Initial Decision for `DQPB`: software for calculating disequilibrium U-Pb ages by Timothy Pollard et al., manuscript *GChron-2022-24*

Noah McLean

December 21, 2022

This is a well-written manuscript describing both U-Pb date calculations with initial isotopic disequilibrium and a useful, open-source software package to quantify and visualize those calculations. The writing is clear and well-organized and the software works as advertised. I agree with the reviewers that this manuscript is well-suited to publication in GChron and suggest minor revisions, as identified by the reviewers and by myself below.

The central concern of the Vermeesch review is handling systems where probability density functions for user-input parameters substantially overlap physically impossible domains. Vermeesch is correct that the results returned by `DQPB` in these scenarios was misleading. The user warning and missing uncertainty described in the authors' reply is a satisfactory remedy, and a description of this behavior in the revised version of the manuscript will benefit readers.

An example, perhaps with synthetic data, illustrating where and how `DQPB`'s algorithms break down with user input of this sort would be informative, but it also risks cluttering an already technical paper. I suggest (but don't insist on) adding this to the text if you can find a place for it, to an appendix if you can't, or to the well-developed online documentation if you don't feel it belongs in the manuscript. I feel strongly that the best geochronology calculations come from a two-way partnership between, on one side, the developers of the software that performs data reduction, error propagation, and visualization, and on the other side, the other geochronologists using that software. On balance, the better the software is documented and its correct use explained, the better the science that comes out the other end. This manuscript and its accompanying software are a nice contribution to the geochronology literature in this respect.

Responses to the rest of Vermeesch's comments, and edits indicated in those responses, all look fine. The final discussion point concerns the overhead of 30,000 Monte Carlo iterations. I think the Monte Carlo approach works fine here, and note that `DQPB` has a setting to adjust the number MC samples generated. There is an error in the mean calculated from Monte Carlo samples that scales with $\sigma/\sqrt{n}$. That's 0.0058 of σ for 30,000 MC trials, which would affect the second significant digit of many `DQPB`-calculated uncertainties and means rounded to the same decimal place. Perhaps it's worth mentioning that n should be increased when calculating dates for publication or when comparing `DQPB`'s output with other calculations.

Responses to the issues raised by reviewer Ickert and revisions proposed by the authors are all appropriate.

Minor edits and suggestions

Line 29 – Igneous minerals are crystallized, not deposited (at least, in this context).

Line 31 – Following on the clarifications suggested by Ickert, monazite doesn't incorporate "an initial excess of Th" but instead an initial ^{230}Th/^{238}U in excess of the ratio in the melt, which is usually assumed to be at equilibrium with respect to the top of the ^{238}U decay chain in U-Pb geochronology.

Figure 2 caption – The ^{207}Pb age described here and elsewhere is, to me, a model age. If this nomenclature has entered the literature and you're set on using it, I think that's ok. But calling this a model age might help others make a connection to a relevant, more broadly applied concept.

Line 147 – The Pb isotope ratios in question don't necessarily come from Pb-rich phases, at least I don't think of K-feldspars as Pb-rich. I think you're looking for low ^{238}U/^{204}Pb (aka μ) here.

Line 154 – The term $D_{Th/U}$ is missing at the end of the line, before "varies across..."

Line 155 – The mineral grains need not be coeval or even cogenetic to do a disequilibrium correction as described here. The Rioux et al. (2012) grains were not assumed coeval, but instead interpreted to have some real spread in age.

Line 156 – The ^{232}Th/^{238}U is directly measured, in the sense that a ^{232}Th beam is measured, in many LA-ICPMS U-Pb studies. The ^{232}Th/^{238}U is not directly measured in the vast majority of ID-TIMS studies, and instead the ^{232}Th is back-calculated from an estimated age and the radiogenic ^{208}Pb (e.g., Schmitz and Schoene, 2007). I'm not certain why the assumption about radiogenic ^{208}Pb needs to be made to estimate Th/U_{min} when there is a direct ^{232}Th/^{238}U measurement, unless it's to justify non back-calculating the initial ^{232}Th/^{238}U.

Line 168 – Variations in Th and U partitioning behavior may constitute a systematic component of error, as suggested here, but it's purely systematic only if you assume that there is no mineral-to-mineral variation in this behavior. Different $D_{Th/U}$ could explain, for instance, the spread in coeval zircon ^{238}U/^{232}Th ratios measured for ^{238}U-^{230}Th dating (e.g., Cooper and Reid, 2008, and references therein). Propagating $D_{Th/U}$ uncertainty as purely systematic does not account for scatter derived from this variation, or alternately/additionally differences in Th/U in a compositionally heterogeneous magmatic system. However, there is often significant systematic uncertainty in the mean of $D_{Th/U}$

or the magma Th/U. Including this source of systematic uncertainty as correlated age uncertainties is commendable.

Line 179 – Reference the definitions of F and G above.

Figure 3 Plots – Are the uncertainties in the text boxes for the plots $\pm 1\sigma$, $\pm 2\sigma$, or 95% CIs? For the y-intercept, it would be more readable to express the result without scientific notation, as 0.8137 ± 0.0015. In the caption, please mention that s is the spine width and reference the appropriate section of the text (Section 4? You might usefully subdivide Section 4 into two sections for 'classical' and robust fitting, then reference 4.2). I appreciate that (a) does not show the oldest reaches of the concordia curve, which is meaningless in this application but is often plotted anyway.

Figure 3 Caption – Change Mid- to Middle. The word ellipses need not be in quotes. What is the confidence level of the ellipse representing the MC-ed concordia intercept points?

Figure 4 – Thanks for emailing the plot for this figure. It shows up when the submitted manuscript is opened in my Chrome browser but not, as reviewer Ickert points out, in Adobe Acrobat Reader. The same comments from Figure 3 apply here — please indicate whether age uncertainties are reported in the plot text boxes as $\pm 1\sigma$, $\pm 2\sigma$ or other. Likewise for the uncertainties in the dates reported in the caption, alongside their MSWD and n, for maximum clarity.

Section 8.2 – Please indicate that the uncertainties in $D_{Th/U}$ and $D_{Pa/U}$ are propagated as purely systematic uncertainties. You might also explain that this involves the assumption that the $D_{Th/U}$ and $D_{Pa/U}$ are unknown, but are identical for all measured data points, if this is how you are treating the uncertainty propagation (this is my assumption from the dark vs. light blue uncertainty bars in Figure 5b).

Figure 5 – Please indicate whether age uncertainties are reported in the plot text boxes as $\pm 1\sigma$, $\pm 2\sigma$ or other. The caption states that the dashed blue lines project from the y-axis through the measured data points to the concordia intercept, but it looks like the blue line corresponding to the discordant data point doesn't continue to the concordia curve. In the caption, please indicate in the description of (a) that the dark blue ellipses are the "data ellipses," to distinguish them from the white concordia uncertainty ellipses. Please re-state the uncertainties in $D_{Th/U}$ and $D_{Pa/U}$ from Section 5.2 for maximum clarity, as they are responsible for the yellow band.

Line 456 – Change 'which' to 'that' or reword.

Line 463 – Insert the word 'for' after 'framework'.

Line 476 – Change 'spline' to 'spine'.