jAgeDisplay: software for evaluation of data distributions in U-Th-Pb geochronology

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During the past 10–15 years, analytical innovations in geochronology have greatly enhanced the application of geochronological data to geological problems. The advances are mainly driven by developments in laser ablation inductively coupled plasma mass spectrometry (LA-ICPMS) which allows for rapid determination of U-Th-Pb ages of mineral grains in large sample sets. LA-ICPMS has now become the most common tool in the application of zircon geochronology to a host of different geological problems.

One of the most regularly used approaches to evaluate complex U-Th-Pb geochronological data populations is to use a diagram that combines a binned frequency histogram and a probability density distribution plot (PDP), as described by Sircombe (2004) and Ludwig (2003). This type of diagram is particularly common in sedimentary provenance studies using large sets of age data (Morton *et al*. 1996; Pell *et al*. 1997; Rainbird *et al*. 1997; Sircombe 1999; Fergusson *et al*. 2001). It is also useful for the analysis of complex age patterns in metamorphic and igneous rocks. The Microsoft Excel workbook AgeDisplay (Sircombe 2004) has often been used to produce these diagrams but it is not supported by versions of Excel that are newer than 2003. Stand-alone software for PC written in Java was therefore developed by the Geological Survey of Denmark and Greenland (GEUS). It is based on the same formulae as described in Sircombe (2004), thus the name jAgeDisplay (with j for Java), and has additional features and graphic improvements. Here we present the setup, operation and capability of the software with examples from single-grain U/Pb age data obtained by LA-ICPMS spot analysis.
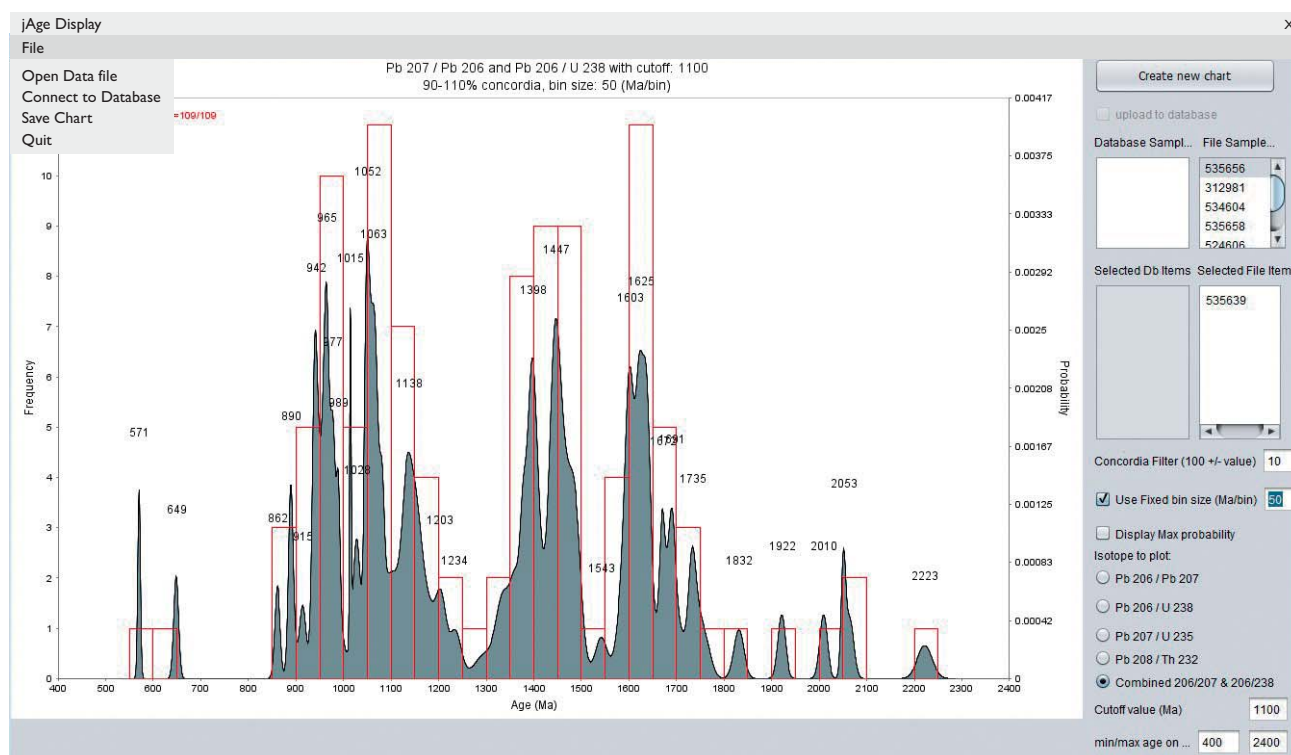

Fig.1. Combined 400–2400 Ma histogram and PDP chart with calculated maximum probability ages for distinct distribution peaks of zircon populations from a single sample, using coupled ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb age pairs. A crossover age of 1100 Ma is used, where ^{206}Pb/^{238}U ages and ^{207}Pb/^{206}Pb ages are used below and above this age, respectively. A *Fixed bin size* of 50 Ma/bin and a *Concordia Filter* of ±10% were used.

Setup and operation of jAgeDisplay

The jAgeDisplay package (current version 1.0) for PC includes an executable Jar file, a Java MS DOS batch file, a HTML readme file, a brief manual and a folder with test data files. The application is available as shareware from the corresponding author, and it is installed by copying the files you receive to any PC with Java.

jAgeDisplay supports both comma-separated (CSV) and tab-delimited (TAB) input text files, with the same table headers and data types as in AgeDisplay, Iolite (Paton *et al.* 2011), and GEUS' in-house Zirchron software and database. The input file can include age data from one or more samples, which are loaded from the *File* menu in the main window (Fig. 1) using the *Open Data file* option. The input file includes four commonly used radiogenic U-Th-Pb age pairs, viz. $^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, $^{207}Pb/^{206}Pb$ and $^{208}Pb/^{232}Th$, together with the sample identification, the name or number of individual analyses, the name of the analytical sequence and information about correction for common lead content. Output charts can be saved in PDF or PNG file format through the *Save Chart* option in the *File* menu.

The main window consists of a chart area to the left and the selected sample parameters to the right. When an input file has been loaded, the samples available for plotting are found in the *File Samples* field or, if loaded from a database, in the *Database Samples* field. To plot one or more of the loaded samples, they are dragged and dropped in their respective *Selected File Items* or *Selected Db Items* fields. The parameters to be used for the chart are selected, and the *Create new chart* button is pressed.

Combined histograms and probability–density plots for each radiogenic age pair ($^{206}Pb/^{238}U$, $^{207}Pb/^{235}U$, $^{207}Pb/^{206}Pb$, $^{208}Pb/^{232}Th$) can be produced. In addition, charts combining the $^{206}Pb/^{238}U$ and $^{207}Pb/^{206}Pb$ age pairs can be made by manually setting a specific age (denoted *Cutoff value*) that controls the change from using $^{206}Pb/^{238}U$ ages for the younger age range to $^{207}Pb/^{206}Pb$ ages for the older age range of the chart (Fig. 1). The frequency in terms of number of analyses for each bin in the histogram is shown on the left y-axis, and the calculated probability distribution of zircon ages for the data set on the right y-axis. Thus, the probability–density distribution provides an estimate of the true mineral-age distribution for a given rock sample.

The plots can be adjusted by the following parameters:
* *Concordia Filter* is the maximum allowed discordance (in per cent) for analyses to be considered as concordant, and is determined as 100 ± Set#Value. This separates the age data used for the plot into two different fields representing 'concordant' and 'discordant' data. In detrital zircon provenance studies a value of ±10% is often used, where this threshold is used as a measure of the quality of the calculated ages. In contrast to AgeDisplay, the complete data set including the 'discordant' data is not shown behind the 'concordant' data, but separately using the same axis as for the concordant data.

* *Use Fixed bin size (Ma/bin)* allows a histogram of filtered ages to be plotted (based on the concordant data obtained via the *Concordia Filter*), where the bin size in million years (Ma) is manually chosen. If this checkbox is deselected, a calculated value for the bin size is used, based on the formulae in Doane (1985).

* *Display Max Probability* (checkbox) shows the ages of the calculated probability peaks for the 'concordant' data set.

* *Min/Max age* controls the age range to be shown in the chart.

Additional parameters can be set through right-clicking on the produced chart, where the title, chart title, axis range, appearance and colours can be modified.

jAgeDisplay can display a single chart for one data set or stacked charts of several data sets (Fig. 2). Stacked charts are useful for comparison of data sets sampled, e.g. at different geographical, stratigraphical or lithological locations in order to identify trends or differences in the age distributions. The stacking follows the order chosen in the *Selected File Items* (or *Selected DB Items*) window at the right, and can be rearranged as appropriate. As the purpose of stacking is to compare, the stacked data sets are displayed for the same age range as set by the *Min/Max age* control.

Use of jAgeDisplay in sedimentary provenance and petrological studies

Detrital studies typically aim to characterise the age population(s) from a sample by means of a large number of single grain analyses, e.g. obtained by LA-ICPMS. In statistical terms the goal of such studies is to estimate the so-called probability density function that gives the relative *likelihood* of the different ages in the population (Vermeesch 2012). Zircon is the most common mineral used for detrital studies, but other mineral phases like rutile and titanite are increasingly being employed in order to obtain supplementary information (e.g. Zack *et al.* 2004; Stendal *et al.* 2006; Meinhold *et al.* 2008; Thomsen *et al.* 2015;
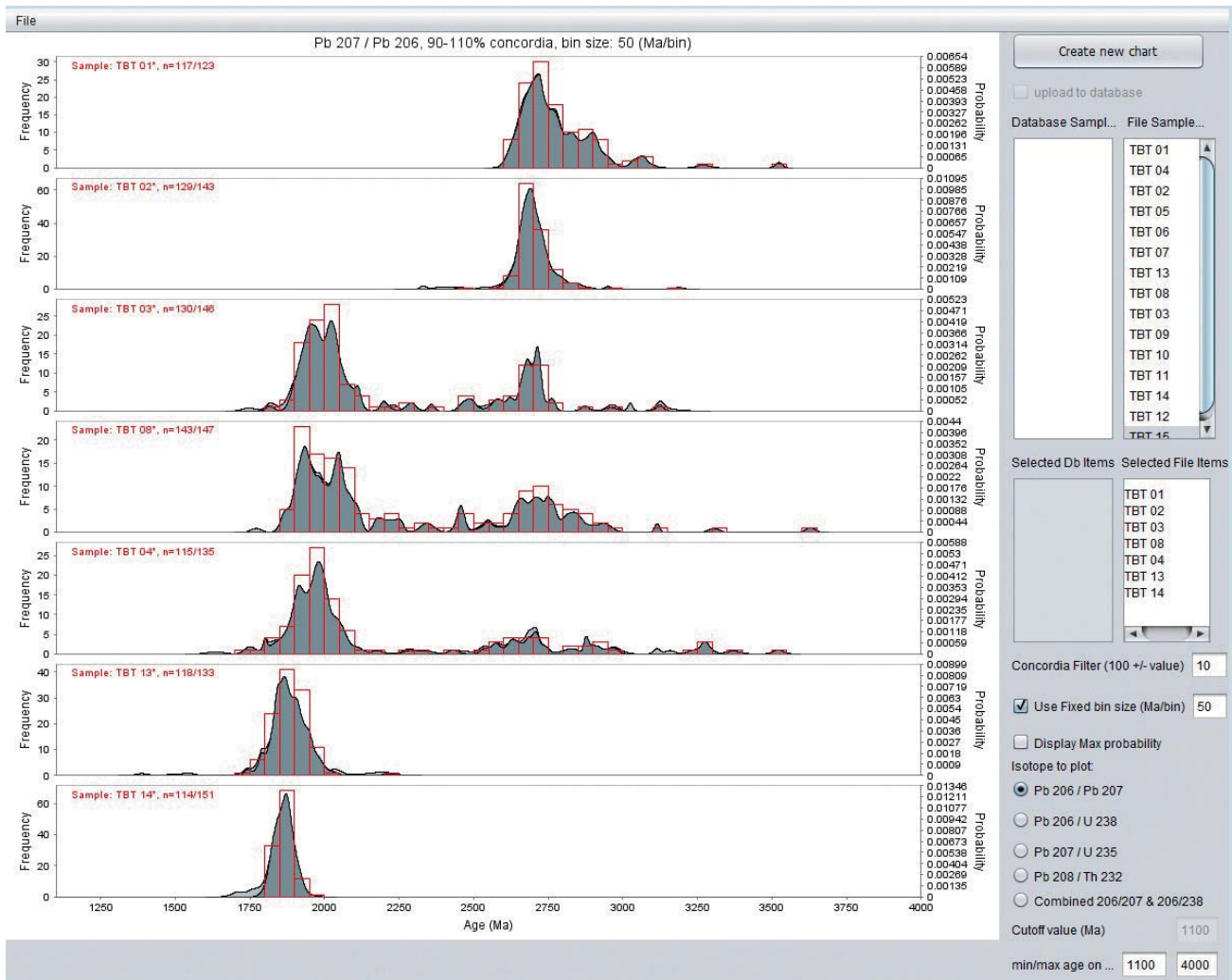
Fig. 2. Stacked chart of combined histograms and PDP charts from 1100 to 4000 Ma of zircons from seven samples using ^{207}Pb/^{206}Pb ages, a *Fixed bin size* of 50 Ma/bin and a *Concordia Filter* of ±10%.

Bruand *et al*. 2016). Signatures of sediment sources not represented in the zircon data set may be present in detrital titanite, rutile or apatite populations. In addition, age data on these minerals may provide further chronological and petrogenetic insight into the tectono-thermal history of their source regions (e.g. McAteer *et al*. 2010, 2014; Knudsen *et al*. 2015; Thomsen *et al*. 2015). Similarly, in metamorphic and magmatic petrology, complex zoning patterns that correspond to distinct geological events can be recorded in zircon, baddeleyite, titanite, rutile, apatite, monazite, xenotime, allanite or any other accessory mineral phase for which the age can be determined by U-Th/Pb methods and can be assessed in probability density plots diagrams through the jAgeDisplay software.

Future options in jAgeDisplay

Although PDPs constitute the most widespread method used today for displaying detrital age distributions, they lack a firm theoretical basis as probability density estimators, and this may produce counter-intuitive results when the number of analyses and/or their quality (precision) is high (Vermeesch 2012). Accordingly, an alternative and robust standard statistical technique, the Kernel Density Estimation (KDE) as described in Vermeesch (2012), will be included in jAgeDisplay, so that users can compare the two methods. We also expect to include a more versatile option for age distribution plots, where any two isotopic pairs can be used in a PDP or KDE diagram, in a similar way as the built-in option for combined ^{206}Pb/^{238}U and ^{207}Pb/^{206}Pb age distributions.

Detailed statistics reporting information on the calculated maximum probability peaks can be useful for improved age differentiation of, e.g. magmatic or metamorphic episodes. At present, this information is only indirectly reported through the plot axis. We expect to include this information in pop-up windows for single peaks and as a print-out option including the statistics of all peaks or a chosen age section of the plot.

Finally, the jAgeDisplay software offers an option to load input files from a database through a local server connection (*File => Connect to Database*). At present, this option only allows reading of certain data types from GEUS' Oracle server. It is our intention to expand this and thus provide users with access to data from a local server repository.

Additional remark

In this presentation only U/Pb geochronological data obtained by LA-ICPMS analysis on zircon are used. jAgeDisplay can of course also evaluate U-Th-Pb data acquired by other instrumentation and complex age distribution patterns measured from other accessory phases such as titanite, rutile, apatite, monazite, allanite, perovskite, xenotime or other minerals that can incorporate U or Th into their crystal structure.

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