Supplementary Information to: **DQPB: software for calculating U-Pb disequilibrium ages** by Timothy J. Pollard, Jon D. Woodhead, John C. Hellstrom, John Engel, Roger Powell, and Russell N. Drysdale

DQPB v0.0.1 USER GUIDE

html and pdf versions of this document will be made available for download from the DQPB GitHub repository. These online documents will be updated to reflect future changes to the software.

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1. Overview

DQPB is a GUI application for geochronology that focuses on calculating disequilibrium U-Pb ages and plotting results, although it can also be used for computing standard equilibrium U-Pb ages, performing linear regression and computing weighted averages. The software allows isotopic data to be read directly from open Microsoft Excel spreadsheets, and results (both graphical and numerical) printed back to the same sheet once computations are completed. In this way, it aims to emulate the ease of use of Ken Ludwig's popular Isoplot/Ex program. The program is distributed on Windows and macOS as a stand-alone application that does not require a pre-existing Python installation to run.

DQPB can be used to:

- Calculate disequilibrium U-Pb concordia-intercept ages on a Tera-Wasserburg diagram
- Calculate disequilibrium ^{238}U-^{206}Pb and ^{235}U-^{207}Pb isochron ages
- Calculate disequilibrium ^{206}Pb/^{238}U and ^{207}Pb/^{235}U (single analysis) ages
- Calculate modified ^{207}Pb ages using an approach similar to Sakata (2018)
- Calculate initial equilibrium U-Pb ages using the above approaches
- Compute "concordant" initial [^{234}U/^{238}U] values from isochron age data using the routine described in Engel et al., (2019)
- Perform linear regression using algorithms that are based on classical statistics (i.e., the model 1, 2, and 3 popularised by Isoplot (Ludwig, 2012), or robust statistics (i.e., the spine algorithm of Powell et al., (2020) and a new "robust model 2" algorithm).
- Compute weighted averages that optionally account for error covariances using both classical and robust algorithms
- Plot data points and disequilibrium concordia curves on a Tera-Wasserburg diagram

The functionality of DQPB is also available as part of a pure Python package for more experienced Python users. For this version, see the pysoplot GitHub page.

2. Installation

The easiest way to install DQPB on macOS and Windows is to simply download the latest installer from the GitHub DQPB releases page. These installers provide a stand-alone version of the software, that does not require a separate Python installation.

Mac

1. Download the Mac .dmg installer
2. Open the .dmg and drag the DQPB.app icon into your Applications folder to install the software.
3. Navigate to your Applications folder.
4. Right-click on the icon and select "Open" to launch the Application for the first time.

Note: the application will not launch if you double-click on the icon the first time you try to open it. You must right-click and select 'Open'.

5. A security message may pop up saying that this file is from an "unknown developer" and asking if you wish to continue. DQPB is open-source software distributed free of charge, so we have opted not to pay fees to Apple to codesign the application. Therefore, this warning cannot be avoided.
6. When running DQPB for the first time, you will probably be asked to give permission to DQPB to "control Excel". You must click OK, otherwise DQPB will not be able to read data from Excel spreadsheets and the application will not function.

Windows

1. Download the Windows .exe installer
2. Launch the installer and follow the usual steps to install the software.
3. When opening the installer, a Windows Defender warning may pop up informing you that this is an "unrecognized" app. DQPB is open-source software distributed free of charge, so we have opted not to pay fees to Microsoft or other third parties in order to codesign the application. Therefore, this warning cannot be avoided. Click the 'More info' link, then click 'Run anyway'.
4. The application can now be launched from the start menu. If for some reason the icon does not appear, go to the installation directory (usually C:\Program Files\DQPB\) and double-click the DQPB.exe icon. A shortcut to this .exe file may then be manually added to the start menu or another location.

3. Verifying Installation

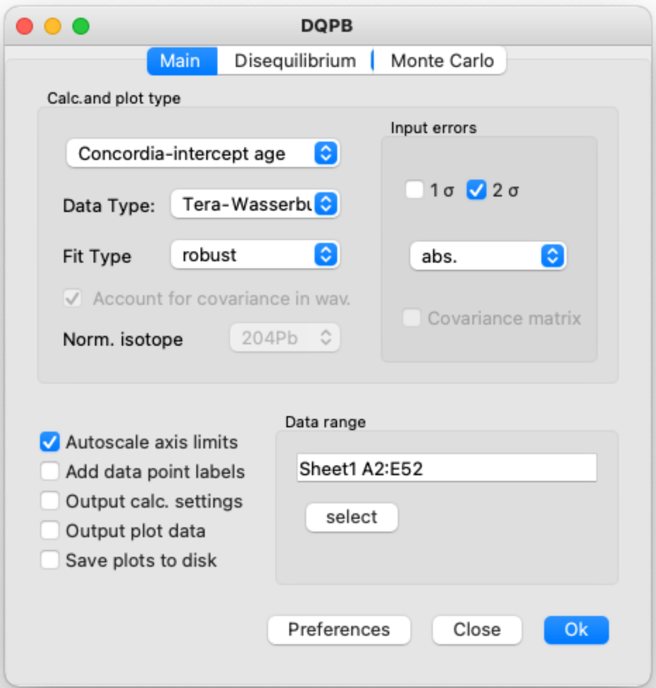
To verify that the installation was successful and explore software features, test data sets may be downloaded from the DQPB Github page.

4. Uninstalling DQPB

- On Mac, simply delete DQPB.app from you Applications folder.
- On Windows, go to the “Add or remove programs” dialog. Click on the DQPB icon and select “Uninstall”.

5. Basic usage

Begin by double clicking on the application icon to launch the main application window. If running DQPB for the first time on Mac, you may need to right-click on the application icon and click ‘Open’.



Main window on Mac

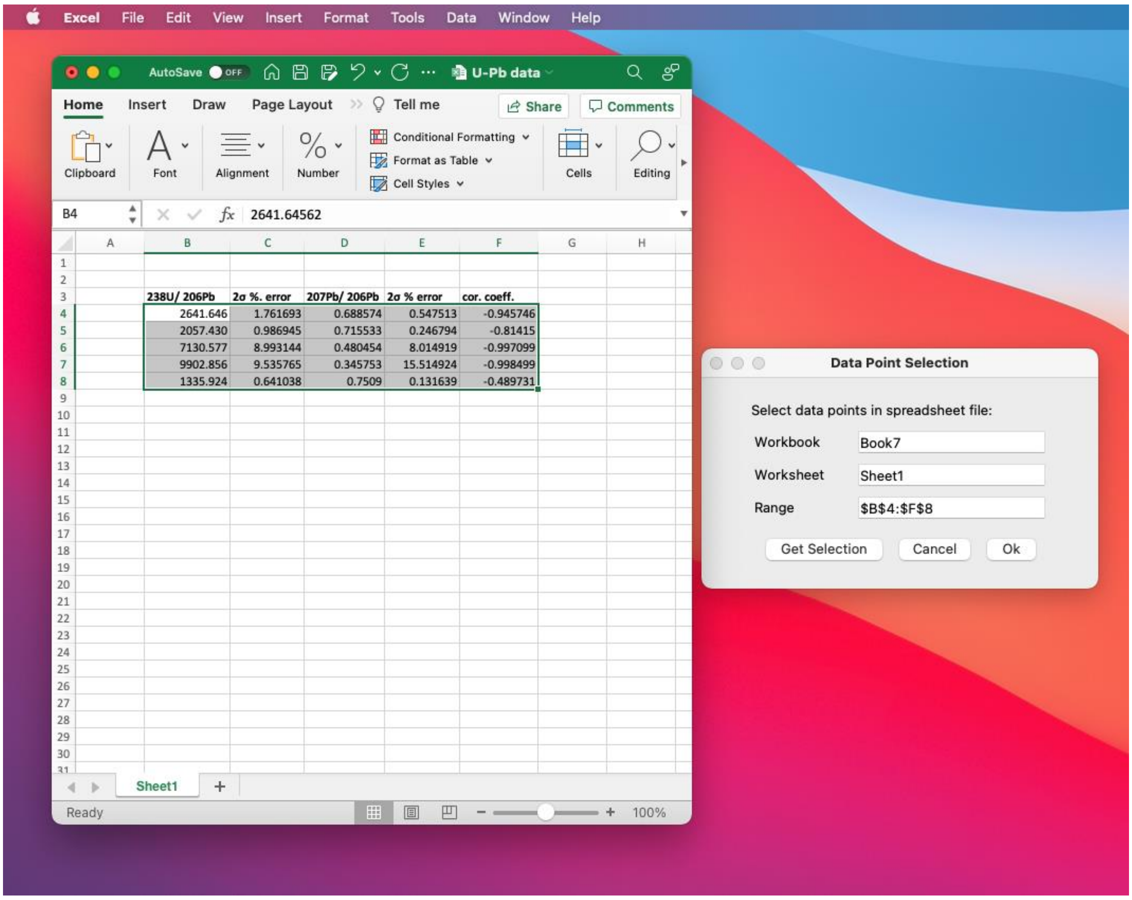
Note: it is recommended that you save and backup your Excel workbook before running DQPB for the first time just in case something unexpected happens (for example, spreadsheet data cells are accidentally overwritten).

5.1. Running a plotting and/or calculation task

All tasks are invoked via the main window, which is displayed when the application is launched. After choosing a task from the drop-down menu, some options on this main menu may be altered, or deactivated if they are not applicable. Further settings may be adjusted via the 'Preferences', 'Type-specific plot settings', and 'Plot format settings' windows.

Basic instructions:

1. Choose an age calculation or plotting task from the task combo box at the top-left.
2. Select the appropriate data type from the 'Data Type' drop-down menu.



Excel data selection dialog on Mac

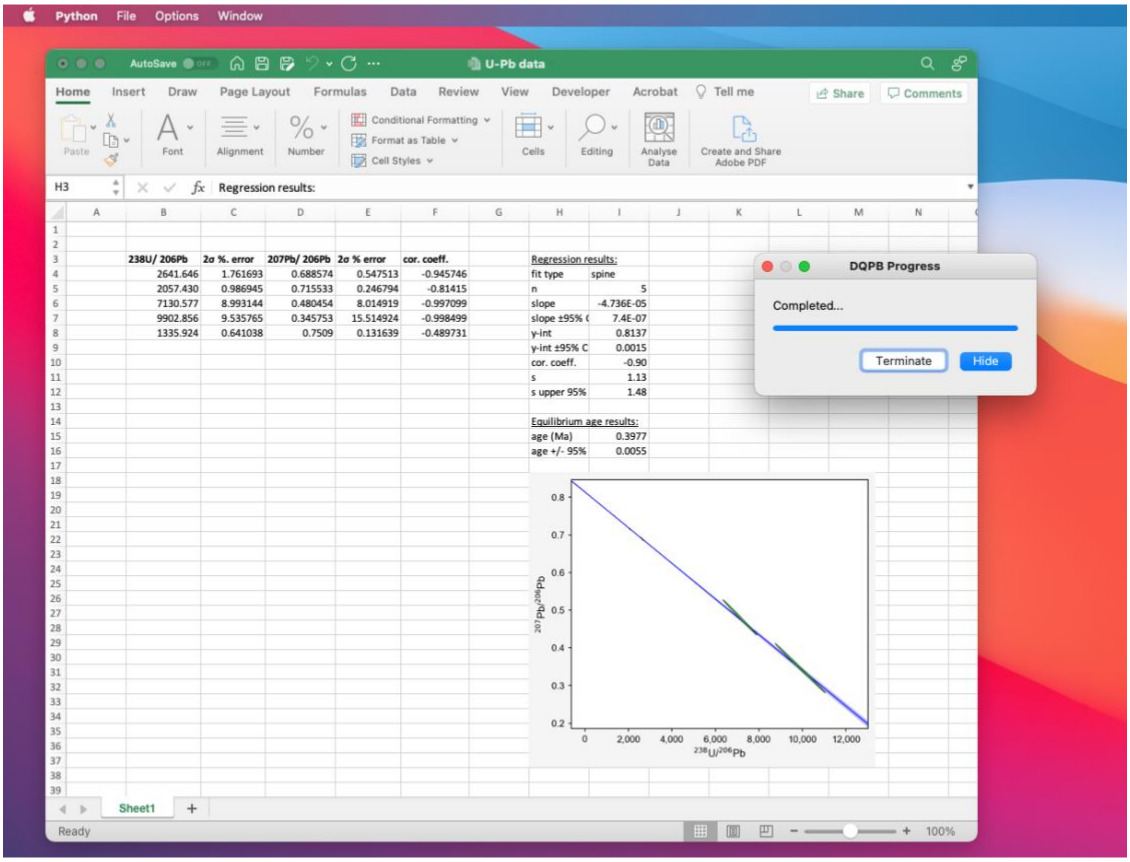
3. Select the input data points from an open Microsoft Excel spreadsheet, by clicking the 'Select data' button. This will hide the main window and launch a smaller data selection dialog. The easiest way to select data points is by navigating to the spreadsheet and highlighting the data in the normal Excel way (excluding headings), and then clicking 'Get selection' on the data selection dialog. DQPB will read the data from Excel. The data selection will typically be *n* rows × *m columns*, where *n* is the number of data points and *m* is the number of variables required.
4. Choose the appropriate input data error type, either absolute (abs.) or percent at the 1 or 2 σ level.

Note: if the incorrect input error type is selected, the task may still run properly but you will receive very strange results. For example, data point uncertainty ellipses may be highly elongated in one direction or completely flat! Keep an eye out for this.

5. Choose a linear regression fit type.
6. Go to the Disequilibrium tab. For a disequilibrium U-Pb age, enter relevant activity ratio values (or Th/U or Pa/U ratio data for single-analysis Pb/U ages). Alternatively, to compute an equilibrium age (using the standard U/Pb equations) check the 'Assume initial equilibrium' option.
7. Click 'Ok'. The main dialog will be hidden, and some further dialogs may pop up asking for additional settings and options to be specified.
8. One of these dialogs will ask you to select where in Excel the data should be output to. A single cell may be selected in any currently open workbook, but care needs to be taken not to overwrite pre-existing data, as the results may be spread over multiple cells down and accross to the right.

Note: data cells that are overwritten by DQPB results cannot be undone in the normal Excel way, so please save and backup important data before running DQPB.

9. Click 'Ok'. A progress bar will then appear showing the progress of the computations.
10. When the task is complete, results and figures (in .jpg format) will be printed back to the Excel worksheet.
11. If an error occurs during the computation (e.g., if no disequilibrium age solutions are found), the task will be aborted, and an error dialog will be displayed. If this happens, check the error log for information on what went wrong.



Progress bar and example of results outputted to spreadsheet on Mac

5.2. Computing concordia-intercept U-Pb ages

Concordia-intercept ages are computed using Tera-Wasserburg diagram variables only (i.e., spreadsheet columns ordered as:

^{238}U/^{206}Pb | ^{238}U/^{206}Pb err. | ^{207}Pb/^{235}U | ^{207}Pb/^{235}U err. | cor. coeff. (optional).

Note that if the data point error correlation coefficients column is not provided, they will be assumed equal to 0 (although this is not a good general assumption for young samples!). Disequilibrium concordia-intercept ages are calculated by solving Eq. (12) in the manuscript using Newton's method. The initial guess for the numerical age solution can either be entered directly (under the 'Disequilibrium' tab of the main window) or set to the lower intercept equilibrium age.

In cases where present-day [^{234}U/^{238}U] or [^{230}Th/^{238}U] values are entered, the disequilibrium concordia curve may loop around quite dramatically and it is possible to have two intercept age solutions in close proximity. In such cases, the algorithm uses a brute force method to search for all age solutions between user defined upper and lower age and activity ratio limits (set in set in the 'Numerical' tab of the 'Preferences' window). Typically, the upper intercept will have a physically implausible initial activity ratio solution, and so the lower intercept is always selected by default, however, the brute force method is implemented to guard against the numerical solution converging to the wrong intercept age.

If the 'assume initial eq.' option is checked, a lower intercept initial equilibrium age will be computed from the standard U-Pb equations using the algorithm of Powell et al., (2020). Note, this algorithm converges rapidly for intercept ages less than ~100 Ma but does not propagate decay constant errors and may not converge for older ages.

For equilibrium ages, age uncertainties may optionally be computed using Monte Carlo methods. To do this, ensure the 'Equilibrium age Monte Carlo errors' option is checked on the main window (note, for disequilibrium ages, Monte Carlo errors are always implemented whether this box is checked or not). Decay constant errors may be included if age uncertainties are computed by Monte Carlo simulation (see the 'Monte Carlo' tab in main window).

For concordia-intercept ages, two separate plots are output by default. The first is an "isochron" style plot showing the data points as 95% confidence ellipses along with the linear regression fit. The second plot is a 'concordia-intercept plot' and shows an enlarged view of the intersection between the regression line and the (dis)equilibrium concordia curve.

5.3. Isochron ages

To compute U-Pb isochron ages the data points should be arranged with columns ordered as:

^{206}Pb/^{20x}Pb | ^{238}U/^{20x}Pb err. | ^{238}U/^{20x}Pb | ^{238}UPb/^{20x}Pb err. | cor. coeff.

or,

^{207}Pb/^{20x}Pb | ^{207}Pb/^{20x}Pb err. | ^{235}U/^{20x}Pb | ^{235}UPb/^{20x}Pb err. | cor. coeff.

where ^{20x}Pb is the normalising isotope (either ^{204}Pb or ^{208}Pb, with ^{208}Pb assumed to be a stable isotope and therefore, applicable to young ages only). Disequilibrium U-Pb isochron ages are calculated by solving the equations given in Sect. 3.2 of the manuscript using Newton's method. As for concordia-intercept ages, the initial age guess can either be entered directly (under the 'Disequilibrium' tab of the main window) or set to the equilibrium age, and age uncertainties may optionally be computed using Monte Carlo methods for equilibrium ages but are always implemented for disequilibrium ages.

5.4. Single-analysis Pb/U and modified 207Pb ages

Typically, multiple single-analyses Pb/U ages will be computed in one go. For Pb/U ages, data points should be arranged with columns ordered as:

^{206}Pb/^{238}U | ^{206}Pb/^{238}U err., or ^{207}Pb/^{235}U | ^{207}Pb/^{235}U err.

and each row as a separate analysis (i.e., a separate mineral grain or spot analysis).

For modified ^{207}Pb ages, data points should be input as Tera-Wasserburg diagram variables (i.e., columns ordered as:

^{238}U/^{206}Pb | ^{238}U/^{206}Pb err. | ^{207}Pb/^{235}U | ^{207}Pb/^{235}U err. | cor. coeff. (optional)

To output a plot of data points on a Tera-Wasserburg diagram, select the 'Output data point plot for mod. ^{207}Pb ages' option in 'Plotting' tab of the 'Preferences' window. A disequilibrium concordia may also be plotted if the Th/U disequilibrium state is input as a constant $D_{Th/U}$ value for all data points, depending on the settings in the 'Type-specific plot settings' window.

For ^{206}Pb/^{238}U and modified ^{207}Pb ages where initial Th/U$_{melt}$ value is set as constant, the Th/U$_{melt}$ values are set in the 'Disequilibrium' tab of the main window, and the Th/U$_{min.}$ values for each data point are selected via a separate dialog that pops up after clicking Ok.

As for other age types, the initial age guess can either be entered directly (under the 'Disequilibrium' tab of the main window) or set to the lower intercept equilibrium age.

To compute a weighted average age from multiple single-analysis ages, select either 'spine' or 'classical' from the 'Fit type' combo box on the main window. To output a plot of the weighted average, ensure 'Output weighted average plot' is checked in the 'Plotting' tab of the 'Preferences' window.

Note that the 'Assume initial equilibrium' option is not yet available for single-analysis Pb/U ages.

5.5. Concordant initial [^{234}U/^{238}U] routine

The 'concordant initial [^{234}U/^{238}U]' routine computes an initial [^{234}U/^{238}U] value that results in agreement (i.e., 'concordance') between the ^{238}U-^{206}Pb and ^{235}U-^{207}Pb isochron ages following Engel et al., (2019). This routine requires two data selections, one to compute a ^{235}U-^{207}Pb isochron ages, and another to compute a ^{238}U-^{206}Pb isochron age. The columns for these data selections should be arranged as described in Sect. 3.3 (of this user guide) above. After clicking 'Ok' on the main window, a data point selection dialog will appear. The initial activity ratio state of isotopes other than ^{234}U may be specified in the 'Disequilibrium' tab of the main window. Typically, for carbonates [$^{230}Th/^{238}U$] and [$^{231}Pa/^{235}U$] will be set to zero. Uncertainties in the initial [234/238U] value are computed using Monte Carlo methods.

5.6. Plot x-y data (and optionally perform a linear regression)

This routine allows arbitrary 2-dimensional data points to be plotted as 95% confidence ellipses, optionally accounting for data point error covariances. Data point columns should be arranged as:

x | *x* err. | *y* | *y* err. | cor. coeff. (optional)

If the 'Data type' is set to 'Tera-Wasserburg', then an equilibrium or arbitrary disequilibrium concordia curve may also be plotted by setting the activity ratios in the usual way, and ensuring appropriate options are set in the 'Isochron' tab of the 'Type-specific plot options' window.

To perform a linear regression, select a regression algorithm from the 'Fit type' combo box, or otherwise, select 'No fit'.

If the 'Data type' option is set to 'other x-y', then axis labels may be set by the 'Axis labels' dialog that pops up after clicking 'Ok'. For mathematical symbols and expressions, LaTeX type syntax can be used (enclosed in dollar symbols). For example, use \$^{238}\$U for ^{238}U or \$\delta^{18}\$O for $\delta^{18}O$.

6. Linear regression algorithms

The following linear regression algorithms may be selected when computing U-Pb concordia-intercept and isochron ages or fitting a regression line to arbitrary x-y data (via the 'Plot x-y data ' task).

6.1. 'Classical'

This routine emulates the default behaviour of Isoplot (Ludwig, 2012). Firstly, a linear regression is performed using the model 1 algorithm. If the MSWD exceeds the lower one-sided confidence interval limit (85% by default, equivalent to a 'probability of fit' value below 0.15), then the fit is accepted as is. If the MSWD is between the lower and upper one-sided confidence interval limits (85-95%, equivalent to a 'probability of fit' value between 0.15 - 0.05), then the slope and y-intercept values are retained, but uncertainties are expanded as per the model 1x fit (see below). If the MSWD exceeds this upper one-sided confidence interval limit then a linear regression is instead performed using the model 2 algorithm for concordia-intercept datasets, or the model 3 for U-Pb isochron datasets. Note that the model 3 algorithm parametrises 'excess scatter' as a strictly Gaussian distributed component of excess scatter. This assumption is not automatically applicable to all datasets and should be carefully considered.

6.2. Spine

Equivalent to the robust line fitting algorithm described in Powell et al., (2020). This algorithm converges to the classical model 1 for 'well-behaved' datasets, but down-weights data points lying away from the central 'spine' of data according to the Huber loss function for more scattered datasets. The spine-width parameter, s, gives an indication of how well resolved the central linear "spine" of data is. Comparing s with the upper one-sided 95% confidence interval, which has been derived via simulation of Guassian distributed data sets, provides a means of assessing whether the 'spine' of data is sufficiently well-defined to obtain accurate results with this algorithm. The spine algorithm may yield unreliable results for datasets where s clearly exceeds this upper limit.

6.3. Robust model 2

A robust version of the Isoplot model 2 (details provided in Appendix C of the manuscript).

6.4. Model 1

Equivalent to the Isoplot model 1. Regression parameters and analytical errors are calculated via the algorithm of York et al. (2004), which yields equivalent results to the original algorithm of York (1969) with errors calculated according to Titterington and Halliday (1979). Confidence intervals on the slope and y-intercept are computed based on assigned analytical errors alone and are not inflated according observed scatter, since any apparent 'excess scatter' is not deemed statistically significant.

6.5. Model 1x

Equivalent to the Isoplot model 1 with 'excess scatter'. Regression parameters and analytical errors are calculated via the York algorithm as above for the model 1. These analytical errors are then multiplied by $\sqrt{\mathrm{MSWD}}$ to account for excess scatter, and further multiplied by the 95th percentile of a Student's t distribution (with *n* – 2 degrees of freedom) to obtain 95% confidence limits following the reasoning of Brooks et al., (1972).

6.6. Model 2

Equivalent to Isoplot model 2. The regression line slope is computed as the geometric mean of a *y* on *x* ordinary least-squares regression, and that of *x* on *y* (see Powell et al., 2020). Uncertainties are calculated following McSaveney in (Faure, 1977) and these are then multiplied by $\sqrt{\mathrm{MSWD}}$ and the 95th percentile of a Student's t distribution (with *n* – 2 degrees of freedom) to obtain 95 % confidence limits.

6.7. Model 3

Equivalent to Isoplot Model 3. This algorithm iteratively adds a uniform component of Gaussian distributed scatted in y to each data point until MSWD converges to 1. This component of excess scatter is returned as an additional model parameter and may have physical significance in some cases. Slope and y-intercept uncertainties are calculated as per the York algorithm and then multiplied by the 95th percentile of a Student's t distribution (with *n* – 2 degrees of freedom) to obtain 95 % confidence limits.

7. Weighted average calculations

The following weighted average algorithms may be selected when computing Pb/U ages, modified ^{207}Pb ages, or invoking the 'Weighted average' routine.

7.1. Classical

This routine computes a weighted average using standard classical statistics equations (i.e., those given in Powell and Holland, 1988; Lyons et al., 1988; McLean et al., 2011, etc.). Where uncertainty covariances are negligible, these equations reduce to the standard error weighted mean (e.g., Taylor, 1997). If the MSWD exceeds a lower one-sided confidence interval threshold value (85% by default, equivalent to a 'probability of fit' value of 0.15) then analytical errors are expanded by $\sqrt{\mathrm{MSWD}}$ in an effort to account for excess scatter, and further multiplied by the 95th percentile of a Student's t distribution (with $n - 1$ degrees of freedom) to obtain 95% confidence limits following the approach of Isoplot (Ludwig, 2012). Where the probability of fit is below a reasonable lower limit (say, 0.05), use of this approach should be considered carefully, and a robust approach should be considered instead.

7.2. spine

A robust version of the spine linear regression algorithm that is capable of accounting for uncertainty covariances (details provided in Appendix A of the manuscript).

8. Main window options

The following options are available in the first tab of the main window:

Account for covariance in wav.	If true, uncertainty covariances are accounted for when computing weighted average ages from Monte Carlo results (applies to Pb/U and modified ^{207}Pb ages only).
Norm. isotope	Normalising isotope (^{204}Pb or ^{208}Pb) for isochron isotope ratios. Only affects plot axis labels, as ^{208}Pb is treated as a stable isotope, and thus should only be used for young samples.
Autoscale axis limits	If checked, plot axis limits will be determined automatically. If not, a dialog will pop up after clicking Ok, allowing the user to specify axis limits for various plot types.
Add data point labels	If checked, labels are added to plotted data points. After clicking Ok, a dialog will pop up asking the user to select the data point labels from the Excel.
Output calc. settings	Output calculation settings (decay constant, activity ratio values, Monte Carlo settings, etc.) to spreadsheet along with age results.

Output plot data	If checked, all data used to construct plots (e.g., data points, regression lines etc.) will be output to a new Excel spreadsheet.
Save plots to disk	Save figures to disk (e.g., to obtain figures in a specific size and/or file type). The save location and file type can be set in the 'IO' tab of the 'Preferences' window. Figure sizes are set in the 'Type-specific plot options' window.
Covariance matrix	Allows data uncertainties to be specified as a covariance matrix when computing weighted averages for arbitrary data via the 'Weighted average' task. If checked, a dialog will pop up allowing the user to select the covariance matrix data from Excel.

9. Monte Carlo options

Note: by default, age uncertainties are computed by Monte Carlo simulation for all disequilibrium U-Pb ages. For equilibrium U-Pb ages, uncertainties will only be computed by Monte Carlo simulation if the 'Equilibrium age Monte Carlo errors' option is checked in the main window.

The following options are available in the 'Monte Carlo' tab of the main window:

Show full Monte Carlo results summary	Include information on cause of failed trials in Monte Carlo results, and additional summary statistics.
Number of trials	Number of age simulations to attempt. For single-analysis Pb/U and modified ^{207}Pb ages, this is the number of trials for individual each individual age.
Include decay constant errors	Include the effects of decay constant errors (set in the 'Constants' tab of the 'Preferences' window). These effects are typically negligible when computing disequilibrium ages for young samples. **Note**: this option does not yet apply to single-analysis Pb/U or modified ^{207}Pb ages.

Include $^{238}U/^{235}U$ errors	As above, but for the natural present-day 238U/235U ratio value. These effects are also typically negligible for young samples.
Reject negative activity ratio trials	Reject any trial encountering a negative activity ratio value, both at the initial randomisation stage or as an initial activity ratio solution where a present-day value is input.
Reject negative age trials	Reject any trials with a negative age solution.
Age histogram	Output a histogram of simulated ages (as well as simulated regression slope and y-intercept values if applicable).
Activity ratio histograms	Output a histogram of simulated activity ratio values and computed initial activity ratio solutions where (for present-day values).

10. Preferences window

The following options are available in the 'Preferences' window:

Plotting

Output weighted average plot	Output a plot showing age points with uncertainties and the weighted average line and uncertainty envelope for Pb/U and modified ^{207}Pb ages.
Output data ellipse plot for mod. ^{207}Pb ages	Plot modified ^{207}Pb data points on a Tera-Wasserburg diagram. A disequilibrium concordia curve is also plotted if the initial disequilibrium Th/U state is specified as a constant $D_{Th/U}$ value.
plot projected lines through modified ^{207}Pb data points	Show lines projected from common $^{207}Pb/^{206}Pb$ value through each data point for modified ^{207}Pb data point plots.
Equilibrium concordia curve limits	The equilibrium concordia curve will not extend beyond these age limits.

Disequilibrium concordia curve limits	The disequilibrium concordia curve on concordia-intercept plots will not extend beyond these age limits. **Note**: different limits are used for (a) curves constructed based on initial activity ratio values only, (b) curves constructed based on a present-day [234U/238U] value but initial [230Th/238U] value, and (c) curves based on a present-day [230Th/238U] value.

Numerical

Min / max age, $[^{234}U/^{238}U]_i$, and $[^{230}Th/^{238}U]_i$	Reject disequilibrium concordia-intercept age solutions (where present-day activity ratio(s) are input) if numerical solutions are outside these limits. See Sect. 4.2 of this document for further explanation.
Classical linear regression fit lower / upper MSWD thresholds	MSWD one-sided confidence limit thresholds. The lower limit is the threshold at which model 1 transitions to model 1x. Upper is the threshold at which model 1x transitions to model 2 / 3. Only applies if the 'classical' linear regression fit type is selected. See Sect. 5.1 of this document for further details.
Wtd. average excess scatter thresholds	MSWD one-sided confidence limit thresholds. If MSWD is above this lower limit, uncertainty on the weighted average result is inflated according to data scatter. The upper limit is not currently implemented. Only applies to the classical weighted average algorithm.
RNG seed	Random number generator seed used to generate reproducible Monte Carlo results. Use an integer seed sequence (e.g., 42) or leave blank for non-reproducible results . See: https://numpy.org/doc/stable/reference/random/generator.html
h value	h value used in the spine linear regression and weighted average routines (default = 1.4).

I/O

Save figures to	Directory (i.e., 'folder') where figures are saved to.
Export file type	Image file format applied to plots saved to disk.
Spreadsheet figure height	Height of figures that are output to spreadsheet (in number of cells). Width is determined by original aspect ratio (i.e., the width and height set in the 'Type-specific plot settings' dialog).
Apply spreadsheet number formats to results	Apply number formatting to results output to spreadsheet (e.g., so that the correct number of significant figures are shown). Complete digits are still retained and are visible in the formula bar when the cell is selected, or if the cell is reformatted in Excel or copied to the clipboard.
Clear cells before printing results	Clear cells of formatting before printing results to spreadsheet (may slow down printing results to Excel a bit).
Font	Apply a non-default font to results in spreadsheet (may also slow down printing results to Excel a bit).
Apply cell colours	Apply a background colour to results that are output to spreadsheet (may also slow down printing results to Excel a bit

11.Type-specific plot settings

Type-specific plot settings that are only applied to plots of a given type. The 'Isochron' settings apply to: isochron diagrams, concordia-intercept 'regression plots', modified ^{207}Pb data plots, and other x-y plots.

All plot types

comma separated thousands	E.g., show 10,000 in axis labels instead of 10000.
hide top and right spines	Remove the top and right-hand side lines bordering the axis window.

lower exponent limit	If axis tick values are less than or equal to 10 ^ (*this limit*) they will be displayed in scientific notation.
upper exponent limit	If axis tick values are greater than or equal to 10 ^ (*this limit*) then they will be displayed in scientific notation.
height	Figure height (in inches). This may be different to the height of the figure output to Excel (which is set as height in number of cells via the 'I/O' tab of 'Preferences'), however, figures exported to disk will be set to this height.
width	Figure width (in inches). As above, this may be different to the width of the figure output to Excel, however, figures exported to disk will be set to this width.
dpi	Dots per square inch of exported figures (only applied to certain image file types such as .png)

Concordia-intercept plots

plot concordia intercept ellipse	Plot the Monte Carlo concordia intercept points from each successful Monte Carlo trial as a confidence ellipse. **Note**: this option is not suitable for plots displaying large intercept age errors.
plot concordia intercept x-y points	Plot the concordia intercept points for each successful Monte Carlo trial as individual markers.
plot concordia uncertainty envelope	Plot uncertainty envelope about the concordia curve representing uncertainty arising from activity ratio uncertainties.
'spaghetti' type concordia envelope	Plot each Monte Carlo simulated curve used to construct the concordia envelope. This can be useful for diagnosing problems with concordia envelope plotting.

plot concordia age markers as ellipses	Plot each age marker along the concordia curve as a confidence ellipse accounting for uncertainty in activity ratio values for disequilibrium curves or decay constant values for equilibrium curves. **Note**: this setting may work poorly if activity ratio values have large errors. May also fail for older ages if present-day activity ratios are set (in such cases, reduce the 'auto markers max age' value).
auto markers max age	Automatically generated concordia age markers / ellipses will not exceed this value.
use manual marker ages	Option to plot concordia age markers or ellipses at user specified locations that are set in the field below.
manual age marker locations	Enter manual concordia age marker locations, separating each age by a space. These should be in same 'units' as the 'age label prefix' option.
show age prefix in label	Show 'Ma' or 'ka' in concordia age marker labels.
rotate labels	Rotate concordia age marker labels according to the settings below.
rotate perpendicular	If checked, rotate perpendicular to concordia line slope at the age marker position (only applies if the 'rotate labels' option is selected). Otherwise, rotate parallel to the concordia line slope.
avoid label overlaps	Any concordia age markers older than the first marker that is overlapped will be removed.
label offset factor	Controls how far concordia age marker labels are offset from markers.

12.Plot format settings

Plot format settings (e.g., colours, line thicknesses, fonts) can be set in the 'Plot format settings' window. These settings are mostly self-explanatory, but keep in mind:

- 'zorder' determines the order in which elements are overlayed on a figure (i.e., those which a higher 'zorder' will be placed on top of those with a lower 'zorder'. These values must be positive whole numbers.
- Setting a linewidth to 0 will make the line (and in some cases the plot element) disappear.
- Alpha is a transparency setting between 0 (clear) and 1 (opaque).
- Colours may be selected from the matplotlib named colours via the drop-down combo boxes. Named colours are shown in Appendix 1 of this document. Alternatively, colours may be entered into the combo box as a case-insensitive (8-bit per channel) hexadecimal RGB string (e.g.: `#0f0f0f`) . These values can be obtained from colour selection dialogs in applications such as Excel.

13. Troubleshooting

13.1. The Log Console

All errors and warnings that are encountered while DQPB executes a plotting or calculation task are logged. To view this log, navigate via the file menu to 'Window' –> 'Log console…'. The content of the log includes information, warnings, and errors logged directly by the DQPB program, and also errors logged by 'third-party' Python modules used by DQPB. The errors (technically speaking, 'exceptions') logged by 'third-party' Python modules are presented as a Python 'traceback'. This may be difficult to interpret for non-python programmers but reading the last line or two will often provide a hint as to what went wrong. The error log console should be your first port of call anytime something unexpected happens and should be routinely checked.

13.2. Unfreezing Excel Workbook

While DQPB is executing tasks, the Excel screen is 'frozen' to increase the speed at which results are printed back to the spreadsheet. If DQPB crashes while executing a task, or is closed by the user, it is possible that the screen will remain locked. To unfreeze the Excel screen, re-launch DQPB and navigate via the file menu to 'File' –> 'Unfreeze Excel screen updating'.

13.1. Overwriting Old Results

Numerical results output to Excel will overwrite any pre-existing cell data if the calculation/plotting task is re-run. To avoid any potential confusion, it is best to delete old results and plots before re-running a task. Also, note that new figures output to Excel will be stacked on top of old figures. If too many figures accumulate this may slow down Excel, so it is a good idea to delete old figures as you go.

13.1. Crowded concordia markers

The concordia curve plotting routine attempts to find a suitable spacing for age markers given the plot axis limits and the concordia age limits (set in the ‘plotting’ tab of the ‘Preferences’ window). However, for Tera-Wasserburg diagrams that span a large range of *x* values (say, 0–10 000), there is often no constant age marker spacing that will deliver satisfactory results, and markers will tend to be bunched together at the left-hand side of the plot. There are at least three possible ways to address this:

a) Set manual age markers (see the ‘Isochron’ or ‘Concordia-intercept’ tabs of the ‘Type-specific plot settings’ window). Tick the ‘use manual age markers’ option and set the ages in the ‘manual age markers’ field below (separate each marker age by a space).
b) Use the auto age marker routine (untick the ‘use manual age markers’ option) but set the ‘auto markers max age’ to a suitable age lower than the concordia age limits.
c) Use the auto age marker routine (untick the ‘use manual age markers’ option), but reduce the concordia age limit. Note this will also truncate the concordia curve line itself.

14. References

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Appendix 1: named colour options

Source: https://matplotlib.org/stable/gallery/color/named_colors.html