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Technical note: Disentangling pre- and post-depositional thermal histories in partially reset samples

Birk P. Härtel, Eva Enkelmann, and Akeek Maitra

Dear Editor,

we appreciate the review comments by Dr. Benjamin Gérard and Dr. Andrea Stevens Goddard. In general, they found no technical flaws in the proposed modeling approach or its presentation, but made valuable suggestions that helped us improve the clarity of the manuscript. In response, we made several minor changes to the manuscript such as: (1) including an explanation for the selection algorithm of high-likelihood thermal-history paths, (2) emphasizing the difference between the conceptualization of our approach and previously suggested strategies, and (3) adding a section about the *PaRACAS* workflow that accompanies the manuscript.

In our opinion, the scope and presentation of our manuscript have strongly benefitted from these changes. We feel that the revised manuscript can be considered for publication. Please find below the specific replies (**A**) to the *reviewer comments* (**R1**, **R2**).

Kind regards,

Birk Härtel for the co-authors

Reviewer #1 (Dr. Benjamin Gérard)

We appreciate the reviewer comments by Dr. Gérard. We are pleased to see that he agrees with the overall concept of the presented approach and are grateful for suggestions to improve the manuscript and the accompanying jupyter notebook.

Please find below the *reviewer comments* (**R1**) and the authors' responses (**A**).

R1: *General comment*

This manuscript presents a new workflow for interpreting partially reset detrital zircon U/Pb–(U-Th)/He double-dating data by combining inverse thermal-history modeling of syn-depositional grains with forward modeling and a likelihood-based evaluation of pre-depositional model ages. Overall, I found the manuscript to be scientifically sound, well-written and well-structured. The study addresses an important methodological problem in detrital thermochronology and provides a practical solution that is likely to be useful for future applications. The manuscript does not aim to introduce a fundamentally new thermochronological model but rather proposes an elegant integration of existing concepts into a coherent and reproducible workflow. In my opinion, this is fully appropriate for a Technical Note in GChron. The methodology is generally clearly presented, the synthetic example effectively illustrates the workflow, and the application to the Canadian Cordillera demonstrates that the approach produces geologically meaningful results consistent with previous independent studies. Importantly, the manuscript remains appropriately balanced regarding the capabilities and limitations of the method. I did not identify conceptual inconsistencies or methodological flaws that would require major revisions. Most of my suggestions therefore concern clarification, presentation and readability. I recommend publication after minor revision.

Main comments of the manuscript

Section 2 – Selection of the best-fitting thermal histories: The use of a knee-detection algorithm (Satopää et al., 2011) to define the likelihood cutoff is an interesting and apparently objective way of selecting acceptable thermal histories. However, this choice is introduced rather briefly. Since this algorithm may not be familiar to many readers in the thermochronology community, I encourage the authors to add one or two sentences explaining the rationale for using this approach and its advantages over a more conventional fixed likelihood threshold.

A: The likelihood of each path depends on many sample-specific factors such as the number of dated grains, their uncertainties, age distribution, and the extent of resetting. That is why we decided not to apply an absolute likelihood cutoff. In contrast, the knee-detection algorithm uses the differences between the ranked likelihoods, choosing the cutoff where the likelihoods cease to change dramatically between paths of neighboring ranks. Thereby it selects a group of highest-likelihood paths with the likelihood spread still allowing to differentiate their fit with the expected age interval. It excludes the less-likely paths that are also more difficult to distinguish by likelihood alone. We agree that a more detailed description in the manuscript is necessary and will add this explanation.

R1: *Section 3 – Practical guidance on selecting inversion grains: One practical aspect I wondered about concerns the initial selection of syn- or near-syndepositional grains used for the inverse thermal-history modeling (blue circles). While the manuscript explains how these grains are identified, it would be helpful if the authors could briefly comment on the extent to which the inferred post-depositional thermal histories are expected to depend on both the number and representativeness of the selected grains for the initial inversion. Even a short qualitative discussion would provide useful practical guidance for future users of the workflow.*

A: We will add a short explanation to section 4.1. In general, we suggest to treat the inverse-modeling step roughly similar as inverse modeling of bedrock samples because the syn-depositional grain population essentially underwent a single thermal history. Therefore, aiming for 3–10 grains as in typical bedrock studies (Reiners, 2005; Flowers et al., 2022) can be a useful rule of thumb. The representativity is not necessarily a problem for our approach, however, using atypical (e.g., very small) grains for the inverse-modeling step can introduce bias towards too-high- or -low-temperature paths requiring more paths to be modeled. We will also expand the discussion on how to model the data if no or not enough syn-depositional grains are available.

R1: *Discussion / Conclusions: The manuscript clearly discusses several simplifying assumptions and possible improvements (e.g., U-Th zoning, radiation damage, He concentration profiles, laser-ablation geometry). It could nevertheless be worthwhile to conclude with a brief perspective on the future development of the PaRACAS workflow. A short paragraph outlining the main priorities for future versions of the code would nicely emphasize that the current implementation provides a flexible framework that can accommodate these refinements.*

A: We agree that such an outlook is worthwhile. We will therefore include a short subsection introducing PaRACAS and its future directions toward apatite (U-Th-Sm)/He and fission-track dating, and He-diffusion modeling for zoned crystals.

R1: *Minor Specific/technical comments*

General: Most figures appear blurred or compressed, particularly when viewed at higher magnification. Providing higher-resolution versions for the final publication would substantially improve readability and the overall presentation quality.

A: We will make sure to provide figures at the right resolution for final production.

R1: *Figure 1: The schematic pre-depositional thermal histories (grey paths) are all illustrated as monotonic cooling trajectories that eventually reach near-surface temperatures prior to deposition.*

While this is perfectly adequate as a conceptual illustration, I wondered whether this representation might inadvertently suggest that the proposed workflow assumes monotonic pre-depositional cooling or complete exhumation of all source rocks prior to deposition. One of the main strengths of the method, as I understand it, is precisely that it does not require prescribing a specific pre-depositional thermal history. It may therefore be helpful to briefly clarify in the text or figure caption that these grey paths are intended only as illustrative examples and are not meant to represent a methodological constraint.

A: We agree this may come off as ambiguous. We will add a short comment to the caption that these are only schematic cooling paths to represent the individual T-t trajectories of each grain.

R1: *Figure 2: The figure is very informative and successfully highlights the differences between the three workflows. If possible, the authors may consider harmonizing the time-axis scales across some of the thermal-history panels or explicitly emphasizing why different time windows are shown. This could facilitate visual comparison between the different approaches.*

A: We will add a note to the description of the three strategies in the text, regarding their different assumptions about the pre-depositional thermal histories with references to the visual elements in Figs. 2c and 2f.

R1: *2f: Unless I overlooked it, the meaning of the vertical grey lines is not explained in either the figure caption or the main text. I assume they indicate the individual U-Pb ages of the synthetic grains, but a brief explanation in the caption or in the text would make the figure more self-contained.*

A: We will add a reference to the grey lines when introducing Fig. 2f.

R1: *Lines 83-85: The authors may also consider citing the following field-based study, which documents the influence of radiation damage on effective ZHe closure temperatures:*
Gérard, B., Robert, X., Grujic, D., Gautheron, C., Audin, L., Bernet, M., Balvay, M., 2022. Zircon (U-Th)/He Closure Temperature Lower Than Apatite Thermochronometric Systems: Reconciliation of a Paradox. Minerals 12, 145. https://doi.org/10.3390/min12020145

A: We will add the reference to the text.

R1: *Line 93: Typo? According to Supplementary Table T1 and Figure 2, the minimum grain radius is 38 μm, not 36 μm.*

A: It is indeed 38 µm. We will correct this typo.

R1: *Line 151: Typo. "each of these**s** paths" >> each of these paths*

A: We will correct this typo.

R1: *Line 176: Grammar. "confirms the validity this approach" >> confirms the validity* ***of*** *this approach*

A: We will correct this error.

R1: *Line 216: Grammar. "25 out 30 grains" >> 25 out of 30 grains*

A: We will correct this error.

R1: *Line 224: Typo. "expected envelop" >> expected envelope*

A: We will correct this typo.

R1: *Line 504: Typo. "misift" >> misfit*

A: We will correct this typo.

R1: *Check consistency of forward-modeling vs. forward modeling. Both spellings appear throughout the manuscript.*

A: We will correct this in the manuscript.

R1: *Likewise, check consistency between temperature-time (**T–t**) and **T-t**.*

A: We will check the consistency and use T-t in the manuscript, introducing it upon first appearance in the text and in the figure captions.

R1: *Notebook documentation: Typo in "1 Load functions": "kneed an seaborn" >> "kneed and seaborn". The installation example could also be updated to include both required packages (e.g., pip install kneed seaborn).*

A: We are grateful for the comments on the errors in the jupyter notebook and its documentation. We will correct the typo and update the installation example in the newest version of PaRACAS (v1.02).

R1: *Run 1 Load functions: The notebook runs correctly, but it raises a minor deprecation warning when importing display and HTML. Replacing "from IPython.core.display import display, HTML" with "from IPython.display import display, HTML" would avoid this warning in recent IPython versions.*

A: We will follow the suggestion and replace the code for importing display and HTML.

R1: *Plot modeling results: The notebook runs well, but I encountered a matplotlib compatibility issue when plotting the modeling results. The error occurs when creating the colorbar in Visualization.py (plt.colorbar(mappable)), with recent versions of matplotlib requiring an explicit* *axis argument. Replacing this with, for example, plt.colorbar(mappable, ax=plt.gca()) appears to solve the issue. This is a minor technical point.*

A: We will fix the problem by adding an explicit axis argument to the plotting functions.

R1: *Plots for zircon raman: The variable axis_range_model_ZR is used in the plotting section but is not defined. It appears that axis_range_model_ZHe should instead be renamed to axis_range_model_ZR. This is a minor typo, but it currently raises a NameError when executing the notebook.*

A: We thank Dr. Gérard for catching this error in the code. We will rename the variable.

R1: *Abrasion helper: The default pit-geometry values are set to zero (r0 = 0, h = 0), which produces NaN values if the cell is run without modification. It may be helpful to either use realistic example values or add a warning that non-zero pit dimensions are required.*

A: We will add warning comments next to the code, set the default values to 10 and 6 μm for the radius and depth, and added a quick check to the code ensuring values greater zero are used.

Reviewer #2 (Dr. Andrea Stevens Goddard)

We thank Dr. Stevens Goddard for the constructive comments on our manuscript. We are pleased that she agrees with the overall scope of our modeling strategy and appreciate her suggestions for improving motivations and the description of the evaluation and outcomes of our new approach.

Please find below the *reviewer comments* (**R1**) and the authors' responses (**A**).

R2: *General Comments:*

This technical note presents a new workflow for interpreting pre- and post depositional histories of partially reset thermochronology data with specific descriptions using the zircon (U-Th)/He system. I appreciate that this contribution provides a practical presentation of this approach using first synthetic data with known thermal solutions as well as an example using real data from a well studied region with additional published thermochronology data to evaluate the effectiveness of the new workflow. The content is well suited to a technical note and will provide valuable guidance for workers interpreting these complicated data sets. The text is well written and the methods are mostly clear with a few opportunities for clarification that will strengthen the manuscript. This is a valuable and practical contribution that will be used in the thermochronology community and I look forward to seeing it published in GChron.

Specific Comments:

1) I think one point of clarity made throughout the manuscript, but introduced really explicitly in the introduction, will help readers follow the goals of the workflow. It took me quite some time to figure out that the "deliverables" were different data types for pre- and post-depositional thermal histories. As I understand it, the workflow delivers a t-T history of the post-depositional thermal history and ZHe model ages that are the calculated ZHe age before subsequent reheating. I think the hang up for me was wrapping my mind around the fact that this workflow does not look at pre-depositional thermal histories. I think this should be easy to make clearer throughout the text. I specifically recommend being clear about what inversion results (from the synorogenic volcanic grains) are being evaluated by the pre-depositional model ages.

A: We agree that avoiding assumptions about the pre-depositional history is the main innovation in our approach and that the actual outcomes of the modeling process can be made more explicit. We will add short notes on these characteristics of our approach to the introduction, and the detailed description of the modeling procedure in section 2.

R2: *2) I find it interesting that the corrected ZHe ages are not put in context of the eU. I realize that using this reconstruction the values have evolved, but I also think eU is such an important part of the story because it is a critical control on the measured cooling age and whether that is reset, unreset, or partially reset (as is put so well in lines 35 – 38!). I would certainly find it* *valuable to see a plot of the correct ZHe age and corrected eU (or maybe even corrected and measured eU??) as I am trying to wrap my brain around this. I am sure these plots exist and there may be a good reason we don't have them, but I think it is the first thing many readers will be curious to see. I leave it to the authors to move forward with that feedback as they see fit.*

A: Tracing the radiation-damage density and its accumulation rate (i.e. eU) over the thermal history of individual grains for quantifying their relative temperature sensitivity is indeed an intriguing possibility. However, the eU concentration is only a useful proxy for lattice damage and its effect on He diffusivity when comparing grains that experienced similar thermal histories. eU concentrations at a specific time (present day, time of deposition, or at the pre-depositional model age) represent only damage-accumulation rates whereas the actual damage densities depend on the unknown pre-depositional thermal histories.

An approach that appears more practical to us is back-tracking present-day radiation-damage measured by Raman spectroscopy throughout the post-depositional thermal history based on the inverse-modeling T-t paths and the damage annealing kinetics. This allows to integrate the radiation-damage evolution into the diffusion-modeling procedure sticking to our premise of not assuming a pre-depositional thermal history. We will add the integration of measured lattice damage and He diffusion to the explanation in section 4.1 of the manuscript.

R2: *3) One thing that I think could be very interesting and valuable to readers is to discuss possible opportunities/next steps for how to treat or group the corrected ZHe ages. In a broad sense, what do we do with these ages? Do we interpret just the corrected ages themselves? Do we model them? It is a new type of data and this is a meaningful opportunity to provide direction on potential interpretation strategies for this (very cool) data. The first place my mind goes is how I put the corrected ZHe ages in context of the U-Pb. The text seems to suggest that individual grains represent unique cooling histories, but the combination of U-Pb with ZHe has the power to identify trends for different sources (defined by U-Pb) and different cooling histories from single sources (defined by U-Pb and clusters of incompatible ZHe ages). This may be a particularly meaningful point for those who are not using ZHe laser ablation, but rather selecting U-Pb grains (with ages already measured) for ZHe. It could be useful to check out Fosdick et al. (2024) in Geology (doi: 10.1130/G52272.1) which defines "U-Pb-ZHe" modes as a strategy for reconstructing thermal histories from detrital data.*

A: We suggest interpreting the coupled U/Pb and pre-depositional ZHe ages in the same framework as unreset detrital ZHe-U/Pb data, e.g., by using the age-age relationship to find populations that cluster around the same ZHe and U/Pb age, or grains that formed at the same time but underwent different pre-depositional thermal histories (e.g., Rahl et al., 2003; Reiners et al., 2005; Malusà et al., 2022; Fosdick et al., 2024). We will add a paragraph to the end of section 2 in the manuscript.

R2: *4) All grains are "syndepositional grains" because they are deposited at the time of deposition (this description is circular). I think what is meant here is volcanic grains that have syndepositional ages. I recommend just saying "volcanic syndepositional grains" for clarity.*

A: Our "syn-depositional" refers to grains that crystallized at our near the time of deposition. While these are likely of volcanic or shallow-magmatic origin, we prefer referring to them as syn-depositional grains for simplicity. We will include this definition early in the manuscript to avoid ambiguity.

R2: *5) I think most thermochronologists are not familiar with a knee detection algorithm. I suggest a brief description of what this is and the goal of using this algorithm in this workflow. 2-3 sentences seems reasonable.*

A: We agree that more details on why we chose this algorithm and how it works are necessary. Our goal is to select high-likelihood paths for further interpretation of the modeling results. The likelihood depends on several factors including the number of dated grains, their uncertainties, age distribution, and the extent of resetting. An absolute likelihood cutoff (e.g., all above 0.05) is therefore not useful when comparing different samples. In contrast, the knee-detection algorithm uses the differences between the ranked likelihoods and sets the cutoff where the likelihood ceases to change dramatically between paths of neighboring ranks. We thus obtain a selection of the highest-likelihood paths with the likelihood spread still allowing to differentiate their fit to the constraints. Conversely, we exclude less likely paths that are difficult to distinguish by their likelihood. We will include this description in the manuscript.

R2: *6) The text is missing a brief description of the zircon raman temperature sensitivity. The description can be very brief, but it should put it in context of the ZHe system.*

A: Our application example cited the PAZ boundaries of Härtel et al. (2021); we will add the information that these ranges overlap the ZHe PRZ.

R2: *Technical Comments:*

Figure 1: t-T space gets young to left which is opposite of most figures (probably because these are HeFTy and QTQt outputs). Also is opposite of Figure 2. Maybe to fit (b) the distribution of single grain ages plot? Consider flipping the x-axis.

A: We will flip the axes in Fig. 1 to make (a) more comparable to the plots in Figs. 2 and 3, but keep the same axis for both subplots.

R2: *Line 35 delete comma after "both"*

A: We will correct this in the revised manuscript.

R2: *Line 36 – by degree, means temperature? (degree meaning magnitude or temperature?)*

A: We will rephrase this sentence to avoid ambiguities.

R2: *Line 40. Replace colon with period and delete "on the one hand"*

A: We will correct this in the revised manuscript

R2: *Line 42: Delete "on the other hand"*

A: We will rephrase this sentence.

R2: *Line 55: It would be helpful to have an example of these assumptions. Or rephrase here (for example "rely on assumptions about the geologic history of the source lithology"*

A: We will add examples for such assumptions such as the timing of initial cooling or the duration and magnitude of heating events in the source regions.

R2: *Lines 77/79: delete "on the one/other hand" – it doesn't match the structure of the argument.*

A: We will rephrase this sentence.

R2: *Line 173: "one the one hand" doesn't match the structure of argument here. Replace with something like, "The strategy preserves*

A: We will rephrase this sentence.

R2: *Line 259: I recommend adding "additional lower-temperature thermochronometers" for clarity*

A: We will modify this sentence as suggested.