Author reply on RC2

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We thank associate editor and reviewer #2 Pieter Vermeesch for their comments on preprint gchron-2024-3. We appreciate the opportunity to clarify what we believe are some misunderstandings about the FDHM method as presented in our paper. Below we respond to each of the comments in detail.

RC2 denotes reviewer #2 comments and **AC** marks the authors' replies.

> **RC2:** *"In a sense, the new method generalises the concept of an 'apparent age' from a single fission track or helium age to a suite of multiple thermochronological age estimates."*

AC: We are not sure what is meant by this statement. The FDHM and the corresponding time of peak cooling should not be thought of as an "apparent age." We are explicit in the manuscript to not describe or treat the FDHM as such. In addition, single vs. multiple thermochronometers have little direct bearing on the FDHM result, but will sometimes affect the uncertainty, as discussed in the manuscript. The FDHM is calculated from the time-temperature (tT) path output from an inversion and is simply a metric for quantifying the model time (± uncertainty) at which ∼50% of the total cooling has occurred within some time interval—e.g., the peak of the total 100 °C of cooling that occurred between 100–20 Ma is at 60 ± 10 Ma (FDHM calculated at the 50 °C isotherm).

> **RC2:** *"It is not clear to me what a 'full time-distribution' means, or what the 'half-maximum temperature' is. According to Figure 1 of the manuscript, the FDHM age should mark the half-way point between the onset and termination of rapid cooling. This is straightforward for simple step histories, but not for more complex cooling curves."*

AC: We thank RC2 and take this opportunity to clarify a fundamental aspect of the FDHM. For the FDHM calculation, a total cooling signal of interest is identified and the midpoint (between min/max temps) for an ensemble of tT histories is determined. The 'full time distribution' is simply a distribution representative of all the points in time [in the tT model] when individual tT paths cross the half-maximum isotherm along the cooling path trajectory. RC2 accurately described the 'half-maximum temperature' in their comment as "the half-way point between the onset and termination of [rapid] cooling." We will clarify this further in the text and add labeled panels in Figure 1 to be more clear about what we are doing.

We agree that determining the half-way/midpoint of a cooling path is straightforward for simple step-like rapid cooling histories, as was discussed and illustrated in our Figure 1 in the manuscript. Much additional discussion and the other examples in the paper are focused on more complex thermal histories, albeit ones that are fairly simple in form with minimal inflection points. Our paper is primarily about FDHM proof-of-concept and simple application, therefore, none of the thermal histories presented in the manuscript are characterized by overly complex tT paths with many wildly divergent inflections. It seems the last sentence on complexity is ultimately aimed at RC2's schematic tT path shown below (Figure 1).

> **RC2:** *"Which isotherm marks the FDHM? The fastest cooling occurs through isotherm A, with a slower but longer period of cooling going through isotherm B. Isotherm C marks the half-way point between the maximum and minimum temperature. It is not clear to me how this cooling history could be summarised with a single FDHM value. It could be reported as two or three FDHM values, but that would defeat the purpose of the method."*

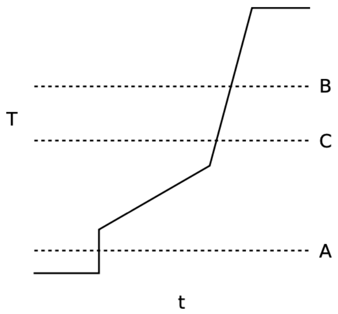

Figure 1: Schematic tT path discussed by RC2

AC: To summarize the point made by RC2, if we consider the cooling path in Figure 1, then isotherms A, B, and C represent half-maximum temperatures for three different cooling segments, depending upon the specific context of the min/max temperature path segments being considered. We thank RC2 for providing the counterexample since it is a good one to utilize for discussion.

If the tT path in Figure 1 is the real, 'exact' path where you know everything perfectly, then you have no need for an FDHM. However, we are dealing with real thermochronology where there is large uncertainty. We would argue, however, that rather than a single path, the overall behavior of a large number of paths is more suitable for FDHM evaluation. We are also not necessarily concerned with "faster" or "slower" cooling rate paths.

To answer the questions asked by RC2 regarding their Figure 1, firstly, we consider that of the three isotherms denoted in the schematic tT path, the minor rapid cooling segment that passes through Isotherm A would almost certainly not be considered geologically meaningful by a thermochronologist. There are many reasons for this since the turning points (or subtle cooling rate changes) along a longer cooling path within a tT inversion may be related to other factors such as the number of random interpolation points available or a lack of tT sensitivity/resolution on the part of the thermochronometer data (as discussed in the m.s.). Nonetheless, if someone wanted to interpret this rapid cooling segment they could do so, and simply define the time domain in the model over which the tT path(s) cross Isotherm A and calculate the FDHM at the midpoint of the cooling segment—as accurately denoted by the dashed line labelled “A” in the diagram. This would be then reproducible by anyone using the same FDHM calculation inputs thereafter.

If we were interested in the ‘total’ cooling signal approximated by the entire path, then Isotherm C would be appropriate. This example most closely aligns with those discussed throughout our manuscript. However, if only the last cooling ‘leg’ was of interest, then Isotherm B would be representative of the FDHM for that segment. Since there are turning points where the apparent cooling rate changes across the entire tT path, then there is no reason that multiple FDHM values could not be calculated—it is up to the user to determine which cooling they want to apply the FDHM. However, as with most interpretive methods, whether or not that is appropriate or geologically reasonable is up to the modeler.

> **RC2:** *“I would like to note that the synthetic data of Table 1 do not make much sense, with the ZHe data being younger than the AFT data and similar in age to the AHe data, even at low eU values. This seems quite unrealistic.”*

AC: This point is noted but we are unsure about what information supports the reviewer’s assertion that the (U-Th)/He data “do not make much sense” or are unrealistic? The trajectories of the 10 °C/Myr and 1 °C/Myr cooling paths set the ages in QTQt by forward modeling. A combination of various factors such as the thermal history style, the radiation damage/diffusivity relationship (eU), and grain size all play a role in generating data that may appear non-intuitive. Importantly, the synthetic zircon and apatite data in Table 1 are *uncorrected for alpha-ejection* and are of quite variable grain size and/or span a broad eU range—i.e., zircons are all small 40 μm spherical grain radius, whereas apatite are low eU but large 75, 60, and 40 μm spherical radius, respectively. All of these points are explained in the text and associated Table 1 caption and were meant to better reflect a complicated but more realistic dataset. The only dataset that appears to more directly correspond with the cooling path behavior in an intuitive way are the apatite fission track data, which obviously do not include the effects of grain size or radiation damage on diffusivity. Reviewer #1 (Murray) also mentioned that the data in Table 1 of the manuscript were difficult to interpret at face value, however, the data provided are the predicted forward model raw dates used in the inverse modeling and are unobscured by various corrections for the sake of reproducibility. Such raw data are the inputs within inverse model software where alpha ejection is accounted for during forward modeling.

We have made comparisons between our reported data in Table 1 and to the ZRDAAM/RDAAM age predictions using the core routines from HeFTy (courtesy of R. Ketcham and P. Zeitler), we note that there are some slight differences in zircon and apatite ages but the overall form of the date-eU patterns are the same. Note that QTQt uses the same age prediction routines. The differences are subtle but are related to the model tT step for diffusion/damage. As stated in the manuscript at lines 177–178: *“The QTQt temperature step for diffusion was set to 3 (AHe) and 6 (ZHe), while the radiation damage step was set to 2 (AHe) and 4 (ZHe).”* HeFTy age prediction routines also allow different age precision options with maximum temperature steps of 10, 2, and 0.5 °C (i.e., maximum temperature change for any time step) for the of ‘Good, Better, and Best’ settings, respectively.

We used a customized time step setting for age prediction only to speed up inversion run time. Reviewer 1 (Murray) also commented that the option to change the step values does not seem to be a publicly available feature in QTQt, but it is in fact included as an option in the model settings for the most recent versions of the code. Ultimately, none of these details are of any real consequence since the data are provided in the manuscript for completeness and can be reproduced by anyone using the same modeling conditions in QTQt. The sensitivity test inversions are employed simply to demonstrate the FDHM on a well constrained ensemble of tT paths. We could move Table 1 to the supplementary materials since it seems to distract in the main text. The cooling age data are not important to the main points of the paper and are only included for reproducibility.

> **RC2:** *"Unrealistic or not, the first example yields an FDHM age of 700 $+7.6/-6.0$ Ma for the slow cooling scenario. Inspection of the true thermal history (dashed line in Figure 2) reveals that nothing special happened at this time. The onset and termination of cooling correspond to geologically meaningful events. The middle of a cooling event does not."*

AC: We appreciate the reviewer's comment, since it allows us to provide some necessary exposition, but we are nonetheless puzzled. Cooling in tT models is most often, but not always, interpreted as a signal of exhumation, which we adopt here as well. If the onset and termination of cooling are geologically meaningful, wouldn't the middle of a cooling event represent the 'middle' of an exhumation event? Put another way, the midpoint of a cooling event would represent the point in time when 50% of the exhumation was complete.

While, it is true that the onset and termination of cooling may be geologically meaningful, it is not a certainty that either are accurately recovered within a tT inversion (particularly the former). For example, if you take a cooling signal and add Gaussian blur, the midpoint is robust while the onset and termination are not. We will add a panel to Figure 1 to demonstrate this point. This is a major argument made regarding the 'onset of cooling' specifically in the discussion of Figure 4 and Figure 5 in the manuscript that deal with accurate recovery of the true 1 °C/Myr thermal history using *only* apatite (U-Th)/He data (see below). The onset of cooling is imprecisely recovered because the apatite (U-Th)/He data do not have sensitivity to that portion of the thermal history. This may seem obvious, but nonetheless such tT models have been a focal point of some papers in the recent literature claiming high resolution of deep-time thermal histories using only apatite He data or, alternatively, only zircon He data that have been reset by fairly recent heating events.

> **RC2:** *"The scientific value of the credible interval for FDHM is also unclear. It reminds me of the story where a statistician took 100 depth measurements of a river; obtained a mean value of 1 m with a standard error of 10 cm; concluded that the river was safe to cross; and then drowned in it."*

AC: We are trying to move away from quoting a single number (i.e., cooling began at X Ma) and show a full distribution of model times at the cooling midpoint. The uncertainty of the FDHM is in essence expressing the uncertainty in the tT path envelope at the cooling midpoint isotherm. If RC2 would like us to recommend several distributions (i.e. quarter way through cooling, halfway through cooling, etc.), we are fine with that and happy to do it.

> **RC2:** *"At various places throughout the manuscript, the FDHM value is claimed to constrain the time of "peak cooling" (Figure 1). However, the second example (U-Th-He dataset) shows that this is not true. For exactly the same history as the first example, it returns a different FDHM value of 634 ± 12 Ma, evaluated at a different isotherm (70°C instead of 140°C). It does not become clear how this closure isotherm is chosen until line 243 of the manuscript points out that 70°C marks the time of maximum temperature sensitivity for the AHe method. This is a very different concept than the time of peak cooling."*

AC: The FDHM can be hypothetically applied to constrain the temporal distribution of model times at *any* chosen 'isotherm' along a model tT path. The cooling 'peak' is a designation.

We are pleased that RC2 recognized the main idea behind the apatite helium-only model in Figure 4 of the manuscript—that a single low-temperature thermochronometer such as AHe cannot adequately resolve a much longer cooling path that extends above the temperature sensitivity of the method. Yes, it is exactly the same history—but the input dataset we inverted is different (i.e., multiple vs. single low-T thermochronometer)—which is the key detail. The AHe-only model and corresponding FDHM are meant as a sensitivity test and cautionary example. Since we know the total amount of cooling from the predetermined tT path, the 140 °C isotherm represents the half-maximum at 700 Ma, which is the 'true' time of "peak cooling." However, the calculated FDHM at that isotherm is 778 +67/−107 Ma—much too 'old' and highly uncertain compared to the real value of 700 Ma (as presented in the manuscript). We fully agree that the FDHM and the 'maximum temperature sensitivity of the [thermochronometric] method' are different things, but they can nevertheless be similarly quantified using the FDHM approach. The FDHM calculated at the 70 °C isotherm (also canonical approx. AHe system closure) is 634 ± 13 Ma—meaning that the AHe technique can only constrain the thermal history $\leq$ that model time and temperature. We will make this more clear in the text.

> **RC2:** *"The concepts of an apparent age and closure/annealing temperature may be crude, but they have the advantage of reproducibility. In principle, two thermochronologists analysing the same rocks should obtain the same AFT central age or pooled helium age, say. I am worried that the same cannot be said about the FDHM method."*

AC: We agree. In principle, two thermochronologists considering the same thermal history using the FDHM method should obtain the same value as output. In terms of reproducibility, a critical aspect of the FDHM is that the user must specify the time interval or time domain within the tT model across which the FDHM is being calculated. The exact time interval over which the FDHM is calculated should be reported if the FDHM is used for interpretation. This also makes the FDHM method reproducible by anyone that uses those same boundary conditions. The FDHM is reproducible for any thermal history if the same variables and steps are repeated, similar to age or annealing temperature calculations. We are open to suggestions and invite RC2 to further test the FDHM on QTQt inversion results to get a sense of code implementation.

> **RC2:** *"Its definition is closely tied to the posterior likelihood space of the QTQt model. For small datasets, QTQt's RJMCMC model will produce simple models that can be easily summarised with an FDHM value (even if this value doesn't correspond to any geologically meaningful event).*

> *However, for large datasets, the solution space will include significantly more complex thermal histories, which will yield different FDHM values, or cannot be summarised with a single FDHM value at all."*

AC: We are not sure what RC2 means when they say the FDHM is closely tied to the posterior space of the QTQt model. Of course, the resolution and complexity of any inverted thermal history will affect the calculated FDHM (this is visible in the FDHM uncertainty bounds). However, this is an indirect result not inherent to the RJMCMC algorithm but is rather an expression of the resolving power of the data with respect to the complexity of the tT history. Furthermore, the multi-chronometer datasets used in our manuscript are *larger* than the majority of datasets commonly encountered in the published literature, and yet fairly simple thermal histories are still recovered in terms of their overall form—large datasets should, in many cases, actually reduce apparent thermal history complexity because more of the solution space is constrained by thermochronometric data. The increase in path 'complexity' (generally expressed as uncertainty—or a broader overall tT path envelope or paths with proportionally greater turning points) is clearly observed in the AHe-only model in Figure 4 of the manuscript or in the Canadian Shield example in Figure 8 where prior to 800 Ma there is high path complexity and low resolution of the thermal history. In terms of multiple FDHMs we refer to our previous comments on the schematic tT path provided by RC2 in Figure 1.

> **RC2:** *"This problem is aggravated by the fact that the RJMCMC algorithm can be tweaked in many ways. As mentioned on line 134 of the manuscript: "The time window, time interpolation step, and the histogram bin size (all in units of Myr) are variables that may require tuning based on the timescale of the specific problem under investigation"."*

AC: The text mentioned at line 134 of the manuscript does not refer to the RJMCMC algorithm in QTQt. The time window (or time domain), interpolation step, and histogram bin size all refer to the code that calculates the FDHM found at: `https://github.com/OpenThermochronology/CoolingFDHM`. For example, tuning of the histogram bin size matters if one has modeled a billion year thermal history vs. another model, like the Bergell example, that only spans a few 10s of Myr, requiring a finer/smaller sub-Myr time bin. This text will be clarified during editing if necessary.

> **RC2:** *"According to lines 178–179, " the option in QTQt to "reject more complex models that do not improve data fit" was not implemented since this explicit penalty is not a formal Bayesian Markov Chain Monte Carlo (MCMC) procedure and we were interested in examining the full suite of accepted histories". These many 'degrees of freedom' open a Pandora's box of 'designer ages'."*

AC: We thank RC2 for the opportunity to clarify a misunderstanding of the manuscript text that will be fixed. The quoted text simply refers to the fact that the RJMCMC algorithm did not explicitly penalize more complex paths with equivalent log likelihood—which is the original QTQt search algorithm formulation in Gallagher (2012). Later, an option was added to specifically prefer simpler histories (by penalizing more complex ones via the LL), which, as far as we are aware, is not a formal MCMC procedure. We are not sure what 'degrees of freedom' and 'designer ages' are referring to in this context. We reemphasize that the time of peak cooling calculated using the FDHM is not a thermochronological age.