Author’s reply to reviewer comments 1 (RC1)

“Technical note: Guidance on setting up Pecube inversions with the neighbourhood algorithm” by Bernard et al is an interesting exploration of how best to use the neighbourhood algorithm. I would recommend minor revisions.

We thank the reviewer for the positive feedback and comments. We updated our manuscript according to the reviewer’s suggestions. Below, we reply to each comment.

The paper does an excellent job at providing the background to different inversion methods but this background is perhaps aimed at a specialised audience. Whereas people that will benefit from this paper are likely people who want to use the NA and Pecube and may not need to know about other methods. If the aim of this paper is to highlight how the NA differs from other methods, then a bit more information is required to introduce these methods. For example, on line 45 the concept of a parameter space is introduced without describing what it is. I am not sure that many people need to know the names of steepest descent, conjugate gradient or Gauss–Newton methods. It is also not clear why these references are chosen. Surely the original references should be used, or maybe examples where these have been used in geomorph or geochron studies. Perhaps the idea of a 2D misfit landscape could be introduced more gently as most people are more used to thinking about a 2D surface than a high dimensional space. This could be tied to Figure 1 and contours of parameter space could help reinforce the idea of a landscape with slopes and curvatures.

We acknowledge that the details provided in the initial version of the manuscript about the inversion methods may be too specialised for the targeted audience, and we followed the reviewer’s suggestion to simplify this part of the introduction. We removed the introduction to local inversion methods to focus on the global or direct stochastic search, which is the inversion category the NA is part of. We also tried to introduce the concept of parameter space more gently in the text (L42-55), and updated figure 1 to include contours of misfit values to highlight the concept of a misfit landscape.

A section on how the NA has been used in other aspects of geomorphology should be included. It has been used in Fox and Shuster (EPSL, 2014) and in Han et al., (Nature Geoscience, 2024). The results presented here are important and useful for these papers too.

We added a sentence in the introduction to briefly acknowledge that NA has been used for inversion of other geomorphological parameters, not only in thermochronology. We added the Han et al. (2024) reference and other references such as Valla et al. (2011) and Fox et al. (2014) (L62-64).

It would be really nice to actually invert the true data to understand how well the model works without any error introduced to the data. At the moment, it is not clear if the inversion is not working because of the noise added to the data or the choice of NA parameters. In particular, the “True” 1D marginals of the posterior density function do not provide the correct values used to predict the data. The relief parameter is relatively flat between 0.2 and 0.7 and the tu parameter has a clear, well defined peak at the wrong location (~15 Ma). The heat production and basal temperature models do not converge to the correct value at all. Is this because of the noise introduced or because the NA is not finding the correct solution?

We performed additional inversions in which we reduced relative uncertainties on each datapoint to 0.1 %. We use a NA configuration similar to inversion 5 (Figure 4d, main text) in which N_m^{1st} = 900 and N_r = 180, corresponding to relatively broad exploration of the parameter space (Inv. A, Figure R1), as well as two additional inversions with NA configurations representing lesser exploration of the parameter space with N_m^{1st} = 36 and N_r = 7 (Inv. B, Figure R1) and N_m^{1st} = 180 and N_r = 36 (Inv. C, Figure R1). As such, we test the robustness of NA to recover the target PPD.

First, reducing uncertainty on the data changes the target PPDs (or the misfit landscape), and reduces deviation between inverted and the target parameter values, demonstrating that NA is able to recover the target parameter under this configuration (Figure R1). While inversion A and C (Figure R1) recover the target PPDs well due to a sufficiently large exploration of the parameter space, inversion B shows large deviation to the target PPDs due to insufficient exploration of the parameter space. This result remains in line with the results in the manuscript showing that an inappropriate configuration of NA leads to inaccurate PPDs. We note that the true values of parameters T_b and H_p are not recovered even for inversions A and C; however, the true near-surface geotherm is recovered. This is explained by the fact that these two parameters show trade-offs, where different combinations of values lead to similar near-surface geotherms (see next reply for more details).

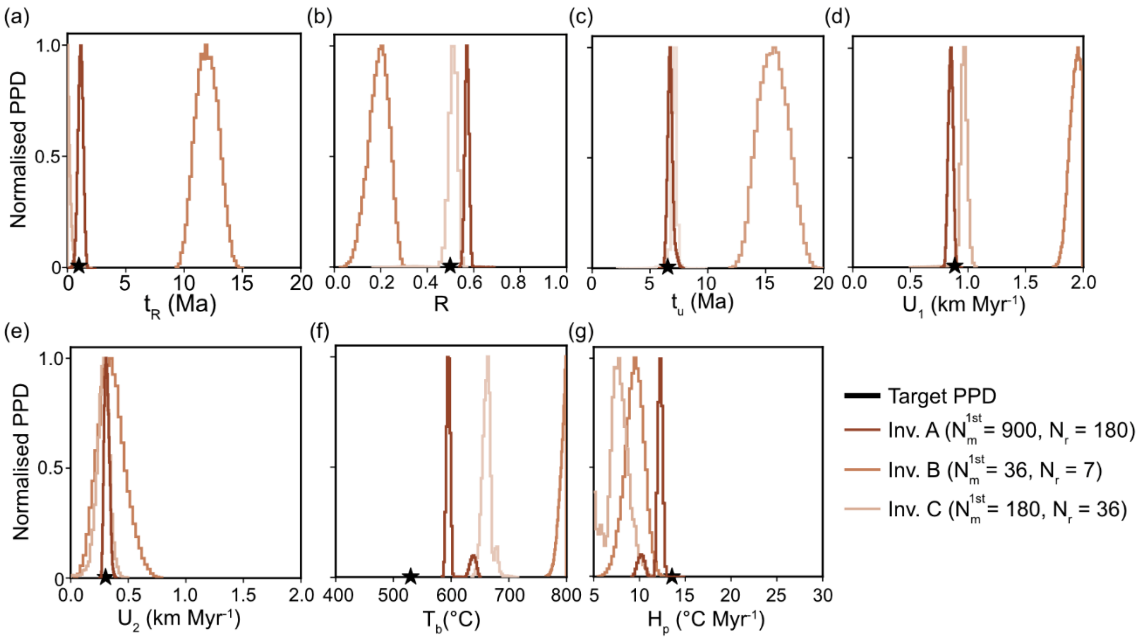

Figure R1. Posterior probability distributions (PPD) of additional inversions with reduced data uncertainties. The PPDs are shown for each inverted parameter and compared to their target PPD.

It would be useful to combine the heat production and basal temperature, with a background average exhumation rate to get an estimate of the near surface geothermal gradient. The data are clearly resolving a geothermal gradient, but because the geothermal gradient is a function of heat production, basal heat flux and exhumation rate, heat production and basal temp can not be independently resolved. The inversions all do a bad job at predicting the correct values of these parameters, but perhaps they do a good job at predicting the correct near surface average present day geothermal gradient. This would simply be an additional plot that could be created from the sampled combinations of parameters, assuming a steady state model, and plotted as a function of misfit. It would be nice to see if this combined parameter is well resolved and would explain why you can't resolve the other parameters. You can also extract the resolution matrices and correlation matrices from the ensemble of forward models. This would also help explain the resolution of the parameters. It would enable you to say that model and data can not resolve the parameters and eliminate the possibility that the NA is not working correctly.

We thank the reviewer for the suggestion and for the relevant comment. We plot in Figure R2 below the extracted near-surface geotherms from all inversion performed, calculated following the steady-state heat equation from Reiners and Brandon (2006):

$$\begin{cases} T(z) = T_s + \left(T_L - T_S + \frac{H_p L}{\dot{\varepsilon}}\right)\frac{1-\exp(-\frac{\dot{\varepsilon}z}{\kappa})}{1-\exp(-\frac{\dot{\varepsilon}L}{\kappa})} - \frac{H_p z}{\dot{\varepsilon}}, Pe > 0.1 & (1a) \\ T(z) = T_s + \frac{(T_L - T_S)z}{L} + \frac{H_p z(L-z)}{2\kappa}, Pe \leq 0.1 & (1b) \end{cases}$$

where T_s and T_L are the surface and basal temperatures respectively, H_p the heat production rate (°C Myr^{-1}), $\dot{\varepsilon}$ the exhumation rate (km Myr^{-1}), κ the thermal diffusivity (km^2 Myr^{-1}), and Pe the Peclet number defined as $Pe = \dot{\varepsilon}L/\kappa$. For all forward models extracted, we consider the temperature, T_s, from the mean elevation of the DEM used in the main text (z = 2.2 km).

Figure R2 clearly shows that the range of estimated near-surface geotherms of 25-35°C km^{-1} from the better fit models (red dots in Figure R2) plot near the target value of ~28 °C km^{-1} from the true exhumation model (white stars in Figure R2), although the PPD peaks at ~35°C km^{-1} (Figure R2c-d). However, this geotherm value is expected from the target PPD, corresponding to the geotherm value the new data constrain due to the addition of deviation and uncertainty from the true data generated by the exhumation model. These results suggest that thermal parameters T_b and H_p cannot be independently resolved from the data but the near-surface geotherm can.

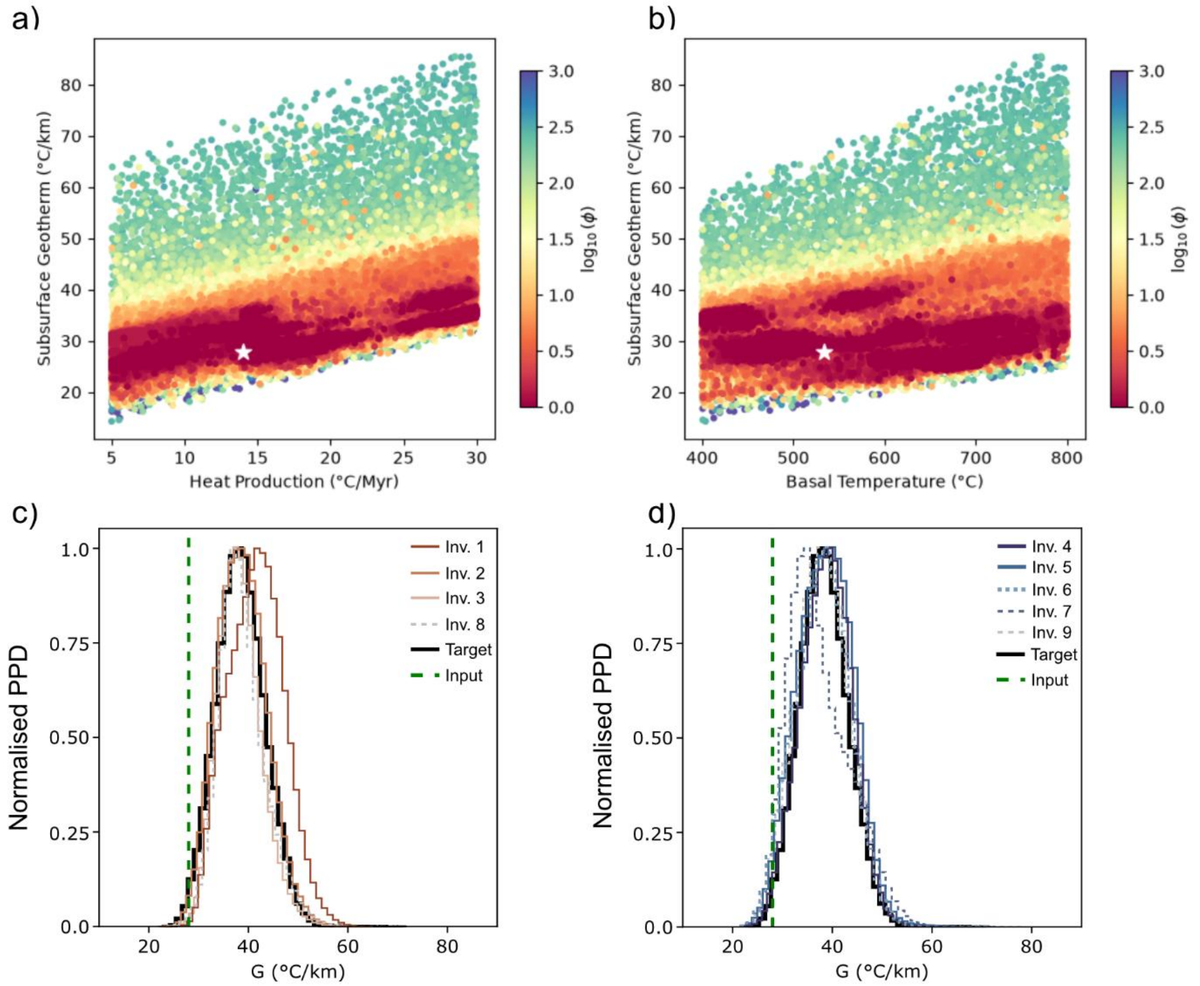

Figure R2. Estimated near-surface geotherm from all NA-Pecube inversions. The heat production rate (a) and basal temperature (b) are plotted against the resulting near-surface geotherm. Each point represents a Pecube model colored by its misfit value. The white stars represent the target values from the true exhumation model. The posterior probability distributions of near-surface geothermal gradients are plotted for the inversion in the danger zone (c, see Figure 4d, main text) and in the safer zone (d), alongside with the target PPD and input value in the reference exhumation model.

We further investigated the correlation among inverted parameters as well as their resolution, as suggested by the reviewer (Figure R3). Unsurprisingly, some parameters show significant correlation with the strongest being the trade-off between t_u and U_1 (Figure R3a, Corr = 0.41, Figure R3b). Correlations are also observed between T_R and U_2 (Corr = 0.36, Figure R3b), T_R and t_u (Corr = 0.30, Figure R3b) and, H_p and T_b (Corr = -0.16, Figure R3b). These trade-offs between parameters are permitted by the data deviation and uncertainties applied for the inversion on the original dataset generated (i.e., 10 % deviation + 5 % uncertainty), which allow multiple solutions to fit the data similarly. This affirmation is supported by the test reducing the uncertainty on the data to 0.1%, leading to retrieval of the true parameter values of the exhumation model considered in this study, with a limited range of solutions (see previous reply). When uncertainties are associated with the data, the resolution to which the data constrain the inverted parameter changes significantly. Only parameter U_2 can be expected to be constrained by the data (Figure R3c, Resolution = 0.88). Other parameters such as t_u and U_1 are reasonably constrained but with broad ranges (Figure R3, Resolution > 0.2). Parameters R, H_p, T_b and T_R are however not constrained by the data (Figure R3c, Resolution < 0.2).

The thermal parameters H_p and T_b are not resolved because of their trade-off when predicting the near-surface geothermal gradient. A similar inversion as shown in Figure R3 but aiming to predict the near-surface geotherm instead of parameters H_p and T_b (i.e., a 6-parameter space), shows a well constrained near-surface geotherm of 35.3 ± 6.2°C.km^{-1} (G in Figure R4a). The geothermal gradient, G, correlates most strongly with parameters T_R (Corr = 0.36), U_2 (Corr = 0.28), and t_u (Corr = 0.27, Fig. R4b) due to the relation between exhumation rate and heat advection in equation 1a. Finally, the resolution value of 0.87 (Figure R4d) suggests that the geotherm is well resolved by the data. We now include a discussion on the near-surface geotherm in section 3.2 (L449-469) and provide Supplements that include further details on how the near-surface geotherm is calculated from the thermal parameters and exhumation rate.

Following these additional tests, we added a paragraph in section 3.3 of the revised manuscript to describe parameter trade-offs, parameter resolution, and the role of data uncertainty in controlling the ability to retrieve a known exhumation scenario. We included Figure R3 as Figure 6 in the manuscript. We also updated our recommendations for using NA-Pecube inversions. We now recommend users to perform a first small inversion (~1000-5000 models) and a subsequent resolution test with their dataset to identify parameters that can actually be constrained by the data. We also provide a new python code to perform this task, available on github (https://github.com/OpenThermochronology/NA-appraisal-Pecube). Additionally, we recommend either fixing the thermal parameters when performing inversion or at most to invert for only one thermal parameter (H_p or T_b), keeping the other fixed, because of the strong correlation between these two parameters.

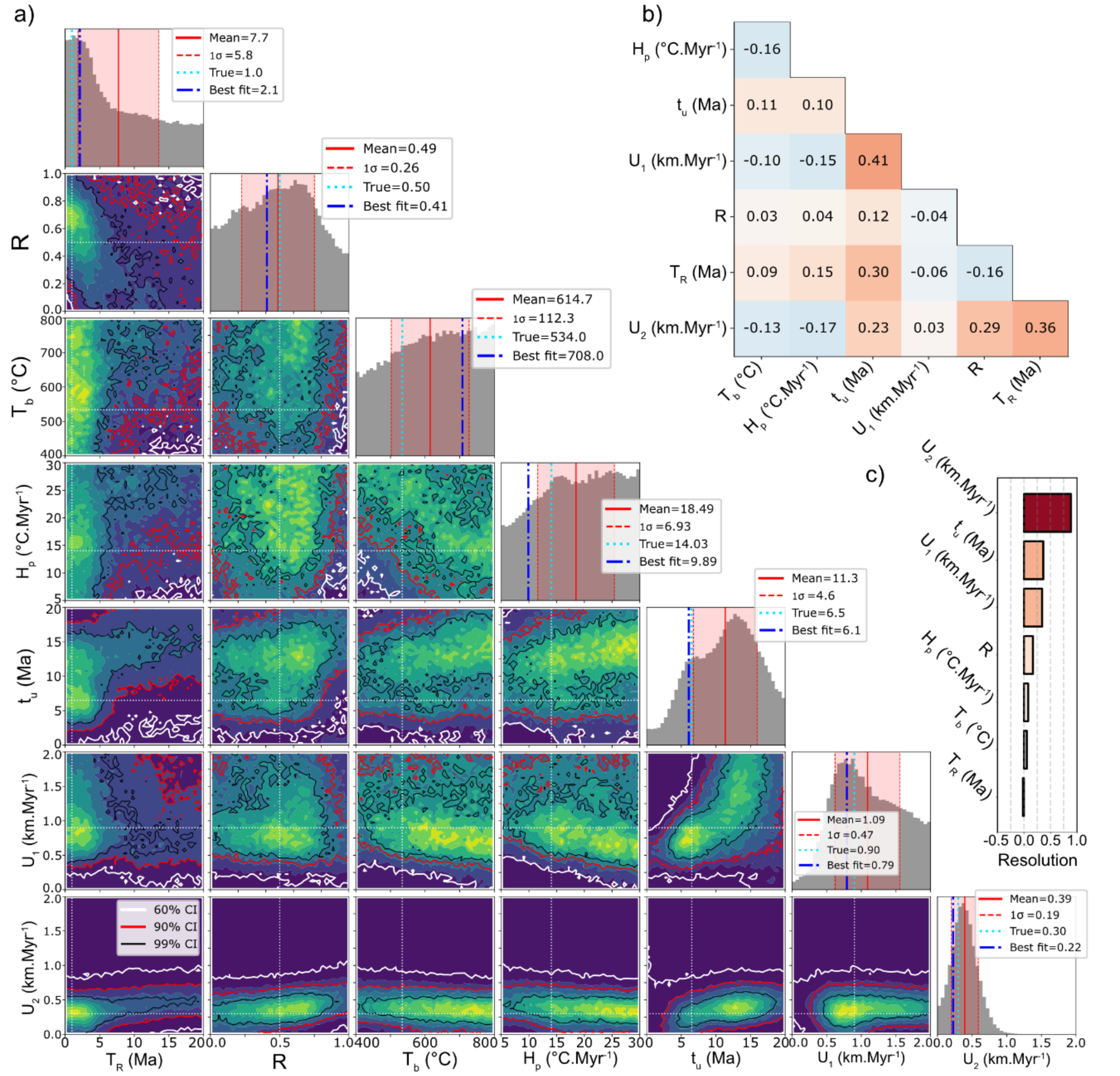

Figure R3. Summary of parameter correlation and resolution for the targeted distribution. Pairwise (2D) parameter distributions are shown in (a) with their associated 1D posterior probability distributions. The correlation matrix of inverted parameters is shown in (b); two parameters are correlated to each other as the correlation value approaches 1 or -1. The resolution of parameters is shown as a bar plot in (c). A resolution value close to 1 means the parameter is well resolved by the data and the model.

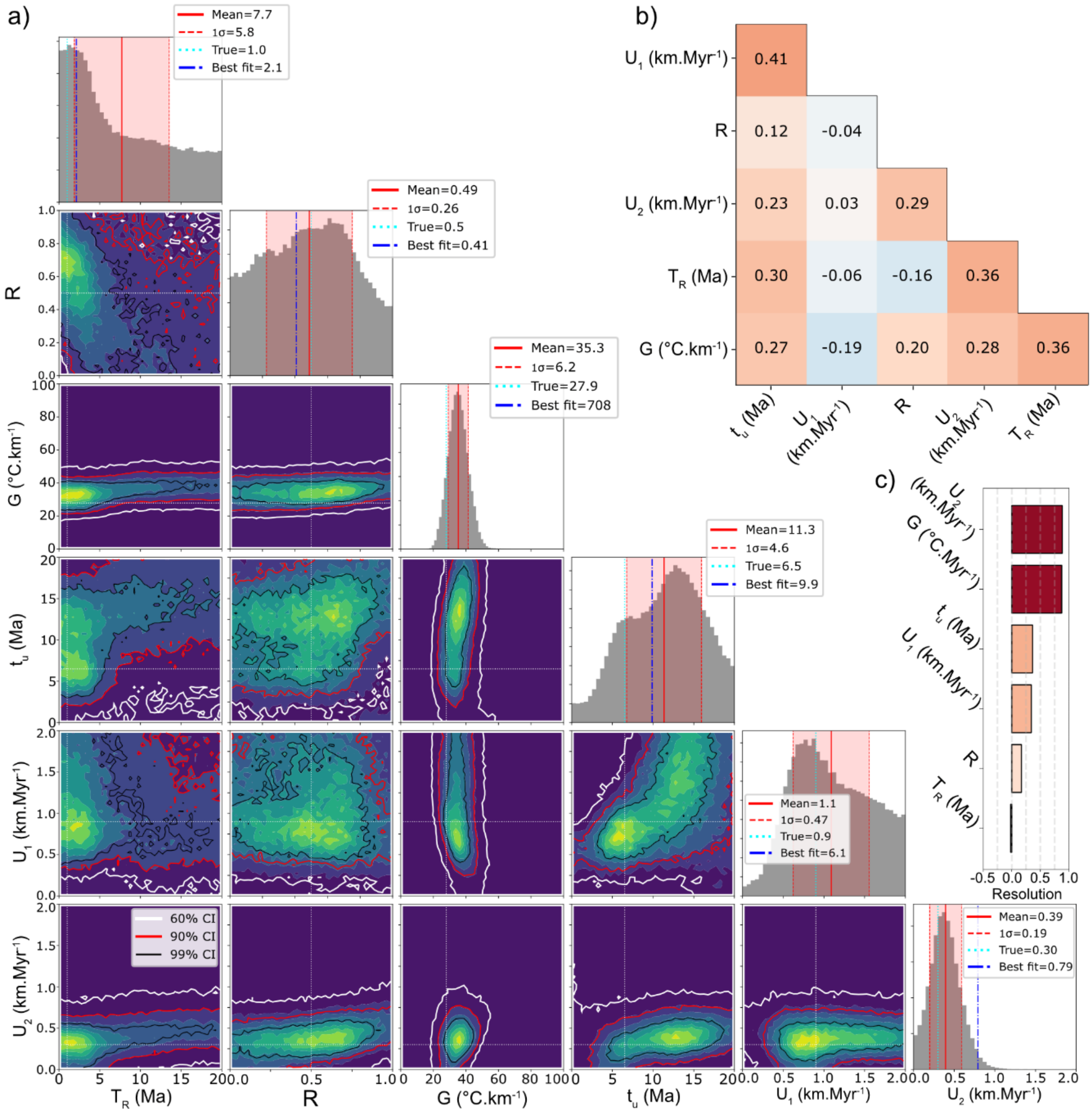

Figure R4. As Figure R3 but for an inversion considering the near-surface geotherm instead of the heat production (H_p) and basal temperature (T_b).

The recommendation should be that people need to do a resolution test. The parameter spaces are all so different and the data sets are all so different, completely different combinations of NA parameters might be required to provide an optimal solution. Ultimately, however, the computational effort required to more fully sample parameter space and rely less on optimization is small compared to the effort of climbing mountains to collect vertical profiles, crushing and separating rocks, picking apatite grains, ….Perhaps the recommendation should be that people should oversample to be on the safe side.

We agree with this comment. A small inversion of about 1000-5000 Pecube models could be first done to estimate the resolution the data provide on each parameter. This would help removing unconstrained parameters from the inversion and help fixing parameters to improve the inversion. We now include this recommendation in section 3.2 of the manuscript (L590-594) as well as in Table 2.

Some of the topic sentences at the start of paragraphs are not very clear. For example "How about Nm?", is not an effective introduction to a paragraph. It also relies too heavily on the previous text. A better topic sentence could be "How does the value of Nm control the ….."

We changed the introduction sentence of this paragraph to "Next, we consider how many models (Nm) should be performed in each iteration".

This topic sentence does not make sense "Lastly, rather than focusing on the number of iterations, the total number of models performed is a more relevant measure when considering the effect of dimensionality.". I think simplifying the text would help here.

We changed this sentence to "Lastly, the total number of forward models evaluated during a NA-Pecube inversion must scale with the dimensionality of the problem. Based on Eq. (2), satisfying coverage of parameter space can generally be expected for $10N \leq N_{total} \leq 50N$, and the number of iterations N_{it} should therefore be tuned to reach this range of models evaluated".

Sincerely,

Matthew Fox

Line comments:

47: "local curvature of the misfit landscape" Are you sure that these algorithms use the curvature of the misfit landscape and not the slope?

Regarding the first comment of the reviewer, we removed the description of local deterministic inversion methods from our introduction.

66: Add Fox et al., (G-cubed), 2014 where the NA was used and correlations in parameter space were assessed.

We added this reference.

277: What does a random noise mean in this instance? Are the ages changed by 10 %? It seems strange to add on 10% error to the data but then estimate the uncertainty to be only 5%. I suppose this is likely what lots of datasets look like, but with much larger errors.

By random noise we mean a random deviation from the generated ages by up to 10 % of their value. This first deviation serves to simulate variation in data that would emerge from any process in nature other than the analytical measurement uncertainty, such as the effect of e.g., local fluids, helium implantation, etc… The 5 % uncertainty we assign simulates the analytical uncertainty that arises from measurement of the data. While this value may be lower than the analytical uncertainties that are usually reported (typically ~10 %), it was chosen to limit the deviation from the true data generated and test the ability of the NA to retrieve the true parameter values of the exhumation model considered, with a relatively precise dataset. We changed "random noise" to "random deviation".

280: It is not appropriate to refer a true distribution. This is never actually shown, instead you show the results of the sampling stage of the NA and 1d marginals through PPD. This is not a "true"

distribution as it is simply inferred with more models, than the other distributions. This should be called something else, maybe target would be best. Especially because the stars are referred to as showing the true parameter values. In fact, after the noise and uncertainty has been added, the target misfit distribution might have minimums that are very far from the actual values used to generate the data. Because of this, the inversions with different NA parameters should be compared with the minimum values of the target distribution not the true values. Please rename the true distributions to something else throughout the manuscript.

We do build the "true" PPD from the sampling stage of the NA considering > 100 000 Pecube forward models. We acknowledge the point raised by the reviewer regarding naming this PPD as the "true" one. This is actually the one that is considered to describe the expected distributions of each parameter, given the data and associated uncertainties. We follow the reviewer's suggestion and now refer to this PPD as the "target" PPD throughout the manuscript.