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Discussion

Reply to Comment on “Thermal history modelling: HeFTy vs. QTQt” by K. Gallagher and R.A. Ketcham

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We would like to begin our Reply by expressing our appreciation for the authors of the Comment. Kerry Gallagher was one of the first to introduce quantitative inverse modelling to thermochronology (Gallagher, 1995), and Rich Ketcham has made crucial contributions to the study of fission track annealing (Ketcham et al., 1999, 2007). Out of respect for these contributions, we invited both authors to review our manuscript prior to publication so as to avoid any misunderstanding. Although they declined this invitation, we welcome the opportunity to engage in an important debate about the role of inverse modelling in thermochronology.

Gallagher and Ketcham’s (2017) Comment essentially rephrases the key points made by Vermeesch and Tian (2014, hereafter referred to as ‘the Paper’). These points are that (a) HeFty struggles to fit large datasets due to a combination of the ‘curse of dimensionality’ and its reliance on *p*-values; whereas (b) QTQt requires careful yet subjective inspection of the residuals to detect inappropriate model fits. In fact, Gallagher (2016) recently used argument (a) of the Paper against a publication co-authored by Ketcham (Flowers et al., 2015), and Ketcham used argument (b) of the Paper in his rebuttal (Flowers et al., 2016). Whilst there are many areas of agreement (“points [made by the Paper] are reasonable and even obvious”), and the Comment even repeats the quote in the Paper from George Box to caution against overinterpreting statistical models, the view was taken that our review was overly simplistic. In response we take this opportunity to clarify, expand, and sharpen the two key points made by the Paper.

1. HeFTy

The Comment maintains that argument (a) “may be valid in some abstract theoretical limit”, but should be of no concern in real datasets. We disagree. If an algorithm does not even work on paper, then how could it be trusted in the real world? Figure 2 of the Comment manages to find some statistically viable t-T paths for the 821-track dataset. The way in which these solutions were found is a perfect illustration of HeFTy’s shortcomings. First, a thermal history was fitted to the smaller (100 length) dataset, allowing only monotonic cooling paths. Then, one (Figure 2.b–c of the Comment) or two (Figure 2.d–e of the Comment) additional box constraints were created to guide the Monte Carlo search for the large dataset. This complex procedure is essentially a ‘hack’ to circumvent the limitations of the HeFTy algorithm. We maintain that our selection of large box constraints[1] is more sensible than the tiny boxes used in the Comment, which have no geological basis whatsoever. Of course such large boxes include many ‘impossible’ cooling paths. But is it not the job of the inverse modelling software to decide what is possible and what is not? This theoretical and practical issue is symptomatic of a deeper problem. To our knowledge, the so-called ‘Frequentist’ algorithm used by HeFTy is not used in any other field of Science. Although the program certainly has its merits in its ability to forward model thermal histories, it lacks the theoretical support to qualify as a bona fide inverse model.

2. QTQt

Fig. 1 of the Comment shows that QTQt can fit polynomial data. Of course it can, but this misses the point. The point that the Paper tried to make is that QTQt-like algorithms are able to find tightly constrained solutions under incorrect model assumptions. This was illustrated in a regression context by fitting a linear model to some polynomial data. A good example of the same problem in a thermochronological context would be the typographical error in Ketcham et al. (2007) that was reported in the Comment. The corresponding bug in QTQt remained undetected for five years precisely because it did not prevent the program from producing thermal history solutions.

A final issue that we would like to address in this Reply is the brief remark about the colour-coding scheme used by QTQt, which the Paper referred to as a ‘graphical trick’. The Comment objects to this term and argues that the colour shading has statistically sound foundations. The shading shows the “marginal distribution of the posterior assemblage of temperature with respect to time”. This procedure (which was inherited from Sambridge et al., 2006) projects 4-, 6- or higher dimensional t-T paths, all of which are highly correlated with each other (Willett, 1997) on a 2-dimensional plane. Unfortunately, a tremendous amount of information is lost in this process, potentially generating misleading results. To illustrate the problem, consider an episodic thermal history

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[1] Initially, we wanted to use a single large box but this even failed to yield a solution for the small dataset.

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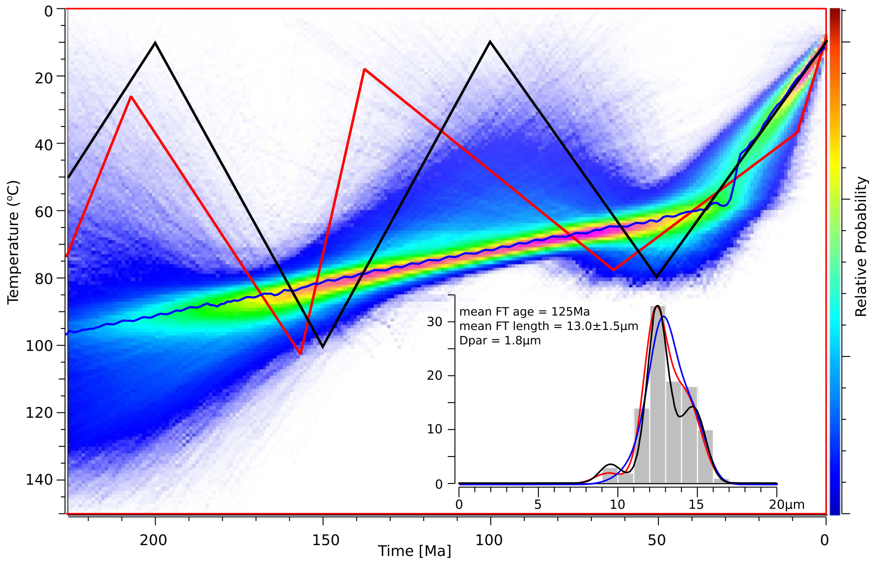

Fig. 1. An example to show that QTQt's colour-coding scheme may produce misleading results. The black line is the true thermal history (main figure) and c-axis projected track length distribution (inset). The grey histogram (inset) represents a random sample of 100 track lengths drawn from this distribution. The red line is the maximum likelihood solution. The blue line shows the 'expected model'. This completely misses the first two cooling episodes. Thermal histories only go back to 250 Ma, which is twice the fission track age, as per QTQt's default settings. An extended version that goes back to 300 Ma is provided in the Supplementary Information. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

that includes linear cooling from 180° C at 300 Ma to 10° C at 200 Ma, followed by linear heating to 100° C at 150 Ma, a second phase of linear cooling to 10° C at 100 Ma, a third phase of linear heating to 80° C at 50 Ma, and a third phase of linear cooling to 10° C at 0 Ma (black line in Fig. 1). This history was forward modelled using HeFTy to create a synthetic fission track dataset of 100 lengths (histogram in Fig. 1). Inverse modelling this synthetic dataset with QTQt yields a best fitting (maximum likelihood) history that approximates the true history reasonably well. Unfortunately, this is not the case for the 'expected' t-T path, which follows a simple hockey-stick trajectory and completely misses the first two cooling episodes. The tightness of the yellow-red shaded zone of the marginal distribution gives false confidence in this oversimplified thermal history. It reflects the tight clustering of the simple models, which graphically dominate the more accurate but less precise models in the posterior distribution.

3. Conclusions

Much can be learnt from visual inspection of grain age distributions, compositions and fission track length distributions. Such an analysis is not necessarily more subjective than the interpretation of continuous t-T reconstructions. Thermochronology is a remarkably powerful tool for understanding upper crustal processes, but it does have limitations. A typical thermochronological dataset comprising 20 single grain age determinations and 100 track length measurements, say, simply does not contain enough information to reliably constrain all but the simplest t-T histories. This conclusion is supported by QTQt's reversible jump MCMC algorithm, which tends to support only crude V-shaped t-T paths. For larger datasets, the ability to constrain continuous t-T paths is hampered by the non-uniqueness of forward models (see Figure 14 of Green, 2012). We agree with the Comment that inverse modelling should be about asking the right questions of a data set. It can be very useful to target specific questions and constrain specific parameters (Braun et al., 2012). But in our view, estimating continuous t-T histories may not always be that right question. The main purpose of the Paper was to provide a fair and balanced review of two popular software packages for thermal history modelling, and to provide non-specialists with basic insights into their inner workings. Our contribution has triggered a lively discussion about the sense and purpose of inverse modelling (Flowers et al., 2016; Gallagher, 2016; Gallagher and Ketcham, 2017; Vermeesch and Tian, 2017). We hope that the thermochronological community will benefit from having this important debate.

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