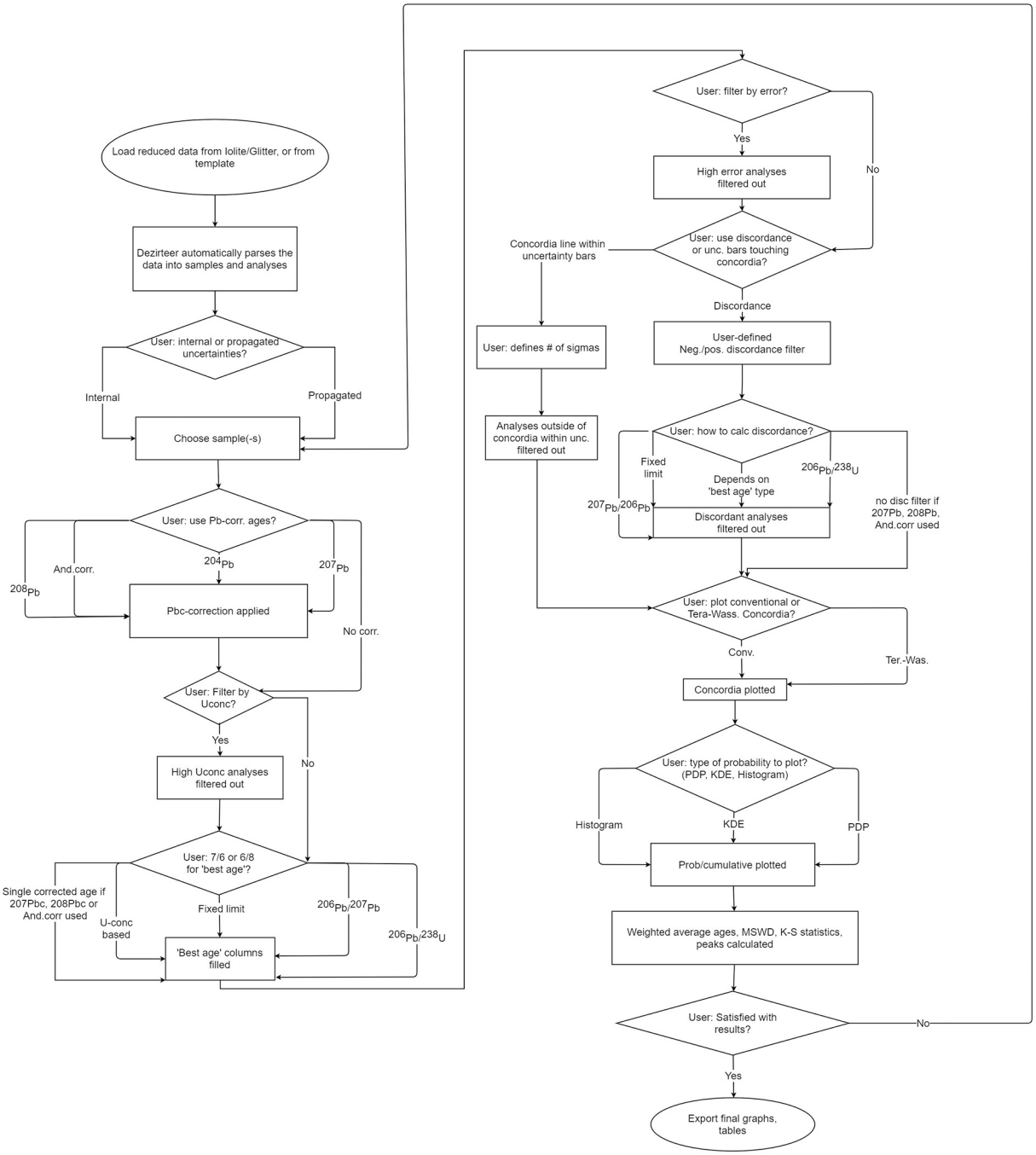

Fig. 3. Illustration of ***Dezirteer's*** workflow.

3.2.2. Data analysis

Data can be analyzed visually and numerically in ***Dezirteer***.

Plotting samples. In the current version of ***Dezirteer***, there are three types of plots available : concordia, probability, and cumulative probability. Concordia graphs are plotted as either conventional or Tera-Wasserburg. Ellipses can be plotted at 1σ (recommended) and 2σ. Individual analysis can be identified on plots by double-clicking on the correspondent line in the table.

Probability and cumulative probability functions can be plotted as KDE with user-defined bandwidth, PDP, and histograms with user-set bin width.

An option is provided to keep previous cumulative plots on screen, allowing easy visual comparison of datasets. In addition, Dezirteer can treat samples separately or join them into a dataset.

Statistics. Dezirteer provides a few statistical calculations to analyze and compare datasets. Samples can be compared by employing K—S statistics; Likeness and Similarity coefficients. Each plotted sample is statistically compared with the previously plotted one. "KS p- and d-val" correspond to K—S P and D coefficients; Likeness and Similarity coefficients are calculated according to Satkoski, Wilkinson, Hietpas, and Samson (2013), and Gehrels (2000), correspondingly.

—

3.3. Data and graphics export

Data are exported by pressing an 'export' button on the action pane as two .csv files. The first one contains all of the data; an additional column specifies whether each analysis passed or did not pass the set

criteria. Employed filters and computation parameters are shown below the data. The second file contains the PDP and KDE values for the age spectra from 0 to 4500 Ma, 1 Ma step. Plots can be exported to a variety of raster and vector formats.

3.4. Current productivity with big data

The productivity of ***Dezirteer*** in analyzing big data was tested in a series of experiments on a Windows-based PC equipped with an Intel Core i7-6820HQ Processor, 16GB of RAM, SSD hard drive. Productivity was measured as the time it took to do all necessary automatic calculations and plot 5000, 10 000, 20 000, and 40 000 analyses (Fig. 4). With the current version, the average time to process and plot one analysis is approximately 0.006 s. Processing of the largest, so far, database such as that of Voice, Kowalewski, and Eriksson (2011), containing ~ 200 000 analyses, will take approximately 20 min using a PC with mentioned performance characteristics. We are planning to optimize the code and substantially decrease these lags in the future versions of the software.

4. Few examples

We will illustrate the use of Dezirteer in assessing the effect various parameters might have on statistical coefficients and geological conclusions. In 5 small examples, we quantitatively compare dZr samples, varying only one parameter at a time, and measuring K—S *p*-value, Likeness, and Similarity coefficients, and, in one example, locations of age peaks on KDE curves.

The file with samples is included in Dezirteer installation package (/dezirteer/examples/iolite_example_with_204.txt) and can be reused by a curious reader. The dZr samples were collected at the Baikal-Patom fold-and-thrust belt, bordering Siberian Craton from the south. TS03, TS14, and TS16 were previously reported in (Powerman, Shatsillo, Chumakov, Kapitonov, and Hourigan, 2015) and belong to Padrinsky Group, Valyukhta, and Zherba Neoproterozoic Formations, respectively.

A few important observations can be made from this simple exercise (partly illustrated in Figure 5). Varying discordance filters can considerably affect the statistical coefficients (Table 1 and 2) and thus change geological interpretations significantly. For example, in Table 2 , K—S p-values dropped as low as 0.05 after loosening the requirements for discordance. Varying discordance filters also affect peaks locations (Table 5). Similarly, changing the calculation of best age from $^{206}Pb/^{238}U$ to $^{207}Pb/^{206}Pb$ (Table 4) and varying % error filter (Table 3) affects statistical coefficients.

By simply varying filtering criteria or 'best age' computation rules, it is entirely possible (and highly likely) to get drastically different statistical coefficients when comparing datasets, potentially resulting in various geological interpretations. Thus, when statistically comparing one dataset to another (e.g., own data with literature data), it is critical to apply the same filters and computations to all datasets.

5. Proposed routine for reporting LA-ICPMS data

To address the challenges summarized in the Introduction, we have defined the following guidelines to improve data robustness, increase the transparency of manipulations with data, and provide a step towards rapid analysis and interpretation of thousands (and potentially millions) of dZr ages.

Aside from the 'final' data table, containing reduced data after applying filtering and algorithms, each publication, in our view, should include:

1. Comprehensive reduction routines; all corrections and analyses exclusion criteria should be transparent. We strongly encourage attaching raw data files from mass spectrometers as supplementary materials.
2. Reduced data table, in editable format, produced by Glitter, Iolite, or a similar instrument (before any further processing, application of filters, and computations). Such data are importable to Dezirteer. Supplementary materials are probably the best place for these data.
3. Comprehensive filtering and computation routines, including rules for calculating the degree of discordance; the isotopic system used for 'best age'; rules for switching between the systems; common Pb correction type, if used; filters used to separate data into 'good' and 'bad' sets. Dezirteer allows applying and exporting these parameters along with processed data.
4. Final data tables with all analyses, including those that have not passed filtering criteria for 'best age' computation. Omitted analyses should be unequivocally marked as such. Dezirteer permits easy export of final data tables in this manner.
5. Final tables must possess sufficient information for the use of others. The following channels should be published: elemental concentrations (if measured); either isotopic ratios or ages derived from these ratios: $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, $^{207}Pb/^{206}Pb$; if measurements were done on isotopic counters rather than less sensitive Faraday cups, the following channels are highly desirable: $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$, $^{208}Pb/^{204}Pb$, $^{232}Th/^{204}Pb$, $^{238}U/^{204}Pb$, $^{204}Pb/^{202}Hg$; uncertainties, internal and propagated (if calculated) reported at 1 sigma. Optional channels include $^{208}Pb/^{232}Th$ (for 208Pbc and for Pb/Th ages), discordances, and ages.

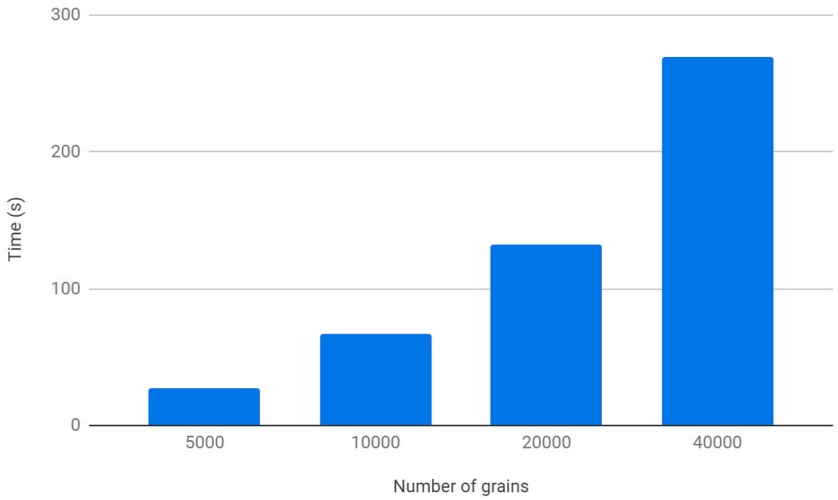

Fig. 4. Diagram illustrating the time required for ***Dezirteer*** to apply necessary filters and calculations and plot the results for the four sets of data.

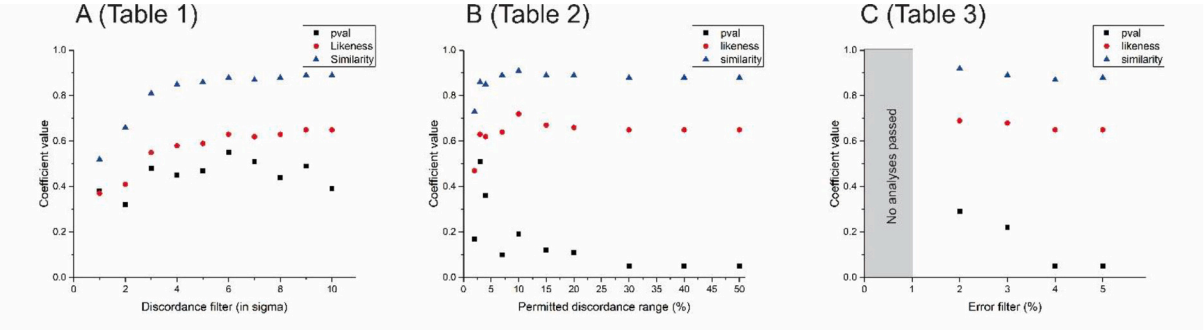

Fig. 5. Relationship between statistical coefficients (KS p-value, Likeness, and similarity) when comparing two datasets after applying filters. Correspond to Table 1, 2 and 3.

Table 1
Statistical comparison of Cumulative KDEs (CKDEs) from samples TS14, TS16 after applying various discordance filter values (uncertainty bars option) in Dezirteer. 'n' (here and further) – number of analyses; K—S p-value, likeness, and similarity coefficients discussed earlier in text.

Discordance filters	n_{ts14}, n_{ts16}	KS pval	Likeness	Similarity
1σ	10, 5	0.38	0.37	0.52
2σ	22, 10	0.32	0.41	0.66
3σ	30, 15	0.48	0.55	0.81
4σ	41, 20	0.45	0.58	0.85
5σ	48, 23	0.47	0.59	0.86
6σ	51, 25	0.55	0.63	0.88
7σ	57, 26	0.51	0.62	0.87
8σ	61, 27	0.44	0.63	0.88
9σ	62, 28	0.49	0.65	0.89
10σ	64, 29	0.39	0.65	0.89

Table 2
Statistical comparison of CKDEs from samples TS16 and TS03 after applying various discordance filter values (positive and negative % values).

Discordance filters	n_{ts16}, n_{ts03}	KS pval	Likeness	Similarity
-1% > d > +1%	18, 11	0.17	0.47	0.73
-1% > d > +2%	27, 17	0.51	0.63	0.86
−2% > d > +2%	33, 17	0.36	0.62	0.85
−2% > d > +5%	54, 26	0.10	0.64	0.89
−5% > d > +5%	69, 29	0.19	0.72	0.91
−5% > d > +10%	82, 34	0.12	0.67	0.89
−10% > d > +10%	83, 34	0.11	0.66	0.89
−10% > d > +20%	86, 37	0.05	0.65	0.88
−20% > d > +20%	86, 37	0.05	0.65	0.88
−20% > d > +30%	87, 37	0.05	0.65	0.88

Table 3
Statistical comparison of CKDEs from samples TS16 and TS03 after applying % error filter on both $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$. Discordant filter is kept constant at −20%, +30%.

Error filter	n_{ts16}, n_{ts03}	KS pval	Likeness	Similarity
1%	0, 0	No analyses passed through filtering		
2%	38, 17	0.29	0.69	0.92
3%	75, 32	0.22	0.68	0.89
4%	83, 36	0.05	0.65	0.87
5%	87, 37	0.05	0.65	0.88
No filter	87, 37	0.05	0.65	0.88

The latter rule yields a much simpler data table than the data-reporting template suggested in Horstwood et al. (2016) and concentrates on a bare minimum of needed information. Discordances and Tera-Wasserburg ratios can be calculated in ***Dezirteer***, a similar program, or an Excel spreadsheet. There is no need to publish both isotopic ratios and the ages derived from them; either one is sufficient for further data interpretation.

Table 4
Statistical comparison of same-sample CKDEs, calculated by $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ methods.

Sample	n_{68}, n_{76}	KS pval	Likeness	Similarity
TS14	73, 73	0.52	0.81	0.96
TS16	37, 37	0.99	0.73	0.92
TS03	87, 87	0.99	0.86	0.97

Table 5
Peaks ages in Ma, calculated by Dezirteer's routine, on the KDE curve (bandwidth = 50) for varying discordance filter (uncertainty bars option). Age calculated from $^{207}Pb/^{206}Pb$, no other filters used.

Sample	1σ filter	2σ filter	3σ filter	4σ filter	5σ filter	10σ filter
TS03	585, 1795. *N* = 8	607, 1753, 1839. *N* = 19	601, 1753, 1839, 2181. *N* = 26.	603, 1757, 1871, 2181. *N* = 35.	609, 1757, 1891, 2181. *N* = 47.	615, 1081, 1863, 2181, 2445. *N* = 70
TS14	591, 829, 1041, 2021. *N* = 10	799, 1381, 1885, 2017, 2551. *N* = 22.	785, 961, 1381, 1883, 2013, 2551. *N* = 30.	785, 1381, 1895, 2551. *N* = 41	781, 1217, 1381, 1725, 1893, 2551. *N* = 48	787, 1259, 1729, 1899, 2533. *N* = 64
TS16	623, 1911, 2227, 2525. *N* = 5.	633, 1893, 2227, 2525. *N* = 10.	645, 1893, 2227, 2509. *N* = 15.	643, 975, 1893, 2227, 2509. *N* = 20.	647, 975, 1915, 2225, 2509. *N* = 23.	651, 1917, 2225, 2509. *N* = 29.

Additional two rules are aimed at improving the ease of editing and parsing the published data:

6. Publish final data tables in an editable format (cvs, xls, xlsx, etc.) *in addition* to pdf tables so that data are easily accessible by spreadsheet software (PDF tables are not).
7. Make sample numbers separated from analysis numbers by one of the recommended symbols (underscore: '_', dash: '-', comma, or dot), allowing for easy parsing by **Dezirteer** or similar software.

The presented software, ***Dezirteer***, greatly simplifies data preparation in accordance with these rules. It allows rapid analysis of large data sets; choosing the desired filters and computations; visualizing results; calculating statistics; exporting data, filtering and computation parameters, and plots.

Data treatment in ***Dezirteer*** should happen after they are reduced in

Iolite or Glitter. The ideal workflow in our view should include the following steps:

● Recording the ICPMS signals by the instrument-specific software.
○ (optional, but desired) Publishing raw data files from ICPMS in Supplementary section.

● Reducing the collected data (in Iolite, Glitter, or similar software):
○ Importing data files;
○ Applying baseline, downhole and instrument drift corrections; calculating isotopic ratios and approximate elemental concentrations; propagating uncertanties;
○ Exporting data tables with ratios and concentrations. No 'best ages' should be assigned at this step.
○ Publishing exported tables with reduced data in the Supplementary Materials.
○ Publishing reduction routines (software used; detrending algorithms, corrections; integration regions and reasons for exclusion; channels exported).

● Applying filtering and computational logic to the reduced data (in **Dezirteer** or a similar instrument):
○ Importing reduced data;
○ Setting the rules on discrodance, best age and Pbc calculations and applying them to the dataset;
○ Setting the filters (degree of discordance, Pbc, Uconc, uncertainty) and applying them to the dataset;
○ Analyzing the effect of filtering and algorithms on results using plots and statistic;
○ Exporting final data tables with ratios, best ages, and logic used to filter and compute;
○ Publishing the resulting data tables with 'best ages' identified;
○ Publishing clear instructions on how the reduced data were filtered and how 'best age' columns were derived;

Following these rules, in our opinion, would greatly improve the reusability of published data by others, improve data trustworthiness, and open new horizons of big data approaches in dZr studies.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Required structure of Iolite-, Glitter- or template files to be imported to Dezirteer

Data are required to be in the comma-separated values format (.csv) and should meet several criteria to be flawlessly imported into ***Dezirteer***. Analyses names must possess proper separator symbols between sample and analysis numbers: underscore ('_'), hyphen ('-'), comma (','), or dot ('.'). This is essential for the program to group analyses into samples. For example, given the pool of analyses: [SB1_01, SB1_02, SB2_01, SB2_02] the software will recognize two samples (SB1 and SB2), each of which has two analyses (01,02). If no proper separation symbol is used (example: [SBA01, SBA02, SBB01, SBB02]), the program will not be able to group analyses into samples and will treat them as individual samples, each containing a single analysis.

Iolite (currently Iolite version 2.3 is supported; newer versions will be supported in coming releases of **Dezirteer)**. The following channels *must* be present in Iolite-reduced data files:

● Analysis name
● *Final206_238, Final206_238_Int2SE*;
● Final207_235, Final207_235_Int2SE;
● *Final207_206, Final207_206*_Int*2SE;*

In addition to the required channels, the following Iolite-produced channels can be used in Dezirteer:

● *U/Th ratios required to calculate 208Pb/232Th age, common Pb-corrected (208Pb and Andersen) ages: Final208_232, Final208_232_Int2SE*;
● Uranium concentration for use during filtering: *Approx_U_PPM, Approx_U_PPM_Int2SE;*
● *Pb204, Pb204_Int2SE*; this channel allows ***Dezirteer*** to apply ^{204}Pb common Pb correction.
● Error correlation between ^{206}Pb/^{238}U and ^{207}Pb/^{235}U systems: *ErrorCorrelation_6_38vs7_35*; if channel is absent, ***Dezirteer*** calculates the rho value.
● Error correlation between ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb systems: *ErrorCorrelation_38_6vs7_6*; if channel is absent, ***Dezirteer*** calculates the rho value.
● *Final206_204, Final206_204_Int2SE;*
● *Final207_204, Final207_204_Int2SE;*
● *Final208_204, Final208_204_Int2SE;*
● *Final232_204, Final232_204_Int2SE;*
● *Final238_204, Final238_204_Int2SE;*

Any propagated uncertainty: <channel_name>_Prop2SE.

Glitter. The following isotopic ratios and uncertainties are required to be present in Glitter-reduced data files:
● Analysis name.
● *Pb207/Pb206.*
● *Pb206/U238.*
● *Pb207/U235.*
Optional:
● *Pb208/Th232.*
● *Th232/U238.*

Template. The following isotopic ratios and uncertainties are required to be present in user-filled csv-template:

Required columns: Analysis name, 206Pb_238U, 207Pb_235U, 207Pb_206Pb, and 1 s (1σ uncertainty) for each column.
Optional columns: U(ppm), Pb204(ppm), 206Pb_204Pb, 207Pb_204Pb, 208Pb_204Pb, 232Th_204Pb, 238U_204Pb.

Appendix B. Algorithms

Calculation of ages and uncertainties:

$$^{206}Pb/^{238}U\ age = 1\Big/\lambda_1 \bullet \ln\left(^{206}\mathrm{Pb}/^{238}\mathrm{U} + 1\right)$$

$$^{207}\mathrm{Pb}/^{235}\mathrm{U}\ \mathrm{age} = 1\Big/\lambda_2 \bullet \ln\left(^{207}\mathrm{Pb}/^{235}\mathrm{U} + 1\right)$$

$$^{208}\mathrm{Pb}/^{232}\mathrm{Th}\ \mathrm{age} = 1\Big/\lambda_3 \bullet \ln\left(^{208}\mathrm{Pb}/^{232}\mathrm{Th} + 1\right)$$

where $\lambda_1 = 1.55125 \bullet 10^{-10}$, $\lambda_2 = 9.8485 \bullet 10^{-10}$ and $\lambda_3 = 4.9475 \bullet 10^{-11}$ year^{-1}, which are decay constants of ^{238}U, ^{235}U and ^{232}Th, respectively. ^{207}Pb/^{206}Pb age is estimated by solving this equation for age (t):

$$^{207}Pb/^{206}Pb = \left(e^{\lambda 2 \bullet t} - 1\right)\Big/\left(\mathrm{e}^{\lambda 1 \bullet t} - 1\right) \bullet \mathrm{k}$$

where k = 1/137.817 (Livermore, Connelly, Moynier, and Bizzarro, 2018).

Common formula for all Pb/U(Th) age uncertainties:

$$\sigma\ (\mathrm{t}) = (1/\lambda)^{*}\sigma(\mathrm{ratio})/(\mathrm{ratio} + 1)$$

$^{207}\mathrm{Pb}/^{206}\mathrm{Pb}$ age uncertainty

$$\sigma\ (\mathrm{t}) = \left[1/\mathrm{k}^{*}\sigma(\mathrm{ratio})\right]\Big/\left[\lambda_2 {*} exp.(\lambda_2 {*} \mathrm{t})\Big/(exp(\lambda_1 {*} \mathrm{t}) - 1) - \lambda_1 {*} exp.(\lambda_1 {*} \mathrm{t}) {*} (exp(\lambda_2 {*} \mathrm{t}) - 1)\Big/(exp(\lambda_1 {*} \mathrm{t}) - 1)^2\right]$$

Calculation of 'best' ages:

'Best' ages are derived from one of the two isotopic ratios — ^{207}Pb/^{206}Pb or ^{206}Pb/^{238}U. Currently there are four programmable options:

1. From the lesser error: for each analysis, the age with the lowest uncertainty (%) is chosen;
2. Fixed limit (Ma): User sets a value in Ma; if ^{206}Pb/^{238}U age < value, ^{206}Pb/^{238}U-derived age is chosen, else the ^{207}Pb/^{206}Pb age is used;
3. ^{207}Pb/^{206}Pb-derived ages for all analyses;
4. ^{206}Pb/^{238}U-derived ages for all analyses.

Calculation of Discordances:

Discordance can be calculated between two sets of ages:

1. Discordance between $^{207}Pb/^{235}U$ & $^{206}Pb/^{238}U$ ages: $D = (((^{207}Pb/^{235}U\ age)\ /(^{206}Pb/^{238}U\ age) - 1) \bullet 100.$
2. Discordance between $^{207}Pb/^{206}Pb$ & $^{206}Pb/^{238}U$ ages: $D = (((^{207}Pb/^{206}Pb\ age)\ /(^{206}Pb/^{238}U\ age) - 1) \bullet 100.$

Currently there are four options how Dezirteer chooses one of the two types of discordance for analyses:

1. Lesser of 2. In this option the program chooses the discordance with the smaller % value;
2. Fixed limit (Ma). User sets a value in Ma; if ^{206}Pb/^{238}U age < value, Discordance between $^{207}Pb/^{235}U$ & $^{206}Pb/^{238}U$ *is used;* ELSE Discordance between $^{207}Pb/^{206}Pb$ *is used;*
3. Discordance between $^{207}Pb/^{206}Pb$ & $^{206}Pb/^{238}U$ ages for each analysis;
4. Discordance between $^{207}Pb/^{235}U$ & $^{206}Pb/^{238}U$ ages for each analysis.

Common Pb corrections:

Calculated by pbc_corr function in the math_module. The function defines fraction (f) of common Pb in measured ^{206}Pb, ^{207}Pb *and* ^{208}Pb *isotopes*:

$f_{206} = (^{206}Pb/^{204}Pb)_c\ /\ (^{206}Pb/^{204}Pb)_m$,

$f_{207} = (^{207}Pb/^{204}Pb)_c\ /\ (^{207}Pb/^{204}Pb)_m$,

$f_{208} = (^{208}Pb/^{204}Pb)_c\ /\ (^{208}Pb/^{204}Pb)_m$,

where c and m indexes denote common Pb and measured isotope ratios, respectively. The value of radiogenic Pb/U and Pb/Th isotope ratios is then calculated from the next expression (in general form):

Radiogenic ratio = (1 - f) •(measured ratio).

Radiogenic Pb/Pb ratio can be defined as:

$(^{207}Pb/^{206}Pb)_r = (1 - f_{207})\ /\ (1 - f_{206})\ \bullet(^{207}Pb/^{235}U)_m\ /\ (^{206}Pb/^{238}U)_m\ \bullet\ ^{235}U/^{238}U.$

or

$(^{207}Pb/^{206}Pb)_r = (^{207}Pb/^{235}U)_r\ /\ (^{206}Pb/^{238}U)_r\ \bullet\ ^{235}U/^{238}U,$

where r index denotes radiogenic isotope ratio.

Andersen method assumes the initial concordance of all isotope ratios of the U-Th-Pb system. True age (t1 - upper intercept age) of mineral is defined by solving eq. (7) in Andersen, 2002.

Dezirteer's Pbc calculated values are in a good correspondence with those calculated on the same datasets with Isoplot and ComPb. Comparison

tables are in Appendix 4.

Probability functions (KDE/PDP/Histogram) and cumulative probability functions:

A probability density plot (PDP) is a density plot of probability density function (PDF):

$PDF(x) = 1/N * \Sigma_{i=1}^{N} \exp.((x_i\text{-}x)^2/(2\sigma_i^2))/(\sigma_i * \mathrm{sqrt}(2\pi))$.

where x_i and σ_i is the i-th measurement of age (of the certain sample) and their uncertainty, which is an expectation/mean of Gaussian function, x is the age variable, N - total number of measurements.

The cumulative probability density function (CPDF) or simply cumulative distribution function (CDF) is given as:

$CDF(x) = \Sigma_{xj<x}^{N} PDP(x_j)$.

Kernel density estimation:

$KDE(x) = 1/(Nh) * \Sigma_{i=1}^{N} K((x\text{-}x_i)/h)$.

where K is the kernel, h - bandwidth, x_i is the i-th measurement of age (of the certain sample), N - total number of measurements. In the present program Gaussian kernel is only used:

$K(t) = \exp.(-t^2/2)/(2\pi)$.

The value of h is user-defined.

Weighted average age, MSWD:

Weighted mean is calculated as:

$\underline{x} = \Sigma_{i=1}^{N} w(x_i)\, x_i$.

where x_i is the i-th measurement of age (of the certain sample), $w(x_i)$ is the weight of x_i, N - total number of measurements. The weight is:

$w(x_i) = \sigma_i^{-2} / \Sigma_{i=1}^{N} \sigma_i^{-2}$.

where σ_i is the i-th age measurement uncertainty.σ.

Mean square of weighted deviations (MSWD):

$MSWD = 1/(N\text{-}1) * \Sigma_{i=1}^{N} (x_i\text{-}\underline{x})/\sigma_i^2$.

Kolmogoroff-Smirnov statistics:

Maximum distances between empirical cumulative distribution functions of two samples:

$D = \sup|CDF_1(x)\text{-}CDF_2(x)|$.

Equivalent size of samples:

$Ne = N_1N_2/(N_1 + N_2)$.

where N_1 and N_2 are the sizes of samples.

The significance of D or "P" value (the probability that two samples from the same population):

$P = 2\, \Sigma_{k=1}^{\infty} (-1)^{k-1}\exp(-2k^2\lambda^2)$,

where $\lambda = D*\mathrm{sqrt}(N_e)$.

If the *P*-value is higher than 0.05 significance level, there is a 95% confidence that the difference between two samples is not significant.

Likeness coefficient:

As per Satkovski et al., (2013), Likeness, or L, represents "the percent of "sameness" between two unitized PDPs, and is calculated as one minus the summation of absolute differences between all PDP values divided by 2.

$L = 1 - (\Sigma_{i=1}^{N} |a_1\text{-}b_1|/2)$.

N is the number of ages in both probability density functions; a, b are the y-axis values for any given age i. Values approaching 100% correspond to a high degree of likeness between two distributions.

Similarity coefficient:

The Similarity coefficient measures whether samples have overlapping modes, and similar proportions in each mode. Gehrels (2000) defines it as.

$S = \Sigma_{i=1}^{N} \mathrm{sqrt}(f(i)g(i))$.where f (i) and g(i) are the PDPs or KDEs and i are ages between 1 and n. A value of 1 indicates samples that are perfectly matched both in the modes and modal proportions, while a value of 0 indicates that the two samples share no modes.

Peaks and their statistical weight:

Peaks are recognized by simple algorithm: If the following condition is true:

$(PDF(x_{k\text{-}1}) < PDF(x_k) > PDF(x_{k+1}))$,

where $x_{k\text{-}1} < x_k < x_{k+1}$.

then x_k variable is the peak age of PDF.

Statistical weight of a peak (number of age measurement per peak) is defined on the basis of the following condition:

$x_i - 2\sigma_i < (\text{peak age})_n < x_i + 2\sigma_i$.

where x_i and σ_i is the i-th measurement of age (of the certain sample). If it is true, then x_i makes a significant contribution to the n-th peak.

Decay constants.

By default, the software uses for the age calculations ^{235}U and ^{238}U decay constants as recommended by [Steiger and Jager, 1977]. Any changes in the decay constant of ^{235}U and ^{238}U are expected to be insignificant for the practical reasons of dating of dZ by the LA-ICPMS. For the decay constant of ^{232}Th we use the value obtained by [Amelin and Zaitsev, 2002] via comparison of $^{206}Pb/^{238}U$ and $^{208}Pb/^{232}Th$ dates for zircon and baddeleyite. For the $^{238}U/^{235}U$ ratio we use the refined value of [Livermore, Connelly, Moynier, and Bizzarro, 2018]; this can be manually overridden in the const.py file.

Error correlations coefficients (rho).

If error correlation values are not reported in imported files, Dezirteer calculates them following (Gerdes and Zeh, 2006):

corr_coef_75_68 = (rat68err / rat68) / (rat75err / rat75).

corr_coef_86_76 = (rat68err / rat68) * (rat76 / rat76err).

In case if any correlation coefficient results in value >1, Dezirteer inverts such value.

if corr_coef >1: corr_coef = 1 / corr_coef

Appendix C. Software installation and instructions

Installation instructions.

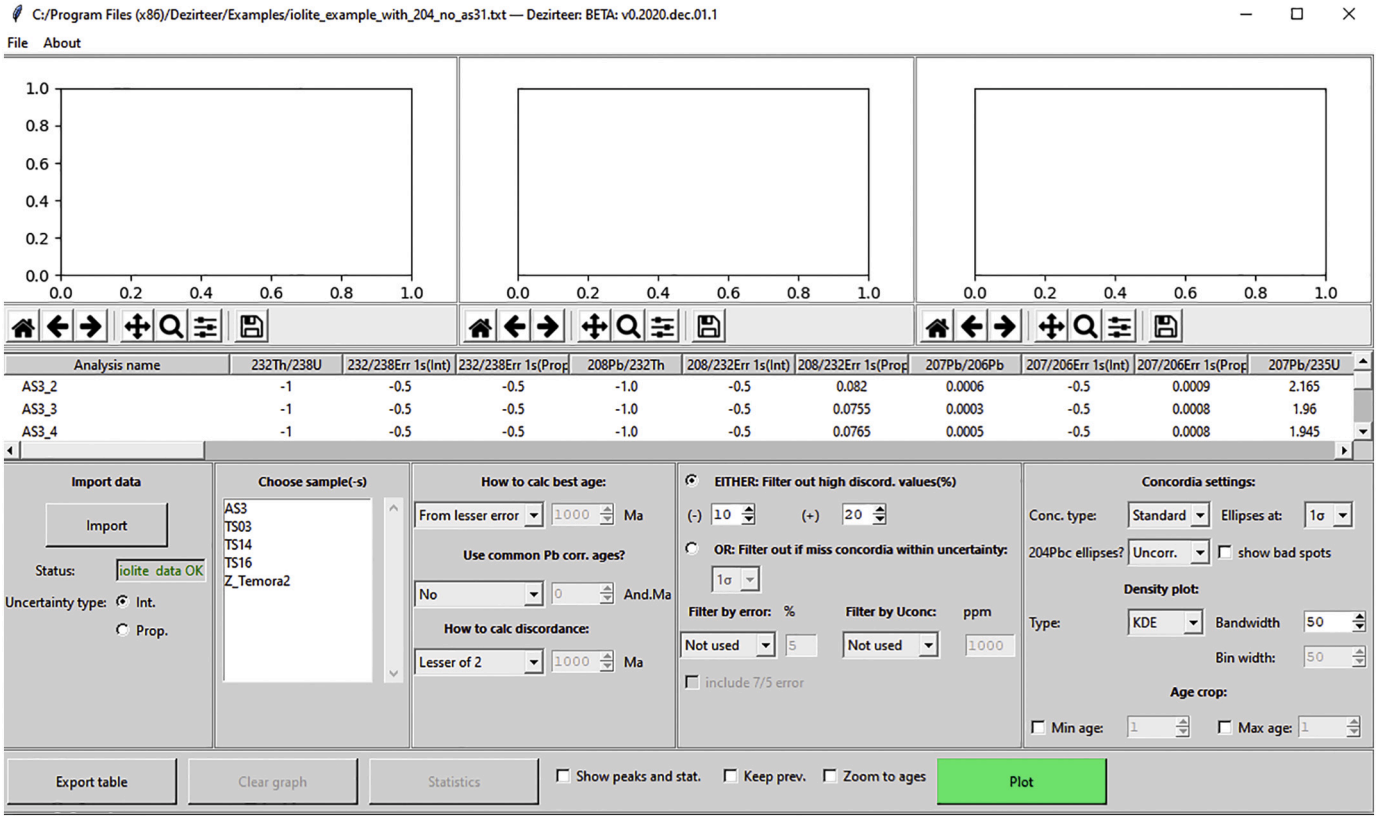
There are 2 ways to install Dezirteer: as a Python package, and as a Windows executable file.

Python package requires Python (version≥3.5). Installation is done by cloning the GitHub repository (https://github.com/dazdraperma/dezirteer) and running the command "python main_gui.py". In order to use it in a Python environment, the following modules should be installed: Scipy, Numpy, Matplotlib, Tkinter, Math.

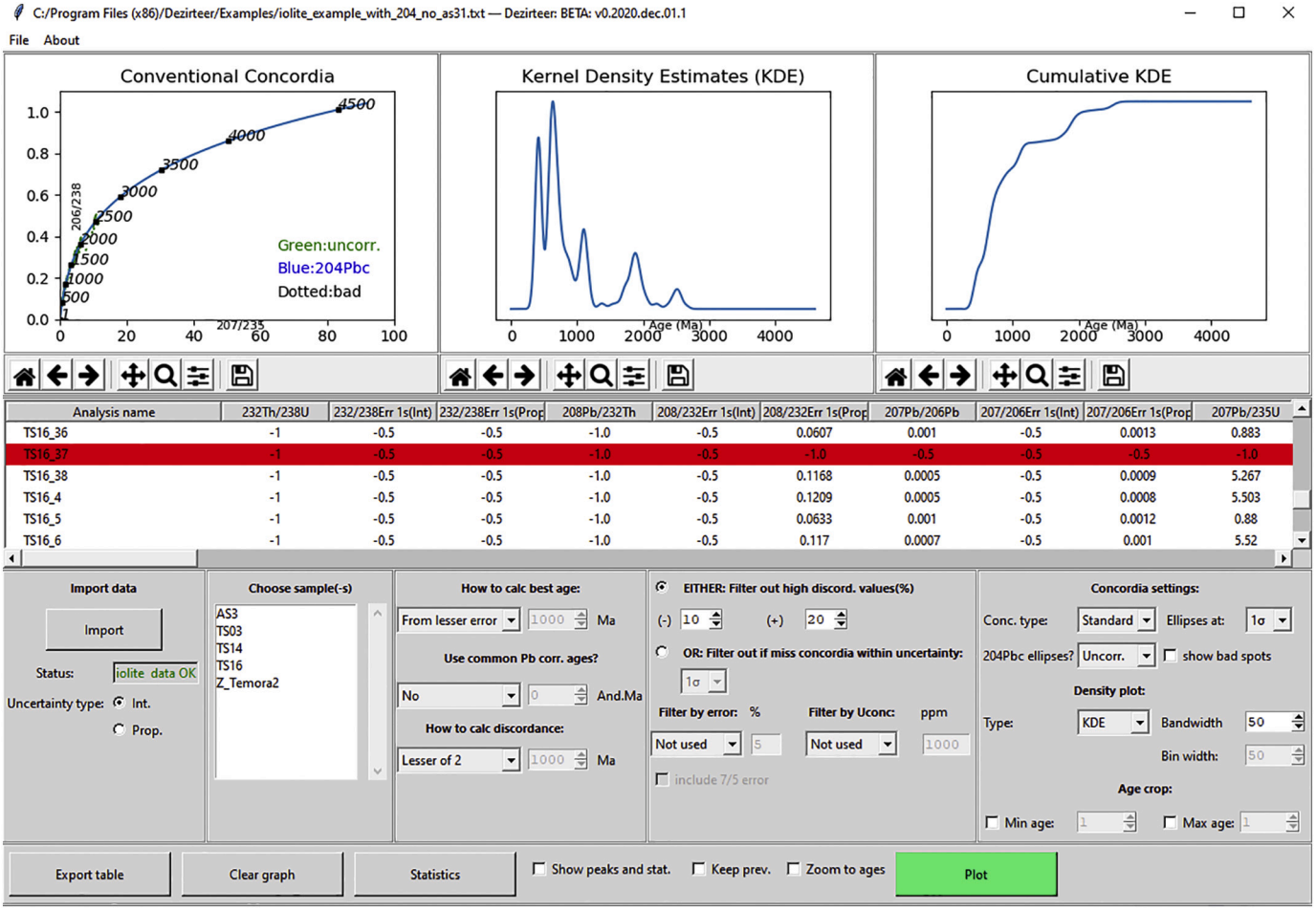
The executable installation file is available for download from http://dezirteer.com/downloads. It runs on 64-bit Windows 10 (if we get requests, we will create similar installation files for other versions of Windows). Currently, the installation file has not been signed, therefore users might get warnings during download and installation. Please ignore such warnings, Dezirteer is perfectly safe for your system. In the future, we are planning to purchase proper software signing to avoid such problems.

Sample workflow

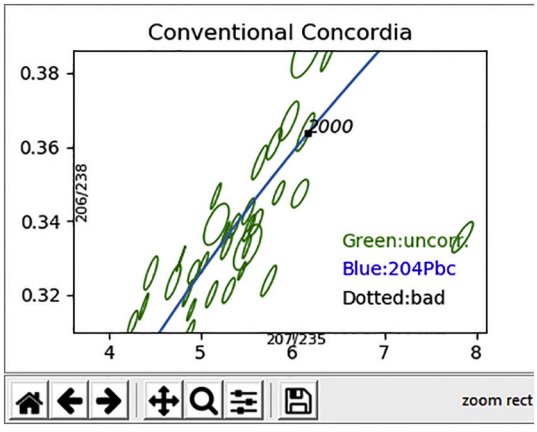
- Install Dezirteer on a Windows 10 OS.
- Open dezirteer.exe from the installed folder (by default: c:\program files (x86)\Dezirteer\)
- Press "import". A default folder (/examples) opens.
- Choose any of the three files: "glitter_example.txt", "iolite_example.txt", "template_example.csv". If any of these files is not visible, choose "all files" option in the lower right of the dialog. The following example is based on the "iolite_example.txt".
- Data is loaded into the table; listbox with sample names is populated:



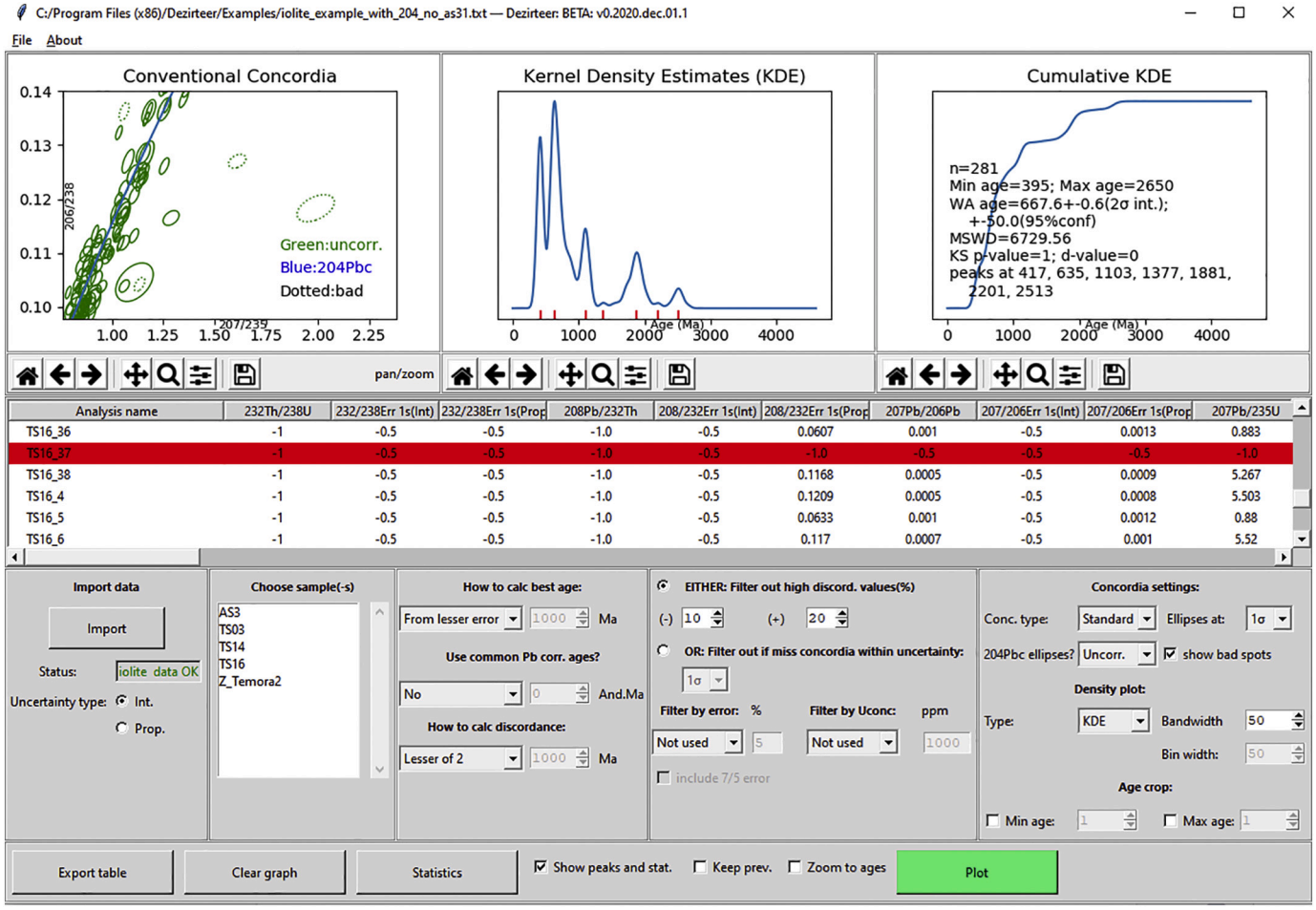
- Choose any sample from the "Choose sample" listbox by clicking on it.
- Press "Plot" button. Result: (1) analyses that have been filtered out are not graphed and are highlighted by red in the table; (2) concordia, probability and cumulative probability diagrams are plotted:



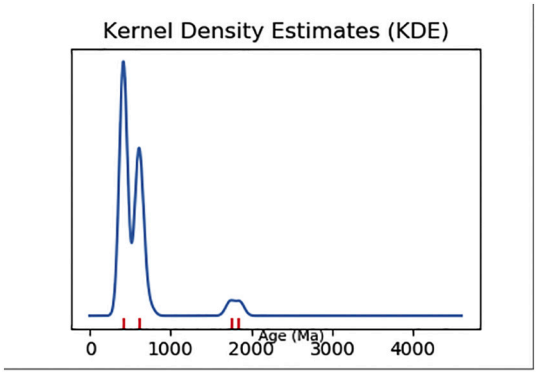
- Use the magnifying glass button to zoom into a graph. Return to the initial view by pressing the “home” button.
- Check “show bad spots” to see discarded analyses:



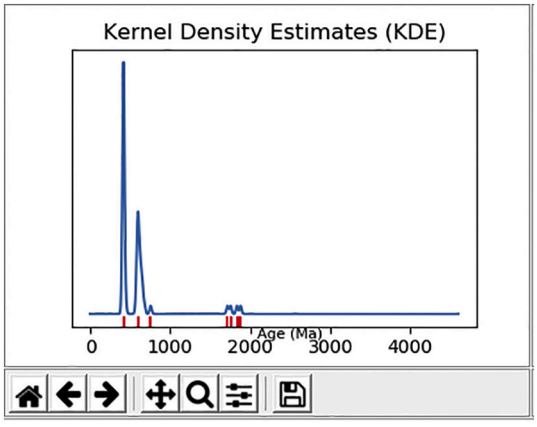
Check “show peaks and stat.” checkbox. Result: (1) in the probability diagram peaks are shown; (2) limited statistical data is plotted in the cumulative diagram:



- Try changing filtering and computational settings: best age rules, discordance calculation. Press “Plot” button again to plot the updated data.
- Zoom in on the plots by pressing the magnifying glass button, return to the initial view by pressing “home” button.
- Change KDE bandwidth; see how it affects the distribution.

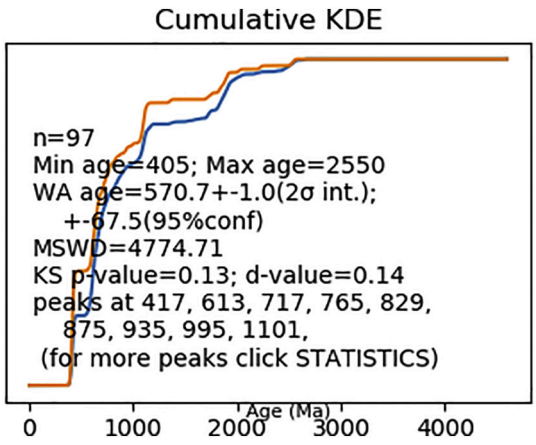


Bandwidth = 50

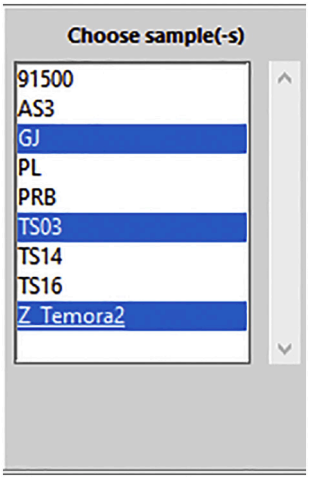


Bandwidth = 13

- Change probability diagram type to PDP or Histogram.
- Plot as KDE again. Check the checkbox “keep prev.” (to keep the graph once the next one is plotted). Click on another sample in the “choose sample” listbox. Press “(re-)draw” button. Results: (1) two samples are plotted; (2) K—S statistics is shown on the Cumulative plot.



- Press "import" again. Choose another file. Once prompted, answer "yes" to keep the previous file. Result: table and listbox is populated with both data files. Now you have the option to compare data from two sources.
- Uncheck the "keep prev." checkbox to clear the graph.
- Choose several samples in the listbox by clicking on them while holding the "ctrl" button pressed. Result:



- Press the draw button. Result: several samples are combined into one and plotted as one.
- Save a session (menu: file → save session).
- Continue exploring the data. Once happy with it, press "export table". In the dialog, choose a destination folder.
- Press the "save" (diskette) buttons on the plots to save graphics.
- Go to the destination folder. You should see the following files: name.csv, name_prob_cum.csv. The first file has the exported table and information about used filters and computations. The second one has probability and cumulative probability data.
- Open the first table in Excel.
- Find the column "is grain good?"
- Sort by the values in this column. Now you have "true's" and "false's" combined. "True's" stand for the analyses that passed your set filters; "false's" didn't pass.
- Find the column "best age system". "0" stands for age calculated from $^{206}Pb/^{238}U$, "3" for $^{207}Pb/^{206}Pb$.
- Go to the table's bottom. It has information about filters and computations.

Appendix D. Relating Dezirteer's computations to other instruments

Table A4. Comparison of common Pb correction algorithms between Dezirteer, Isoplot and ComPbn
A4.i: Dezirteer vs Isoplot, ^{204}Pbc.
A4.ii: Dezirteer vs Isoplot, ^{207}Pbc.
A4.iii: Dezirteer vs Isoplot, ^{208}Pbc.
A4.iv: ComPb, Andersen-correction; U238_U235 = 137.88; LAMBDA_232 = 4.9475E-11, U238_U235 = 137.88.
A4.v: Dezirteer, Andersen-correction; U238_U235 = 137.88; LAMBDA_232 = 4.9475E-11, U238_U235 = 137.88.
A4.vi: Dezirteer, Andersen-correction; LAMBDA_232 = 4.934E-11, U238_U235 = 137.817.

A4.vii: Dezirteer vs Intercept age offsets.

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