

We thank Dr. Kirkland for reviewing this manuscript, and his comments will help us substantially clarify the manuscript.

This study continues the concept of extracting age information from discordant zircon U-Pb data, particularly in detrital zircon suites. Traditional geochronology often discards discordant data, but this approach leverages discordance to date post-depositional geological events like fluid alteration and contact metamorphism. The paper applies a technique introduced by Reimink in 2016. The method is validated using synthetic data and applied to zircons from the Alta Stock metamorphic aureole, successfully dating a ~23 Ma alteration event. This technique should have implications for dating fluid flow, low-temperature metamorphism, and sedimentary basin evolution.

Introduction & Framing

The study builds upon Reimink et al. (2016) by introducing a useful refinement to an existing core technique. As such, it may be more effectively presented as a technical note that directly highlights the specific methodological improvement. Specifically, I am not convinced that the introduction needs to be structured with the basic conceptual framework of U-Pb geochronology and its uses. I would have thought that most / all readers of this journal would be well informed of the basic concepts. Also, there are elements of similarity with some previous works on the subject area starting the work in this way. In any case, I think it would be more efficient and productive for this work to be more direct about inverting discordant data to better understand its effect. So, in short, the work could commence around line 78 without any detriment to the new insight the work aims to convey.

This comment is similar to that of Dr. Ickert and it will be relatively simple to modify the manuscript to accommodate these suggestions. We have removed the first several paragraphs of the basic conceptual framework material, start the introduction with a discussion of discordance in U-Pb data, and treatments of such data (see below). We have expanded the already present discussion of discordant data treatments, as highlighted in specific responses below.

How the Study Represents the Field

I am concerned that the general depiction of the field, as not aiming to use discordant data, is not an accurate portrayal of the current community knowledge. Please let me elaborate on this: U-Pb discordance has long been known and modelled via discordia regressions and their lower intercepts interpreted with various success as the times of meaningful geological events. Clearly with additional scatter from a single Pb loss line interpretation of the timing of radiogenic Pb mobility becomes difficult if not

impossible to determine using conventional regression approaches. However, as I am sure the authors are well-aware there is now a wide range of works that have proposed methods to address this complexity and extract meaningful times for Pb loss. Specifically, the following works all introduce methods to invert discordant data to resolve Pb loss times.

Sharman, G. R., & Malkowski, M. A. (2024). Modeling apparent Pb loss in zircon U-Pb geochronology. *Geochronology*, 6(1), 37-51. <https://doi.org/10.5194/gchron-6-37-2024>

This paper was not initially cited because the modeling approach outlined in that work was designed to identify Pb-loss from a single population of magmatic grains, with the goal of better resolving igneous or volcanic ages. That work did not fundamentally use discordant data in the way other work we cited did. However, Dr. Kirkland makes a good point that the Sharman and Malkowski work deals with new approaches to discordant data, and citation in our manuscript is therefore useful to readers. We have included a discussion and citation in the revised introduction.

Morris, G. A., Kirkland, C. L., & Pease, V. (2015). Orogenic paleofluid flow recorded by discordant detrital zircons in the Caledonian foreland basin of northern Greenland. *Lithosphere*, 7(2), 138-143. <https://doi.org/10.1130/L420.1>

The Morris, et al., 2015 manuscript is cited in the manuscript in the section where discordant data treatment approaches is outlined. By our reading, this was the original derivation of the method that eventually came to be called Concordant-Discordant Comparison and was cited for that reason. We have developed a more robust introduction and description of this, and related, methods in the newly revised introduction, following the earlier comments by Dr. Kirkland and Dr. Ickert.

Kirkland, C. L., Abello, F., Danišík, M., Gardiner, N. J., Spencer, C., & (2017). Mapping temporal and spatial patterns of zircon U-Pb disturbance: A Yilgarn Craton case study. *Gondwana Research*, 52, 39-47. <https://doi.org/10.1016/j.gr.2017.08.004> 747

We had not initially cited the Kirkland et al., 2017 work as it derives the fundamental methodology from Morris, et al., 2015. However, it does appear to be the first time that the CDC method is introduced by name, so this paper is now referenced in the newly revised introductory text, which is outlined below.

Kirkland, C. L., Johnson, T. E., Kinny, P. D., Kapitan, T., & (2020). Modelling U-Pb discordance in the Acasta Gneiss: Implications for fluid-rock interaction in Earth's oldest dated crust. *Gondwana Research*, 77, 223-237.
<https://doi.org/10.1016/j.gr.2019.07.017>

This manuscript was not cited as it did not appear to advance the methodology, but applied the existing discordant zircon treatment methods to a different sample location.

My point simply is that a lot of emphasis is being placed on the term “most” in the statement “most modern U-Pb studies aim to minimize its effect rather than understand or use it”.

We apologize that our wording in this sentence has led to a mischaracterization of the manuscript. Our intention was to highlight the relative lack of focus on discordant zircon U-Pb data (several papers in the past several years) as compared to the broader uses of zircon U-Pb data (several thousand papers in the same timeframe), which we believe was appropriate.

Nevertheless, we do not wish to give the impression that zero work has gone into evaluating discordant zircon U-Pb data (work which is highlighted later in the manuscript). The changes outlined for the introductory text will hopefully alleviate these concerns.

Nothing would be lost from the advance this work makes by better framing it in the context of the existing field working on exactly the problem addressed in this paper.

We have now added in a full discussion of the approaches outlined above, including a discussion of the CDC method’s performance on the Alta DZ data presented here.

So, it would seem reasonable to also acknowledge there are a range of other techniques which also aim to invert discordant data to arrive at the most likely time of radiogenic-Pb mobility. Providing this context would better frame the advance of this work.

This comment has been addressed by restructuring the manuscript to begin the introduction with a discussion of discordance and provide more detail about the various approaches that different methodologies have used to extract age information from discordant data.

We now start the manuscript with a short introduction to discordant U-Pb data, then outline various approaches to treating discordance, using one paragraph for each general class of models – traditional approaches, sedimentary zircon discordance events, the CDC test specifically, resolving age mixtures, and the quantified removal of discordance (Pb-loss).

This then flows directly into the model presented in the present work, which concludes the shortened introduction while also giving a more thorough overview of the various approaches to discordance (or Pb-loss as it is called by other works).

Methodological comments

I am not convinced that the statement in line 96 is accurate “Without the constraint of a single, shared geologic history, no discordant datum can be confidently related to another datum, whether it is discordant or concordant.”

We apologize for the wording that led to this misreading of our intention. Our phrasing here is only meant to explain that a single discordant data point cannot be interpreted on its own. That basic concept may not need to be pointed out to the readership of Geochronology.

As shown from other works seeking to invert discordant data the reality is that discordant data is, more often than not, derived (in your words “related to”) from the same geological provenance (e.g. discordant data and concordant data is ultimately derived from terranes that share one or more connected formation ages). This connection can be probabilistically assessed and used in the inversion problem.

While many zircon datasets may allow for safe use of the assumption that discordant analyses are directly derived from the concordant data, this is still an assumption (for cases where this assumption may not be valid, see Donaghy et al. 2024, Geochronology). In particular, variable discordance may be imposed on different age populations in such a way that any comparison statistical tests aimed at probabilistically assessing goodness of fit are inaccurate (see discussions below regarding the CDC test and the Alta dataset presented here). Responses to later comments show more information regarding this aspect.

Even if there is a perfect statistical match between reconstructed discordant and concordant zircon datasets, that is not a firm guarantee that any lower-intercept age derived from such a comparison is valid. We cannot validate geological relationships with statistical tests, we may only invalidate them. All discordant data treatment methods, including the one presented in our work, and as shown by our modeling, are susceptible to various limitations depending upon the

assumptions involved in the analysis, and caution is required in the treatment of the statistical approaches here.

The revised outline of the introduction would alleviate this particular concern, but this comment helps make the case that our sensitivity and uncertainty modeling test (Section 2) remain in the manuscript to robustly outline the assumptions and limitations of the discordance dating technique, as exposed in the modeling and discussion in those sections of the present manuscript.

Line 98, the concept of “strict” or not in terms of discordance is a bit nebulous and would be better framed as within or outside the analytical confidence bounds.

This comment is easily addressed by changing the wording from “strict” to “discrete”, which better conveys our original meaning of simply using a discordance filter (e.g., 10%, 20%, etc) when treating U-Pb data.

Line 101 the paper at this stage in the text now reverts to acknowledge that there are other approaches to invert discordant data. This creates a bit of a non sequitur with what was introduced around line 80.

Our intention in the earlier sections was to highlight the relative lack of research focus on discordant data, not to give the impression that no other work was done on discordant data. A rewritten introduction as outlined above hopefully satisfies this concern, and we apologize for the way that the original introduction read, it was not our intention. We now fully discuss other discordant data treatment approaches, and have added a full section discussing the outputs of the CDC method in detail.

Also, the list of works focused on this topic is curiously incomplete. I would have thought that the author would have been familiar with the work on Acasta that uses Pb loss modelling to derive most likely times of fluid-rock interaction?

We are well aware of the work referred to here (Kirkland et al., 2019; Gondwana Research). It is not cited here because it simply used the CDC method outlined by Morris, et al., 2015, Lithosphere; Olierook, et al., 2021, Gondwana Research, work that is cited. We did not deem it necessary to cite all papers that have used CDC or equivalent methods for investigating discordant data from a variety of locations.

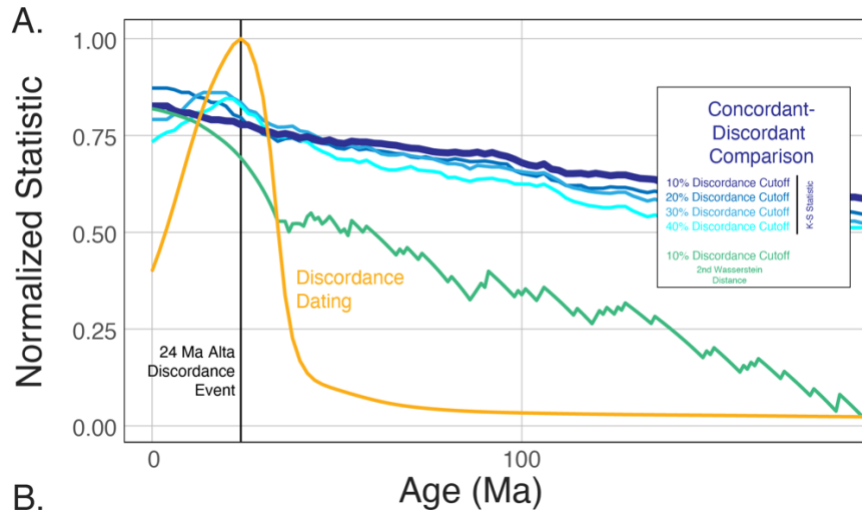
While the method is contrasted against linear regression approaches (e.g., IsoplotR), other discordance modelling techniques (e.g., isotope diffusion modelling, Bayesian approaches) are not considered. A discussion on how this method compares would strengthen its utility.

Apologies, our meaning here was seemingly not conveyed accurately. We do not 'contrast' our approach with linear regression, we are using linear regression to "benchmark our approach against isochron regression techniques". Meaning, we use linear regression to determine the validity of the discordance dating approach.

We did not include a comparison of the modeling conducted here with the CDC method (which we assume Dr. Kirkland means when mentioning Bayesian methods in this comment) because in our initial testing, the CDC method appeared to be inappropriate for the natural data we present, natural data which we modeled the synthetic data after. This is likely due to several reasons (see revised Section 3.3).

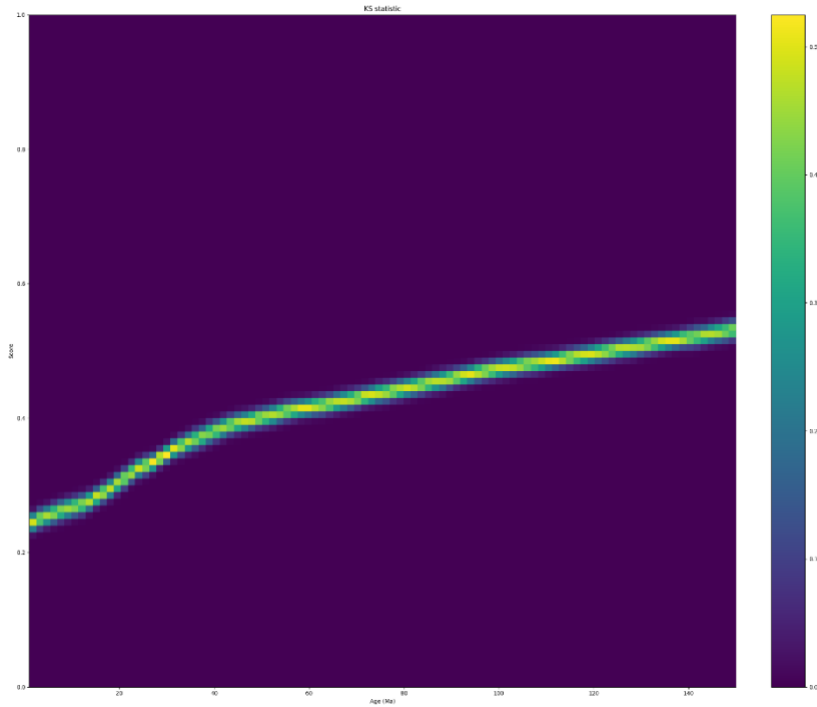
However, Dr. Kirkland is correct that a full discussion of the CDC method strengthens the manuscript and highlights the utility of discordance dating. We now include a comparison of the CDC method as applied to our Alta Tintic formation zircon sample set. The key conclusions are that 1) The CDC method does not resolve the lower intercept age at 24 Ma, and 2) the reason for the CDC method's underperformance is likely to do with the a) reliance on concordant data, and b) the use of K-S or other 'similarity' metrics that rely on not only peak location, but peak height.

This can be seen below. Here we show the outputs from our own calculations that replicate the CDC statistical test. The blue lines are the CDC models applied to the Alta DZ data (71/407 concordant data), with colors corresponding to various discordance cutoffs. Note that we inverted the K-S statistic such that 1 is a perfect match, in order to directionally compare to our discordance dating outputs. No peak is obvious in the CDC data until an unrealistically high discordance filter of 30-40% is used (light blue line), but even then, the peak is small and quite broad. When using the CDC methodology, and using a Wasserstein distance comparison (Lipp and Vermeesch, 2023), the CDC approach does not resolve any peak in the Alta pluton age range.



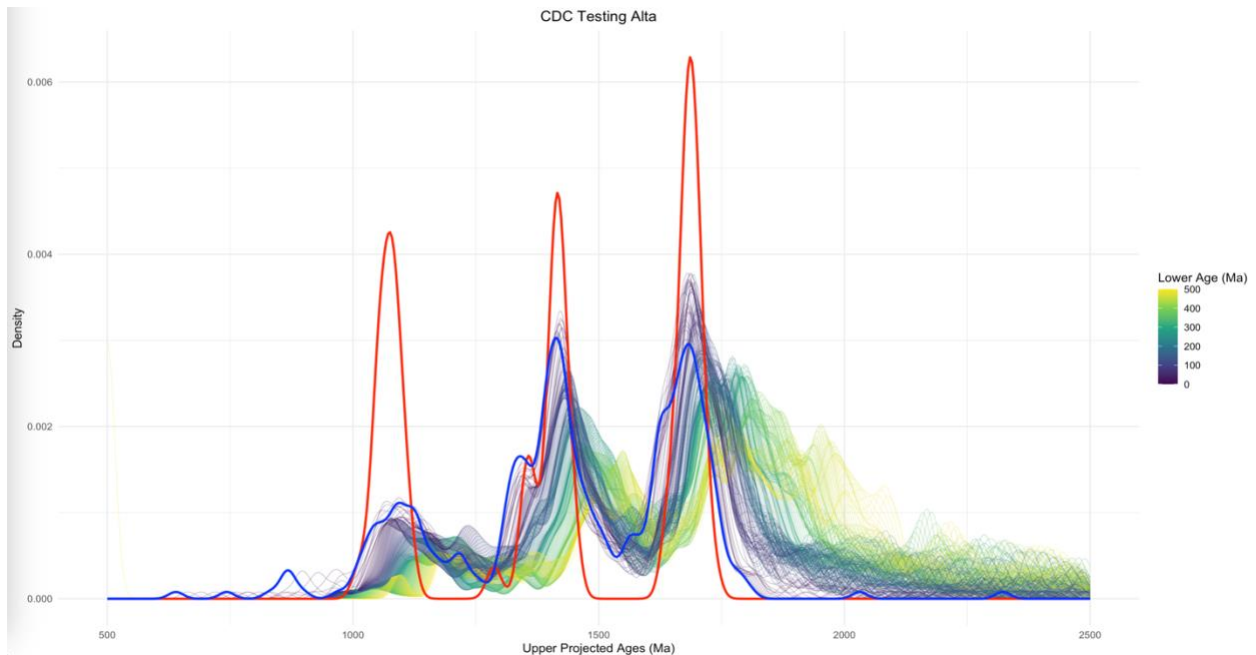
B.

Dr. Kirkland's review made us aware of a paper posted on an archive (Mathieson et al.) that was posted publicly after our manuscript was submitted and reviewers had been assigned. That archived manuscript contains code for CDC modeling that allowed us to validate our internal reproduction of the CDC method, which compares well (shown below). Note that the small differences between the CDC method and our own derivation of the CDC method may be due to the Monte Carlo simulations of analytical uncertainty in the Mathieson et al version of the CDC method, small differences in the K-S statistic parameters between our code and that of Mathieson et al., or the fact that our derivation is calculated using Wetherill concordia as opposed to Tera-Wasserburg concordia space.



Importantly, we highlight that we are not showing this to condemn the CDC method. We are simply documenting that the CDC method should not be expected to perform well with the Alta data due to the relative lack (71/407) concordant data points in the dataset.

In fact, the reason that the CDC method does not return accurate or precise chronology results for the Alta stock data requires further investigation. Our analysis suggests that underperformance of the CDC method is partially due to the reliance on comparison tests (K-S test statistics or comparable methods). Results from our testing of the CDC method are shown below.



In this image, the red lines are the 7/6 ages of the concordant data population (all lines are a kernel density estimators using 15 Ma bandwidth). The other curves are CDC projections from various lower intercept points (the color reflects the lower intercept age) through the discordant data points and we show the distribution of those recalculated upper intercept ages. Importantly, the discordance dating age of 24 Ma is shown in the blue curve.

Using a 24 Ma lower intercept, the resulting recalculated data does indeed return correct peak positions, but the relative height of those peaks does not closely match the concordant data point age distribution, hence the relatively poor comparison metrics. The K-S statistic accounts for differences in relative peak heights as well as positions, so the red and blue curves do not yield highly comparable distributions when using that comparison statistical test.

An improved CDC method that simply compared peak locations between concordant and modeled upper intercepts could possibly remove any potential biases induced by preferential discordance imposed on different populations. For instance, perhaps the 1.1 Ga zircon peak in the Tintic formation was more immune to discordance at 24 Ma than the 1.4 and 1.8 Ga zircon populations. This could be simply due to less radiation damage or some compositional difference in source terrains (higher U or Th in the source rocks for older grains). Thus, the relative peak heights of discordant data would be higher for those older populations than the 1.1 Ga population. Using a peak matching algorithm would decouple the reconstructed peak locations from possible biasing of the peak

heights and perhaps make the CDC test more reliable for samples like the Tintic formation detrital zircons discussed above.

Based on this comment by Dr. Kirkland, we have added a new Section 3.3 (replacing the text recommended for removal by Drs. Ickert and Kirkland), which outlines the results discussed above and includes a single figure discussing the CDC approach.

The description of the Concordance-Discordance-Comparison technique (and its inverse in Olierook) is incomplete, as it is not merely a projection method. Instead, it employs a Bayesian Monte Carlo approach to probabilistically evaluate all possible Pb loss events, ultimately determining the most likely Pb loss age (or the primary crystallization age in the inverse application).

We apologize for the apparent incompleteness. It would be useful if the appropriate reference was mentioned here, as we cannot determine how either Bayesian (i.e., one that generates and interrogates a posterior distribution which is generated by combining the likelihood distribution and the prior distribution), or Monte Carlo approaches are employed in the CDC method as currently published. We do see that Monte Carlo approaches are used to model uncertainty in an archived manuscript in prep (Mathieson, Kirkland, et al) which was not public at the time we submitted our manuscript.

Line 108, the work states a “safe” assumption is that “all the zircon grains have a shared thermal and geological history” yet is this really the case. Specifically, other works have clearly demonstrated (that in some cases) the susceptibility of the zircon cargo to post crystallization modification is highly variable. This is easily demonstrated by considering the heterogeneous alpha dose (or U content) within any detrital zircon population. Effectively, this means that in many situations, components within a chemically heterogeneous zircon population will be “blind” to certain events whereas other grains may record that event.

This is exactly the scenario that, as shown above, may lead to the underperformance of the CDC method in the Alta DZ data presented here. There is a mismatch between the relative heights of concordant data, and reconstructed discordant data upper intercepts.

This assumption, that all zircons will respond to the same event, at least needs to be discussed and considered as it has fundamental implications for when the proposed methodology would be the most effective or not.

This is similar to a comment on the wording raised by Dr. Ickert. It would be straightforward to add some discussion of the kind requested here and in

previous comments by Dr. Ickert. Specifically, by using “thermal and geological” we are referring to events that affected the entire rock sample in question – metamorphism, heating, pluton emplacement, etc.). We do not mean specific processes that could variably affect individual zircon growth zones differently. We will reword this to make this aspect of our meaning clear.

Line 120-122 is a statement I would certainly agree with and has been said various times before, so you probably could support your point with references.

Good point. Our revised introduction will include relevant references to other work that has taken different approaches to address the same issue.

“.....enables geochronologists to extract meaningful geological information from discordant datasets, turning previously discarded data into valuable insights” Mathieson et al., 2024. Turning Trash into Treasure: Extracting Meaning from Discordant Data via a Dedicated Application. G4 in press, 2024. DOI: 10.22541/essoar.173315682.28715367/v1.

“CDC modelling of discordant U-Pb zircon analyses may provide a means to recognise the distal footprint of otherwise difficult to date tectonothermal events and extract useful information from often discarded analyses.”

<https://doi.org/10.1016/j.gr.2017.08.004>

The first quote comes from a manuscript that was posted on an open archive (Nov. 27th, 2024) after the date of submission and assignment of the reviewers of our manuscript (Oct. 28th, 2024).

The work may be improved by considering that discordance in the case study dataset could also relate to physical mixtures (e.g. core-rims).

This was discussed in the manuscript in Section 3.3, but this section is likely to be removed from the text based on the comments made by Drs. Ickert and Kirkland.

The text on many of the figures is illegible (this may just be an issue with the review pdf but the scaling of text especially in figure 2 needs to be made more consistent across the different components of the figure).

This is indeed an issue with the PDF and will be addressed at the manuscript typesetting stage.

Line 294, it would be more informative to know how it performs relative to Sharman, G. R., & Malkowski, M. A. (2024) and the Concordance-Discordance-Comparison test, rather than against linear regression approaches which clearly are not designed to deal with such over dispersion.

We will add discussion of the Sharman and Malkowski paper in the revised and shortened introductory text, and a full comparison to the CDC test is outlined above and will be included in a revised version of the manuscript.

It would be useful to have a more complete consideration / discussion of how uncertainty in the inversion method has been dealt with. Presumably this is a function of the step size the trial cords have been spaced at?

This extra discussion would be straightforward to add. The summed likelihood method employed here is naïve to the underlying data structure (it is not an inversion), and the only impact the node spacing has is to refine the shape of the underlying likelihood curve. Wider node spacing yields a less-smooth likelihood curve shape. Uncertainty is calculated by our bootstrapped resampling approach (Fig. 7), and after Dr. Ickert's suggestion, now also estimated including decay constant uncertainties.

The method relies on a summed-likelihood approach, but it is unclear how it handles data gaps, outliers, or clustering effects. Could certain grain populations disproportionately influence the results?

We address the uncertainty by using a bootstrapped resampling method to address the sensitivity of the discordance dating to data distributions. The model simply reports distributions of data across Pb/U space, which is then left to the geochronologist to interrogate and interpret. Our sensitivity analysis is important in this regard, as it exposes some of the limits of the discordance dating approach, such as the possibility of generating artificially old lower intercept ages. We attempted to make that point clear in Section 2.2, but have added text to more clearly convey this point.

Line 265-266 "and therefore yields more accurate results for complex datasets" more accurate than what? Linear regression? Well obviously, it must, as it is designed to account for dispersion in the data.

As indicated by the text in the introduction to this section, we are merely using linear regression functions to "benchmark our approach against isochron regression techniques". We are using the well accepted linear regression methods to perform an assessment of the sensitivity and accuracy of the discordance dating methods. We did not mean to convey that they are competing methods and have reworded this text to more clearly convey this point.

More accurate than the other Pb loss modelling approaches?

As shown in response to a previous comment by Dr. Kirkland, yes. We now highlight this fact in a revised version of the manuscript by including a discussion of alternative techniques applied to the Tintic formation detrital zircon data.

I would be rather confident in guessing that the answer to that question depends entirely on the underlying geological controls on the dispersion e.g. chemically heterogeneous grains (with heterogeneous age) variably responding to different episodes of Pb loss or chemically homogeneous grains (with heterogeneous ages) undergoing a single phase of Pb loss. The assumption that all zircons in a sedimentary unit share a common post-depositional history is not universally valid.

This is addressed in a reply to a comment by Dr. Ickert. Our discordance dating approach relies on variable response to a discordance-inducing event. This may not be the case for other methods focused on analysis of discordance detrital zircons.

Localized alteration, differential Pb mobility, or variable zircon radiation damage could result in multiple resetting events rather than a single event. How does the method account for this?

We did not intentionally imply that each grain has experienced an identical chemical history. In fact, our model relies on a variable response (among the entire grain/growth zone population) to, in this case, an apparently single discordance-inducing event. This creates the spread in discordance and results in the ability to apply things like discordance dating to date discordance-inducing events. With the Alta dataset, there is a clear single discordance-inducing event, so our model only outputs a single event, because it is simply mapping probability distributions in Pb/U isotopic space. More complex scenarios are considered in Reimink et al., 2016, and the interested reader is directed there for more details on this aspect. As pointed out by Dr. Ickert, the discordance dating presented here is a modified version of the method outlined in that work, and following his suggestion we do not include further discussion of that model apart from the introductory text already in the manuscript.

The model assumes that the youngest discordant grains define the resetting event. However, zircon discordance can result from multiple overlapping processes (fluid mobility, radiation damage, Pb clustering). It would be nice if the paper could clarify how, it differentiates true geologic resetting from more complex Pb-loss mechanisms.

Our discussion in Section 3.3 in part covered this problem, focusing on the structural mechanisms of discordance. However, this section has been cut to shorten the manuscript to a technical note (see comments by Dr. Ickert on this as well).

The model, like most statistical methods, models U-Pb data alone and cannot rigorously evaluate the causes of discordance. Radiation damage does not itself induce discordance. Chemical disturbance of radiation damaged lattice domains can, however, cause discordance. Pb clustering has only rarely been documented and often produces spuriously old ages in very ancient grains. Other mechanisms

for producing discordance, as outlined and summarized in the present manuscript, have a series of shared geologic 'forcing' processes (metamorphism, fluid ingress, thermal perturbation, etc.).

Our goal is to produce a statistical method that allows geochronologists to more fully interpret U-Pb datasets, but ultimately it is simply a statistical model that necessarily leaves the geological interpretation up to the geochronologist. We feel that this is the appropriate approach, as additional information (grain structural information, trace-element data, alteration histories of a particular rock sample, other thermochronology data) can be leveraged into addressing the questions posed in this comment.

While synthetic datasets were tested, real-world zircon populations may exhibit more complex discordance patterns than the simplified scenarios presented. A more robust sensitivity analysis including mixed multi-stage alteration histories could improve confidence in the method.

The synthetic datasets presented here really serve only one purpose – to test the limits of our method when applied to a single discordance-event population, closely mirroring the geological scenario captured by the Alta DZ dataset. Our intention was to test the sensitivity and accuracy of the age information derived from this discordance dating to robustly evaluate the uncertainties. Therefore, we prefer to keep the synthetic data closely resembling the Alta DZ dataset, in part to limit the length of the manuscript. The most important outcome of the modeling is to show that artificially old ages can be created, and that discordance dating is very sensitive to the position of the most discordant analysis. These results help guide the reliable interpretation of results as well as direct future analytical approaches to using discordant data.

A test case where the method is applied to a sample with known independent constraints (e.g., metamorphic zircon rim ages) would validate its accuracy.

It is possible that we don't completely understand this comment, but it appears that the requested test is exactly the test we have conducted using the Alta Stock alteration halo. These Tintic detrital grains have experienced a known resetting event with well-understood age distributions, which are accurately reproduced by the discordance dating method. The age of the Alta stock and surrounding metamorphic aureole are well known, as shown in the papers reference in the present work.

The discussion on whether Pb loss is due to fluid infiltration versus recrystallization is a bit speculative without clear microstructural evidence (e.g., TEM, Raman spectroscopy).

Suggest incorporating or citing complementary methods that could distinguish these processes.

We agree with this comment regarding discordance (not only Pb-loss but possible U-gain or other mechanisms for creating discordance), and were attempting to make exactly this point in the text. However, this section will likely be cut in the next version of the manuscript following comments by Dr. Ickert.

The analytical dataset appears to be of generally high quality, although I note the 207/206Pb values for glass NIST 612 appear a bit low.

This was noted by Dr. Schmitt and is addressed in the response to that comment.