Systematic uncertainty and thermochronology of the Great Unconformity? A review of Fox et al. 2022, gchron-2022-23

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The title of the manuscript by Fox and coauthors poses a clear question:

> *Can the origin of the Great Unconformity be resolved by thermochronology?*

A valid question! However, this is in detail actually quite a different question from that which this manuscript actually addresses, which might be more accurately stated as:

> *Can the origin of the Great Unconformity be resolved* ***by timing alone*** *using* ***single-chronometer ZHe thermochronology at a single location?***

While this may at first seem like a fine point, in the context of recent debate about the Great Unconformity it is absolutely critical that these two should *not* be conflated, given that the answers to these two questions are almost certainly *not the same*: specifically, the answer to the former question is (given enough data from different locations using different and/or multiple chronometers) quite likely **yes**, even though the answer to the latter question is quite likely **no**.

Even this more accurate latter question, however, might be somewhat misleading as a title, as it implies that the issues considered herein are somehow unique or particular to the question of the origin of the Great Unconformity. What Fox and coauthors do present is an analysis of the effects of diffusion model uncertainty on single-chronometer zircon helium time-temperature inversions, with the Great Unconformity chosen as a case study.

Moving past the title, this is a highly worthwhile undertaking. Systematic uncertainty is, in general, often overlooked and underappreciated in the geosciences – and diffusion model kinetics in thermochronology are no exception. More study of the implications of systematic uncertainties affecting thermochronometric t-T inversions (and more funding thereof!) is highly welcome. If recent heated debate regarding the Great Unconformity, and especially the possibility of thermochronologically resolving the timing of exhumation associated therewith [1, 2, 3, 4, 5] can help attract attention to such work, so much the better! Nonetheless, it is I think worth noting that this is far from the only application (or even the only high-profile one) to which questions of systematic thermochronometer uncertainty apply.

I do have some concerns regarding the representativeness of the presented t-T inversions (i.e., Figure 5); in particular, the strong diagonal path density which more or less entirely sidesteps the known Cambrian surface exposure suggests to me given my previous experience with this particular dataset that either the model has not fully converged on the stationary distribution (i.e., too short of a burn in burn-in), that a significant likelihood preference for simple paths has been applied (which it perhaps should not be in this case), or that data uncertainties have been overestimated (possibly due to running age uncertainty resampling on helium age uncertainties that have *already* been expanded by empirical resampling in McDannell et al. [3]), or some combination thereof.

Although it has long been common to run only some tens to at best low hundreds of thousands of steps of burnin, our recent experience with deep-time inversions, especially data rich ones, is that at the very least 500k (e.g. [3]), but more preferably >1M (e.g., [5]) steps of burnin should be run for such inversions, along with at least 500k steps collected post-burnin. Some approaches such as simulated annealing (e.g., van Laarhoven and Aarts [6]) as tentatively implemented for zircon helium in Keller et al. [7] (the `Thermochron.jl` package also used in the Community Comment by McDannell [8]) may reduce the number of required steps, though this requires further study.

As the authors well know, assessing convergence is one of the hardest problems in Bayesian MCMC inversions, and it is always safer to err on the side of *more burnin*. This, along with ensuring that analytical uncertainties are not *doubly* expanded by sequential empirical and hierarchical resampling is my biggest requested methodological change to the current manuscript. These issues are in my view entirely addressable and would not detract from the present manuscript.

One *might* propose that in assessing the influence of kinetic model uncertainty on inversion results, it in some sense may not matter whether the distribution has become fully stationary or whether it reproduces unambiguously known geologic constraints; all that maters is that the inversion results are different with different kinetics. However, if this exercise is going to be broadly useful, what we all are really going to be most interested in is how it applies to inversions that *are* fully stationary, and geologically valid. In other words, the current models with completely overshoot the uncontroversially established Cambrian surface exposure are not representative of how a Bayesian t-T inversion would or should be used in practice for these data, and thus should not form our basis for assessing the importance of systematic kinetic uncertainties on such inversions. Indeed, while I suspect fully burned-in results for these data will be at least probabilistically consistent with the known Cambrian exposure history, it would be most valuable to consider (as [3] did) models that both do and do not impose a Cambrian exposure constraint.

That is to summarize, on the technical side I would recommend that the authors:

- Ensure that uncertainties have not been redundandly expanded
- Run all models with at least 500k steps burn-in (preferably ∼1M)
- For each set of diffusion parameters, run both an "unconstrained" model as well as one that imposes a Cambrian exposure constraint (say, 0-40C, given Cambrian surface temperature uncertainties)

Beyond these entirely tractable issues, there is one more major concern I have at present: the current framing of the manuscript *appears* to imply (possibly unintentionally?) that McDannell et al. [3] were unaware of systematic uncertainties in the zircon helium system, or that these issues significantly undermine or invalidate the results of McDannell et al. [3]. This I find somewhat odd given that a key point of McDannell et al. [3], as opposed to some previous studies, is that a single-chronometer inversions from single localities in isolation are likely insufficient to resolve the origin of the Great Unconformity, and that instead *multichronometer inversions* (which reduce the impact of systematic uncertainty in diffusion kinetics since different chronometers have different systematic kinetic uncertainties, and also more generally increase t-T resolution by widening the range of effective diffusivities and annealing rates considered) and particularly *the spatial pattern of exhumation* are key to obtaining meaningful insight into the origin of the Great Unconformity via thermochronology. This first clearly discussed on Page 2 of McDannell et al. [3], where we note:

> *First, the uncertainty of time-temperature (t-T) paths derived from a single thermochronometer can be large for older rocks a problem sometimes exacerbated by the use of suboptimal inversion methodologies – making it difficult to discern between glacial and tectonic drivers by timing alone. Second, the magnitudes of both glacial and tectonic erosion are expected to be spatially heterogeneous. Fortunately, however, glacial and tectonic processes predict distinct spatial patterns of exhumation with tectonic erosion focusing in tectonically active regions near cratonic margins and ice-sheet glacial erosion focusing in regions of wet-based icenamely, in the models of Donnadieu et al. (33), broad regions of the low-latitude cratonic interiors away from ice divides, narrowing to a more "hit-or-miss" pattern at cratonic margins where basal slip is focused into only a few rapid outlet ice streams, as is observed*

> *at modern Greenland and Antarctic ice margins. Consequently, to resolve the relative contributions of all such climatic and tectonic drivers of erosion in the Neoproterozoic, not to mention their potential interactions, we require higher-resolution tT paths from localities that can address the spatial pattern of Neoproterozoic exhumation at a global scale. [...] The use of multiple thermochronometers with varying temperature sensitivities is critical for such deep-time applications.*

and again on Page 6, where we further note that it is indeed not only thermochronometric uncertainty, but also uncertainty in the timing of tectonic forcings that makes a spatially-aware approach all the more critical:

> ***Spatial Patterns of Tectonic and Glacial Erosion of Continents***
>
> *McDannell et al. (55) and DeLucia et al. (36) came to the conclusion that kilometer-scale Neoproterozoic exhumation occurred after 1 Ga within the North American interior and linked this to formation of the Great Unconformity due to Rodinian geodynamics and/or snowball Earth glaciations. These two hypotheses are not mutually exclusive – it is possible that both tectonics and glaciation contributed to global Earth system disruption (80, 81) during formation of the Great Unconformity. Glaciation would be most effective as a driver of erosion in regions with preexisting topography (be it from rifting or orogeny); therefore, erosional synergy between tectonics and ice sheets is a possibility (82). [...] Direct and meaningful comparisons between tectonic and glacial unconformity hypotheses are complicated by the fact that there are precise estimates for the timing of Snowball glaciations (23), whereas the timing and duration of Rodinia assembly and breakup remain incompletely understood due to discrepancies between paleomagnetic and geologic data (11, 83, 84). Rodinia assembly and breakup occurred episodically and diachronously over at least 250 Ma for each phase, with timing dependent upon location (10, 11).*

and again on Page 7:

> *Cratonic interiors provide the only location to truly test and differentiate the hypotheses of pre-, syn-, or post-Cryogenian formation of the Great Unconformity. Timing is a key component of this signal, but spatial pattern and magnitude of exhumational rock cooling are also critical. Tectonic rifting and glacial erosion will produce opposing spatial patterns of exhumation and different magnitudes of crustal unroofing across a continent. The majority of exhumation associated with supercontinent assembly and breakup would be limited to compressional orogenic belts and extensional (faulted) rift margins, respectively. Rifting will show large exhumation narrowly restricted to continental margins, where tectonic activity is highest, whereas stable continental interiors will experience little to no erosion or even deposition.*

Other key factors noted by McDannell et al. [3] in differentiating between tectonic and glacial causes include the apparent absence of an equivalent "Great Unconformity" phenomenon associated with the breakup of Pangea (or perhaps relatedly, how exactly it is that the "continental rifting" part of the supercontinent cycle is supposed to cause more erosion and exhumation than the "continental collision" part).

Subsequently, we continued to reiterate the importance of relying on more than timing alone in our more recent contribution on the subject [5], wherein we note:

> *The Canadian Shield margin displays many features indicative of late Neoproterozoic rift-related tectonism and is, in principle, consistent with a mantle plume model (i.e., Sturrock et al., 2021), including pre-rift doming, pervasive faulting, dike emplacement, and syn/post rift deposition (Cawood et al., 2001; McClellan and Gazel, 2014). Evidence for such events is, however, absent within the stable cratonic interior. We maintain that tectonic phenomena such as rifting or distal plume impingement (Sturrock et al., 2021) are unlikely to drive >36 km of exhumation within the continental interior, which is far from the western Laurentian*

> *Cordillera margin and more than 2000 km inboard of the Iapetan rift margin. The inferred magnitude of erosion is also greater than models of dynamic topography commonly predict (<3 km; Braun et al., 2013).*
>
> *While these results appear to support a broad pattern of denudation across disparate, stable cratonic regions of North America (e.g., McDannell et al., 2022), we by no means rule out variability in the timing and magnitude of cooling; indeed, such variation is expected even in a glacial endmember hypothesis.*

The only case in which we expect a single t-T inversion could significantly inform our understanding of the Great Unconformity would be in the case of an undisputedly stable cratonic interior where no tectonic forcings for kilometric exhumation are plausible regardless of some nontrivial uncertainty in timing – but even then a multichronometer inversion as in [5] is far preferable, and even then is most meaningful only in the context of a broad spatial pattern supported by numerous independent inversions at different cratonic and marginal localities.

That is, to summarize key points from McDannell et al. [3] and [5] as quoted above:

- We expect that single-thermochronometer inversions have inadequate timetemperature resolution to differentiate between geologic and tectonic causes of exhumation by timing alone, and do not rely upon them (indeed, only one out of our seven presented t-T models between these two papers relies on a single chronometer alone, in significant contrast to the work of some others on the same subject).
- Multichronometer inversions are better, but still technically inadequate to resolve the debate in isolation / by timing alone, considering that tectonic and glacial exhumation may temporally *coincide*.
- Instead, the *spatial pattern of exhumation between tectonically active cratonic margins and tectonically stable cratonic interiors* is most key to differentiating between glacial and tectonic exhumation.

Consequently, I fully agree that systematic thermochrometer uncertainty is an important consideration, but have already taken major steps to ensure that it does influence our conclusions, something which the current manuscript *appears* to suggest the opposite of.

Finally I have some concern from a statistical perspective with the robustness and geologic significance of the "onset of cooling" metric discussed in the current manuscript; the time of half-cooling or width of the distribution at half-cooling is likely more useful, robust, and geologically meaningful in practice for reasons discussed in more depth in McDannell [8]. These issues do not mean that the path density prior to a cooling event cannot be used when discussing variation in the shape of a t-T inversion in the abstract, but should (I would propose) be considered and perhaps acknowledged whenever there is a clear geologic context being discussed.

Given the broader implications of uncertainties in diffusion model kinetics far beyond the Great Unconformity, an additional demonstration of the effects of varying diffusion kinetics on another dataset of interest might also be welcome, though I would not insist upon it. Overall, I find that the current manuscript addresses an important and often little-discussed factor that is quite relevant to the field of thermochronology as whole, despite some tractable potential issues in t-T inversion, framing, and titling.

I recommend Revisions and would be happy to consider a revised manuscript.

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