

1   **An efficient approach for inverting rock exhumation from thermochronologic age-elevation**  
2   **relationship**

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16 **Abstract**

17 This study implements the least-squares inversion method for solving the exhumation history from  
18 thermochronologic age-elevation relationship (AER) based on the linear equation among  
19 exhumation rate, age and total exhumation from the closure depth to the Earth surface. Modelling  
20 experiments suggest significant and systematic influence of initial geothermal model, the *a priori*  
21 exhumation rate and the time interval length on the *a posteriori* exhumation history. Lessons  
22 learned from the experiments include that (i) the modern geothermal gradient can be used for  
23 constraining the initial geothermal model, (ii) a relatively higher *a priori* exhumation rate would  
24 lead to systematically lower *a posteriori* exhumation, and *vice versa*, (iii) the variance of the *a*  
25 *priori* exhumation rate controls the variation of the inverted exhumation history, (iv) the choice of  
26 time interval length should be optimized for resolving the potential temporal changes in  
27 exhumation. To mitigate the dependence of inverted erosion history on these initial parameters,  
28 we implemented a new stepwise inverse modeling method for optimizing the model parameters  
29 by comparing the observed and predicted thermochronologic data and modern geothermal  
30 gradients. Finally, method demonstration was performed using four synthetic datasets and three  
31 natural examples of different exhumation rates and histories. It is shown that the inverted rock  
32 exhumation histories from the synthetic datasets match the whole picture of the “truth”, although  
33 the temporal changes in the magnitude of exhumation are underestimated. Modelling of the  
34 datasets from natural samples produce geologically reasonable exhumation histories. The code and  
35 data used in this work is available in GitHub ([https://github.com/yuntao-github/A2E\\_app](https://github.com/yuntao-github/A2E_app)).

36

37 **Key words:** Thermochronology; Exhumation; Numerical inversion; Age-elevation relationship;  
38 Least-squares method; Geothermal model

39 **1. Introduction**

40 Quantifying rock exhumation from the Earth interior to the surface is important information for  
41 better understanding many geological problems, ranging from orogenic growth (e.g., Zeitler et al.,  
42 2001; Whipp Jr. et al., 2007) and decay (e.g., House et al., 2001; Hu et al., 2006), to resource and  
43 hydrocarbon evaluation and exploration (e.g., Armstrong, 2005; McInnes et al., 2005), as well as  
44 the underpinning endogenic and exogenic processes and their interactions (e.g., Burbank et al.,  
45 2003; Fox et al., 2015; Tian et al., 2015). Various experimental and modeling methods have been  
46 invented for estimating the rock exhumation at different crustal levels (e.g., Braun, 2003; Reiners  
47 and Brandon, 2006; Anderson et al., 2008; Braun et al., 2012; Fox et al., 2014).

48 One type of the methods for estimating the rock exhumation in the middle and upper crust  
49 relies on thermochronologic cooling ages acquired from noble gas and fission-track dating of a  
50 series of accessory minerals, such as Ar-Ar, fission-track and (U-Th)/He analyses (Ault et al., 2019  
51 and references therein). Based on the closure temperature theory (Dodson, 1973), assuming  
52 monotonic cooling, a thermochronologic age records the time duration that a rock cooled through  
53 the corresponding closure temperature, which is a function of the kinematics describing fission-  
54 track annealing and noble gas diffusion, and rock cooling rate (Dodson, 1973). If the depth of the  
55 closure temperature isotherm can be estimated from the crustal temperature field, a time-averaged  
56 exhumation rate can be obtained from the cooling age.

57 Based on the thermochronologic methods and thermo-exhumation modelling, many  
58 analytical and numerical tools have been implemented for inverting the exhumation and/or the  
59 associated cooling history from thermochronologic data. These tools have different functions, such  
60 as inverting temperature history (Laslett et al., 1987; Ketcham, 2005; Gallagher, 2012),  
61 determining time-averaged exhumation rates (Brandon et al., 1998; Ehlers, 2005; Willett and

62 Brandon, 2013; Glotzbach et al., 2015; Van Der Beek and Schildgen, 2023), spatiotemporal  
63 changes in exhumation (Sutherland et al., 2009; Herman et al., 2013; Fox et al., 2014; Willett et  
64 al., 2020), and evolution of exhumation in two or three dimensions given a tectonic framework  
65 (Batt and Brandon, 2002; Braun, 2003; Van Der Beek et al., 2010; Valla et al., 2011; Braun et al.,  
66 2012).

67 Convincing estimate of exhumation history for a region requires both a proper sampling  
68 strategy for thermochronologic data and a robust modeling approach for exhumation inversion,  
69 especially when the rock exhumation and its spatiotemporal changes are tectonically controlled  
70 (Ehlers and Farley, 2003; Schildgen et al., 2018). A routine and efficient sampling strategy  
71 acquires themochronologic ages from an elevation transect over a significant relief and a relatively  
72 confined spatial distance. Plotting the age versus elevation, i.e., the age-elevation relationship  
73 (AER), and analyzing the slope changes of the plot can provide first-order understanding of the  
74 exhumation history (Fitzgerald et al., 1986). Because both the subsurface geothermal field and  
75 closure temperature of thermochronometers are functions of the thermal advection and cooling  
76 during rock exhumation (e.g., Dodson, 1973; Brandon et al., 1998), as well as the long-wavelength  
77 topography (Braun, 2002; Ehlers and Farley, 2003; Glotzbach et al., 2015), Estimating reliable  
78 exhumation rates requires to account for temporal variations of the thermal field caused by changes  
79 in the thermal and kinematic boundary conditions.

80 Fox et al. (2014) reported a linear inversion modeling method that solves exhumation  
81 history from AER, given a combination of *a priori* exhumation rates and assumed geothermal  
82 parameters. However, as shown in that study, the inverted exhumation history depends highly on  
83 these *a priori* values and geothermal assumptions. Building on that study, we here provide a

84 detailed test on the method and report an improved modeling method that makes use of both the  
85 AER and the modern geothermal gradient for inverting exhumation history.

86

87 **2. Linear inversion method**

88 Our inversion of exhumation from thermochronologic data followed the linear inversion  
89 approach of Fox et al. (2014). Rock Exhumation from the closure depth of a thermochronometer,  
90  $z_c$ , to the Earth's surface can be described as an integral of the exhumation ( $\dot{e}$ ) from the cooling  
91 age ( $\tau$ ) to the present (Brandon et al., 1998; Fox et al., 2014). For a set of correlated bedrock  
92 samples with a shared history of exhumation rates ( $\dot{e}$ ), their thermochronologic ages ( $\mathbf{A}$ ) and the  
93 corresponding closure depths ( $\mathbf{z}_c$ ) can be expressed by the following equation.

94 
$$\int_0^\tau \dot{e} dt = z_c \quad \Rightarrow \quad \mathbf{A}\dot{e} = \mathbf{z}_c , \quad (1)$$

95 where  $\mathbf{A}$  is a model matrix, with  $n$  rows (the total number of samples) and  $m$  columns (the total  
96 number of time intervals). Each row of the matrix is a discretization of a sample age, which is  
97 composed of a number of time lengths ( $\Delta t$ ) followed by an age residual ( $R_i$ ) and a number of zeros.

98 The  $\dot{e}$  is a  $m$ -length vector of exhumation rates, and the  $\mathbf{z}_c$  is  $n$ -length vector of closure depths.

99 This linear equation can be solved using the Least-Squares Regression approach assuming  
100 the Gaussian uncertainties and *a priori* mean exhumation rate ( $\dot{e}_{pr}$ ) and associated variance ( $\sigma_{pr}$ )  
101 (Tarantola, 2005; Fox et al., 2014). Such an approach requires a  $m*m$ -sized parameter covariance  
102 matrix,  $\mathbf{C}$ , and a  $n*n$ -sized data covariance matrix,  $\mathbf{C}_\epsilon$ , which includes the uncertainties on the  
103 closure depths. These two matrices can be constructed as equations 2 and 3, respectively.

104 
$$C_{ij} = \begin{cases} \sigma_{pr}^2, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} \quad (2)$$

105 
$$(C_\epsilon)_{ij} = \begin{cases} \dot{e}_{pr}\epsilon_i, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases} , \quad (3)$$

106 where  $\dot{e}_{pr}$  and  $\sigma_{pr}$  are the *a priori* exhumation and the associated variance, and the  $\varepsilon$  is analytical  
 107 uncertainty of the age data. The construction of the data covariance matrix assumes the age data  
 108 are uncorrelated. Worth noting is that previous studies used different constructions of the data  
 109 covariance, changing from using the analytical age uncertainties (Fox et al., 2014; Fox et al., 2015)  
 110 to constant values (Jiao et al., 2017; Stalder et al., 2020).

111 Given the above model parameters, the equation 1 has a maximum likelihood solution for  
 112 the exhumation rate vector:

$$113 \quad \dot{e}_{po} = \dot{e}_{pr} + \mathbf{C}\mathbf{A}^T(\mathbf{A}\mathbf{C}\mathbf{A}^T + \mathbf{C}_\epsilon)^{-1}(\mathbf{z}_c - \mathbf{A}\dot{e}_{pr}), \quad (4)$$

114 where  $\dot{e}_{pr}$  is a n-length vector of  $\dot{e}_{pr}$ ,  $\mathbf{z}_c$  is the n-length vector of closure depths calculated using a  
 115 combination of exhumation and geothermal model parameters (see section 3). The  $\dot{e}_{po}$  is the  
 116 posteriori maximum likelihood estimate of the exhumation rate, with a covariance matrix,  $\mathbf{C}_{po}$ ,  
 117 which provides an estimate of the uncertainties on the model parameters (equation 5).

$$118 \quad \mathbf{C}_{po} = \mathbf{C} - \mathbf{C}\mathbf{A}^T(\mathbf{A}\mathbf{C}\mathbf{A}^T + \mathbf{C}_\epsilon)^{-1}\mathbf{A} \quad (5)$$

119 The method also provides a model resolution matrix,  $\mathbf{R}$ , which gives a measure on how  
 120 well the model estimates correspond to the true values:

$$121 \quad \mathbf{R} = \mathbf{C}\mathbf{A}^T(\mathbf{A}\mathbf{C}\mathbf{A}^T + \mathbf{C}_\epsilon)^{-1}\mathbf{A} \quad (6)$$

122

123 **3. Closure depth and topographic correction**

124 Inversion of the exhumation using the equation 1 requires accurate estimates of the closure  
 125 depths of the thermochronologic ages ( $\mathbf{z}_c$ ), i.e., the depth of the closure temperatures (Fig. 1). The  
 126 latter can be determined by modelling the temperature of the crust using a 1D thermal-kinematic  
 127 model, which accounts for heat conduction, advection and production (Turcotte and Schubert,  
 128 2002):

129 
$$\frac{\partial T_m}{\partial t} = \kappa \frac{\partial^2 T_m}{\partial z^2} + \dot{e} \frac{\partial T_m}{\partial z} + A_b, \quad (7)$$

130 where  $A_b$  is the heat production (in  $^{\circ}\text{C}/\text{Myr}$ ). This function can be numerically solved using a  
 131 Crank–Nicolson time integration with a set of initial and boundary conditions, such as an initial  
 132 geothermal gradient ( $G_0$ ) at the start time of the model and surface temperature ( $T_s$ ) (Turcotte and  
 133 Schubert, 2002; Fox et al., 2014).

134 The closure temperature ( $T_c$ ) of a thermochronometer is a function of cooling rate ( $\dot{T}$ ) at  
 135 the closure time and kinetic parameters of Helium and Argon diffusion and fission-track annealing  
 136 in mineral phases (Dodson, 1973):

137 
$$\dot{T} = \frac{\Omega R T_c^2}{E_a} \exp\left(\frac{-E_a}{R T_c}\right), \quad (8)$$

138 where  $\Omega$  and  $E_a$  are the diffusion frequency factor normalized by the mineral size and geometry,  
 139 and activation energy, respectively. Parameter  $R$  is the gas law constant. See reviews by Reiners  
 140 and Brandon (2006) for the  $\Omega$  and  $E_a$  parameter values for different thermochronometers.

141 The cooling rate ( $\dot{T}$ ) can be computed from the derivative of transient geotherms,  $T_m(t, z)$   
 142 that can be computed using equation 7 (Fox et al., 2014):

143 
$$\dot{T} = \frac{\partial T_m}{\partial t} + \dot{e} \frac{\partial T_m}{\partial z}, \quad (9)$$

144 where  $\dot{e}$  is unknown exhumation that can be computed through the equation 1.

145 Combining the equations 7-9, the closure depth of a thermochronological system ( $z_{c,m}$ ) can  
 146 be numerically computed. This depth also needs a topographic correction, because of the  
 147 topographic perturbation,  $p$ , on the isotherms (Braun, 2002; Ehlers and Farley, 2003; Fox et al.,  
 148 2014; Glotzbach et al., 2015). Such a perturbation can be determined by the following equation  
 149 (Mancktelow and Grasemann, 1997; Fox et al., 2014):

150 
$$p(\lambda) = \left(\frac{\gamma_0 - \gamma_a}{\gamma_{z_m}}\right) \exp\left(-z_m\left(\frac{\dot{e}}{2\kappa} + \sqrt{\left(\frac{\dot{e}}{2\kappa}\right)^2 + (2\pi\kappa)^2}\right)\right) h(\lambda), \quad (10)$$

151 where  $\gamma_a$  is the atmospheric lapse rate,  $\gamma_0$  and  $\gamma_{z_m}$  are the thermal gradients at the model surface and  
 152 at the depth  $z_m$ . The  $h(\lambda)$  is a cosine function expression of the model surface topography, which  
 153 can be determined using the discrete Fast Fourier Transform at the frequency domain. Here we use  
 154 the SRTM30 data for computing the topography of regions of interests.

155 Finally, the closure depth of the  $z_c$  is corrected by the topographic perturbation (e.g.,  
 156 Brandon et al., 1998):

$$157 \quad (z_c)_i = (z_{c,m})_i - p_i + h_i, \quad (11)$$

158 where  $z_{c,m}$  is the closure depth calculated using the 1D geothermal model,  $p$  and  $h$  are the  
 159 topographic perturbation and elevation difference with respect to the mean elevation at the sample  
 160 site (Fig. 1), and the  $i$  denotes the  $i$ -th age.

161 As shown by the equations 7, 8 and 9, the closure depth is a non-linear function of rock  
 162 cooling and exhumation. Therefore, the problem of interest is non-linear, which can be addressed  
 163 by iterative numerical modelling methods. In this work, the solution of exhumation is  
 164 approximated by coupling and iterating the linear inversion and closure depth modeling. As shown  
 165 in Tarantola (2005) and Fox et al. (2014), the algorithm converges in a few iterations and produces  
 166 stable outputs.

167

168 **4. Model evaluation**

169 Quantitative model assessment relies on a misfit value, i.e., the difference between  
 170 observed and predicted ages weighted by the observed analytical uncertainty:

$$171 \quad \Phi_\tau = \sqrt{\frac{1}{N} \sum_{i=1}^N \left( \frac{\tau_{prd,i} - \tau_{obs,i}}{\varepsilon_i} \right)^2}, \quad (12)$$

172 where  $\tau_{obs,i}$  and  $\tau_{prd,i}$  are the observed and predicted  $i$ -th age calculated from the exhumation history,  
 173 and  $\varepsilon_i$  is the uncertainty of the observed  $i$ -th age. Following Fox et al. (2014), both the *a priori* and

174 *a posteriori* misfits,  $\Phi_{\tau, pr}$  and  $\Phi_{\tau, po}$ , are determined for the models. The difference between these  
175 two misfit values provides a measure of the model improvements. A smaller posteriori misfit value  
176 indicates an improved model result, and *vice versa*.

177 To evaluate the geothermal parameters, we also determined the misfit value of the  
178 predicted to the observed modern geothermal gradient value using the following equation:

179

$$\Phi_{\gamma} = \sqrt{\left(\frac{\gamma_{prd} - \gamma_{obs}}{\varepsilon_{\gamma}}\right)^2}, \quad (13)$$

180 where  $\gamma_{prd}$  and  $\gamma_{obs}$  are the predicted and observed geothermal gradients, and  $\varepsilon_{\gamma}$  is the uncertainty  
181 of the observed value. Because the depth-temperature curves are slightly non-linear, the predicted  
182 geothermal gradient ( $\gamma_{prd}$ ) is calculated as a mean value for the upper 1 km of the model. Similar  
183 as the assessment of age data, we also determined the *a priori* and *a posteriori* misfits,  $\Phi_{\gamma, pr}$  and  
184  $\Phi_{\gamma, po}$  values for assessing the geothermal parameters.

185

186 **5. The reference inverse model**

187 Following Willett and Brandon (2013) and Fox et al. (2014), here we use the published  
188 AFT data acquired from Denali Massif (Fitzgerald et al., 1995) for method demonstration (Fig.  
189 2a). A break-in-slope is shown by the AER at ~7-6 Ma, indicating a coeval change in slope, i.e.,  
190 the apparent exhumation rate (Fitzgerald et al., 1995), increasing from  $0.17 \pm 0.04$  km/Myr to  $1.2$   
191  $\pm 0.6$  km/Myr (Fig. 2b). AER regression of young dates from the lower part of the transect  
192 (between 4.3-2.0 km) also predicts a closure depth that is the intercept at  $-3.3 \pm 3.4$  km (Fig. 2b).  
193 However, using the present geothermal gradient ( $38.9$  °C/km) (Fox et al., 2014) and a nominal  
194 closure temperature of AFT method ( $110$  °C) (Reiners and Brandon, 2006) and a  $-12$  °C surface  
195 temperature (Fox et al., 2014), the closure depth is predicted as ~3.1 km beneath the mean elevation

196 (~4 km), which is equivalent to an elevation of ~0.9 km. This closure depth is significantly higher  
197 than the intercept ( $-3.3 \pm 3.4$  km). Such a difference indicates the AER slope of the lower part  
198 overestimates the exhumation rates since ~7-6 Ma.

199 Following the protocol outlined in Fox et al. (2014), the reference inverse model uses the  
200 following parameters, a start time at 25 Ma, a time interval ( $\Delta t$ ) of 2.5 Myr, a 4020 m mean  
201 elevation, a  $-12$  °C surface temperature, *a priori* exhumation rate of  $0.5 \pm 0.15$  km/Myr, a  $24$  °C/km  
202 initial geothermal gradient, a  $38.9$  °C/km present geothermal gradient, a model block with a  
203 thickness of 80 km, and a  $30$  km $^2$ /Myr thermal diffusivity.

204 The exhumation history output of the reference model is shown in Fig. 3. The inversion  
205 results reveal an more than two-fold increase of exhumation rate to a value of ~0.6 km/Myr at 7.5  
206 Ma (Fig. 3b), consistent with the development of the break-in-slope in the AER. The model also  
207 shows a gradual decrease of exhumation rate from *a priori* exhumation rate (0.5 km/Myr) to 0.3  
208 km/Myr from 25 Ma to 7.5 Ma. The invariant exhumation during the starting stage resulted from  
209 the fact that all ages are younger than 17.5 Ma, and thus the data have no resolution for the time  
210 span. These results are similar to those of Fox et al. (2014). The posteriori misfit for the age is  
211 1.88, significantly smaller than that of the priori model (4.51), suggesting the improvement by the  
212 inverse modeling (Fig. 3b). Such a model also provides reasonable fit to the modern temperature  
213 field, as shown by the small misfit (0.39) in the geothermal gradient (Fig. 3b).

214 The resolution of the inverted exhumation history can be assessed by the resolution matrix  
215 **R** (equation 6). Imaging of the matrix shows the model provides no resolution for the time period  
216 before 17.5 Ma (Fig. 3c), consistent with the fact that the oldest input age is younger than  $16.1 \pm$   
217 0.9 Ma. For the time span between 15 and 5 Ma, the model resolution is high, as shown by the  
218 diagonal elements of the matrix, with the highest resolution at 7.5-5 Ma span, including eight age

219 date points (Fig. 3c). The most recent two phases of exhumation (5-0 Ma) are less resolved, as  
220 shown by the nearly equal resolution values for the two phases, i.e., the latest four pixels of the  
221 matrix (Fig. 3c). This is because no input ages fall into this time span, when the modeled  
222 exhumation results are time-averaged values. The slight decrease in the last stage reflects changes  
223 in geothermal gradient.

224 For assessing the correlation among model parameters, the calculated covariance matrix is  
225 scaled by the diagonal covariance matrix (Fox et al., 2014):

226

$$\hat{C}_{\xi\beta} = \frac{C_{\xi\beta}}{\sqrt{C_{\xi\xi}}\sqrt{C_{\beta\beta}}} \quad (14)$$

227 The correlation matrix for the reference model is shown in Fig. 3d. The diagonal correlation  
228 values are 1 and off-diagonal ones are dominantly negative, indicating anti-correlated uncertainties  
229 (Fig. 3d), which suggests exhumation parameters were not resolved independently by the modeling.  
230 In fact, it is expected to have the anti-correlation, because, given two steps of rock exhumation,  
231 decreasing the exhumation during one step would increase that of the other step.

232

## 233 **6. Dependence on model parameters and proposed solutions**

234 Here we use the Denali data set for demonstrating the influences of (1) the initial  
235 geothermal parameters, (2 and 3) the *a priori* mean and variance values of the exhumation rates,  
236 and (4) time interval length on the inverted exhumation history. Also discussed in this section are  
237 the solutions for optimizing the model setup for these parameters.

238

### 239 **6.1. Dependence on initial thermal model**

240 Different initial model geothermal parameters would lead isotherms to shift either  
241 downward to greater depths or upwards to the Earth surface, and either compression or expansion

242 among isotherms. Therefore, the initial thermal models have systematic influence on the closure  
243 depths and consequently the *a posteriori* exhumation.

244 This is demonstrated by modelling experiments presented in Figure 4. Using a relatively  
245 lower initial geothermal gradient produces relatively higher *a posteriori* exhumation rates  
246 (comparing the models shown in Figs. 4a-4f), and *vice versa*. Such an influence is significant even  
247 for the time and elevation intervals with multiple age constraints (10-5.0 Ma). For example, using  
248 relatively lower geothermal gradients of <22 °C/km would yield significantly higher average  
249 exhumation rates of >0.75 km/Myr for the last two stages (<5 Ma) (Figs. 4a-4c) than those (<0.6  
250 km/Myr) using higher initial geothermal gradients of ≥26 °C/km (Figs. 4d-f). Further, it is also  
251 shown that models using higher and lower prior geothermal gradients of <20 °C/km (Figs. 4a-4b)  
252 and >30 °C/km (Figs. 4e-4f) yield worse misfits ( $\Phi_{\gamma, po} > 1$ ) for the observed present-day  
253 geothermal gradient than those ( $\Phi_{\gamma, po} < 1$ ) using medium initial gradients (22-26 °C/km) (Figs. 3  
254 and 4c-4d).

255 These results highlight the importance of taking geothermal parameters into account in  
256 inverting the exhumation history and model evaluation. We proposed to run a set of models using  
257 different *a priori* geothermal parameters, especially the initial geothermal gradient, to search for  
258 the proper initial geothermal setup that provides reasonable fits to both the ages and the modern  
259 geothermal gradient (see section 7 for details).

260

261 **6.2. Dependence on the *a priori* exhumation rate**

262 Both the mean and variance of the *a priori* exhumation rate have important influences on  
263 the model solution for the maximum likelihood estimation method. Our modeling experiments  
264 show that the mean value of the *a priori* exhumation has systematic influences on the inverted

265 exhumation. Similar to the reference model, exhumation of the preceding three stages (25-17.5  
266 Ma) without age constraints is the same as the *a priori* input. For the following stages, a relatively  
267 higher mean value of the *a priori* exhumation results in relatively lower *a posteriori* exhumation  
268 rates (comparing different models presented in Fig. 5). For example, models using the mean *a*  
269 *priori* exhumation of  $\leq 0.4$  km/Myr yield *a posterior* exhumation of 0.5-0.9 km/Myr for the stages  
270  $< 7.5$  Ma (Figs. 5a-5c), whereas those using a higher *a priori* value ( $\geq 0.6$  km/Myr) result in *a*  
271 *posterior* exhumation of 0.45-0.6 km/Myr for the same stages (Figs. 5d-5f). This is because a  
272 relatively higher *a priori* value, which would be used for calculating thermal models, would lead  
273 to a quicker increase in geothermal gradient and thus relatively shallower closure depths and  
274 relatively lower exhumation rates.

275 The variance of the *a priori* exhumation rate has important influence on both the  
276 exhumation rates and the posterior variance. Models with lower *a priori* variances yield less  
277 variations in the *a posterior* exhumation history, and *vice versa* (comparing models in Fig. 6).  
278 Further, models using the input variance of the *a priori* exhumation of 0.2-0.3 km/Myr (40-60%  
279 of the mean value), the variation of the inverted exhumation history becomes stable (Figs. 3, 6c-  
280 6d). Given that the uncertainty of the input age data, which is often 10%-20% at a two-sigma level,  
281 larger variance of the inverted exhumation would be unreasonable (Figs. 6e-6f), especially when  
282 multiple age data are available at different elevations.

283 We proposed to run a set of models using different *a priori* mean value of erosion rates to  
284 search for the one that provides appropriate fits to both the ages and the modern geothermal  
285 gradient. As to the *a priori* variance, we propose to use a value 30-70% of the *a priori* erosion rate.  
286 Future applications of the method may need to test a set of the variance inputs so as to get a stable

287 exhumation output. Larger *a priori* variance would lead to larger uncertainties for the exhumation  
288 rates, which is unreasonable and non-meaning for geological studies.

289

290 **6.3. Dependence on time interval length**

291 Constraining the onset time of major changes in exhumation rates is one of the important  
292 tasks for inverting the exhumation history from thermochronologic data. Using a large time  
293 interval length cannot accurately capture the potential transition time of exhumation rates. As  
294 shown in the Figs. 7b-7d, models using time lengths of  $\leq 3.5$  Ma show an abrupt increase in  
295 exhumation at 7-6 Ma, consistent with that shown in AER plot. However, the models using a large  
296 time interval length ( $\geq 4.5$  Ma) overestimate the onset time of the enhanced exhumation (Figs. 7e-  
297 7f). Further, a relatively shorter time length would smooth temporal changes in exhumation rates,  
298 leading to an underestimating of the variations. For example, as shown in the Fig. 7a, the model  
299 using a relatively shorter time length (0.5 Ma) yields an exhumation variation between 0.35-0.60  
300 km/Myr, significantly lower than those using relatively larger time interval lengths (Figs. 7b-7f).  
301 In addition, a shorter time length also significantly increases the computational time and resources,  
302 especially when processing a large number of vertical transects.

303 Given the interests in major exhumation changes, we propose the time interval length ( $\Delta t$ )  
304 should be optimized for constraining the transitional time and the associated exhumation changes.  
305 Therefore, the time interval length should be set as the absolute uncertainty at two sigma levels at  
306 the break point ( $\tau_b$ ) (equation 15). If the break point is unclear in AER, we suggest to use the  
307 absolute uncertainty at two-three sigma levels at the median age value ( $\tilde{\tau}$ ) (equation 15), so as to  
308 focus on the time intervals where ages cluster.

309 
$$\Delta\tau = \begin{cases} \delta\tau_b, & \text{if a break in slope exists} \\ \delta\tilde{\tau}, & \text{if no clear break in AER} \end{cases} , \quad (15)$$

310 where  $\delta$  is the relative age uncertainty at two sigma levels, varying between 10%-20% among  
311 different studies. Following this method, the Denali case should use a time length of  $\sim$ 1.5 Ma (7  
312 Ma  $\times$  20%), slightly lower than that used in the reference model (Fig. 3).

313

314 **7. A new modeling guideline**

315 Following the modelling protocol outlined above, a stepwise modeling guideline is  
316 developed for addressing the model dependencies on the initial geothermal parameter, the *a priori*  
317 exhumation rates and time interval length. As illustrated in the Figure 8, the approach includes the  
318 following three steps.

319 (i) Estimating a time-averaged erosion rate. Dividing each nominal closure depth, which  
320 can be estimated from the nominal closure temperatures and the modern geothermal gradient, by  
321 the corresponding age results in a time-averaged erosion rate. Then, a mean value can be  
322 determined by averaging the rates. Such a mean value and assumed variance (30% - 50% in this  
323 work) will be used as the *a priori* erosion rate.

324 (ii) Optimizing the fit to the modern geothermal gradient. This step runs a set of inversion  
325 models (20 in this work) using different geothermal gradients, ranging from 50% to 120% of the  
326 modern value, together with the *a priori* erosion rate estimated in the first step, for determining  
327 the initial geothermal gradient that yields the maximum fit to the modern value, i.e., the minimum  
328  $\Phi_\gamma$  (equation 13).

329 (iii) Optimizing the fit to both the age data and the geothermal gradient. Given the model  
330 dependence on the geothermal parameters (see section 6.1), a comprehensive evaluation of the  
331 models should assess not only the age misfit ( $\Phi_\tau$ ), but also that of the geothermal gradient ( $\Phi_\gamma$ ). In  
332 the third step, a set of inversion models (20 in this work) are run using different *a priori* erosion

333 rates, changing from 10% to 200% of the mean value estimated in the first step, together with the  
334 estimated geothermal gradient by the second step, to search for the model that provides the best fit  
335 to both the age data and the modern geothermal gradient. This study uses the following compound  
336 misfit function to evaluate the models:

337 
$$\Phi = \Phi_\tau + \Phi_\gamma / \sqrt{N}, \quad (17)$$

338 where  $\Phi_\tau$  and  $\Phi_\gamma$  are misfit values for the age and geothermal gradient calculated using the  
339 equations 12 and 13, and  $N$  is the number of age inputs. Dividing  $\Phi_\gamma$  by the square root of  $N$  in this  
340 equation, as also done for calculating the  $\Phi_\tau$  (equation 12), means that the modern geothermal  
341 gradient is given the same weight as an age input for evaluating the model.

342

343 **8. Synthetic models for testing the new modeling guideline**

344 We firstly test our stepwise inversion scheme by synthetic datasets generated by thermo-  
345 kinematic models modified from Braun et al. (2012) (their Fig. 9). The synthetic age dataset is  
346 produced by *Pecube* using the following parameters: a steady-state topography with a 20-km  
347 wavelength and a 2-km relief, a model block thickness of 30 km with a basal temperature of 600 °C,  
348 a thermal diffusivity of 25 km<sup>2</sup>/Myr, a sea level temperature of 10 °C, a lapse rate of 5 °C/km.  
349 Worth noting is that these parameters are the same as Braun et al. (2012). For model details, see  
350 Braun et al. (2012). For model setup see the supplementary Figure S1.

351 Synthetic AFT and AHe ages (supplementary Tables T1) were calculated for both surface  
352 and borehole samples for four different exhumation histories. The synthetic models a and b are  
353 characterized by a sudden decrease in exhumation rate from 1 km/Myr to 0.1 km/Myr (model-a,  
354 same as the that shown in the Fig. 9 of Braun et al. 2012) and 0.3 km/Myr (model-b) at 5 Ma,  
355 respectively. The models c and d include a sudden increase in exhumation rate from 0.3 km/Myr

356 (model-c) and 0.1 km/Myr (model-d) to 1 km/Myr at 5 Ma, respectively. All models start from 40  
357 Ma. Except for the synthetic age data (plotted in the first row of Fig. 9), these four models generate  
358 modern geothermal gradients of 26.5 °C/km, 28.6 °C/km, 35.5 °C/km and 34 °C/km for the  
359 uppermost 2-km crust, respectively.

360 Inversion of rock exhumation history used a start time of 20 Ma and a time interval length  
361 of 1.0 Myr for all synthetic datasets, which were assigned with a 6% uncertainty. As shown by the  
362 modelling output visualized in Fig. 9a, our inversion of the rock exhumation from the synthetic  
363 dataset-a finds an optimal initial geothermal gradient of 22 °C/km and *a priori* rate of  $0.85 \pm 0.25$   
364 km/Myr, and yields a decrease in exhumation rates from ~0.9 km/Myr (before 6 Ma) to 0.3-0.1  
365 km/Myr (4-0 Ma), via a gradual decrease during 6-4 Ma. The data has no resolution for the  
366 exhumation history before 10 Ma. Comparing to the synthetic model (abrupt decrease from 1  
367 km/Myr to 0.1 km/Myr at 5 Ma), the rates before 5 Ma are underestimated by 0.1 km/Myr, whereas  
368 the values after 5 Ma overestimated by 0.1-0.3 km/Myr.

369 The inversion for the synthetic dataset-b results in an optimal initial geothermal gradient  
370 of 21.7 °C/km and *a priori* rate of  $0.81 \pm 0.24$  km/Myr, and an increase in exhumation rates from  
371 ~0.85 (before 5 Ma) km/Myr to 0.4-0.5 km/Myr (4-0 Ma), via a gradual decrease during 5-4 Ma  
372 (Fig. 9b). Comparing to the synthetic model (abrupt decrease from 1 km/Myr to 0.3 km/Myr at 5  
373 Ma), the rates before 5 Ma are underestimated, whereas the values before 5 Ma are overestimated  
374 by ~0.1-0.2 km/Myr.

375 The inversion for the synthetic dataset-c yields an optimal initial geothermal gradient of  
376 24.3 °C/km and *a priori* rate of  $0.55 \pm 0.17$  km/Myr, and a decrease in exhumation rates from  
377 ~0.45-0.3 km/Myr (before 5 Ma) to 1.0 km/Myr (3-0 Ma), via a gradual increase during 5-3 Ma  
378 (Fig. 9c). Comparing to the synthetic model (abrupt decrease from 0.3 km/Myr to 1.0 km/Myr at

379 5 Ma), the rates during 5-3 Ma are underestimated, whereas the rates before 5 Ma overestimated  
380 by 0-0.15 km/Myr.

381 The inversion for the synthetic dataset-d produces an optimal initial geothermal gradient  
382 of 24.5 °C/km and *a priori* rate of  $0.25 \pm 0.08$  km/Myr, and an increase in exhumation rates from  
383 ~0.1-0.2 km/Myr (before 5 Ma) to 1.0 km/Myr (3-0 Ma), via a gradual decrease during 5-3 Ma  
384 (Fig. 9d). Comparing to the synthetic model (abrupt decrease from 1 km/Myr to 0.3 km/Myr at 5  
385 Ma), the rates before 5 Ma are slightly overestimated, whereas the values during 5-3 Ma are  
386 underestimated.

387 To summarize, the inverted rock exhumation histories for the four synthetic datasets match  
388 the whole picture of the synthetic “truth”, but the variations in exhumation are underestimated,  
389 and the sharp changes at 5 Ma are smoothed. It is worth noting that inversions using only surface  
390 samples produce similar results (supplementary Fig. S2).

391

## 392 **9. Natural examples for testing the new modeling guideline**

393 Below we use three examples to demonstrate our new method. The Denali data is used  
394 again for demonstrating the efficiency of our method in finding the proper initial geothermal  
395 gradient and the *a priori* exhumation rate. Then, we further test our method using the Himalayan  
396 Dhanladar range and KTB borehole (the Continental Deep Drilling Project in Germany)  
397 thermochronologic data for representing regions of fast and slow erosion, respectively.

### 398 9.1 The Denali transect

399 Using the stepwise inversion modeling guideline, the Denali transect yields an exhumation  
400 history generally similar with that of the reference model (Fig. 10a). Differences in the *a priori*  
401 parameters include that the new inversion finds and uses an initial geothermal gradient of

402 25.2 °C/km (slightly higher than that of the reference model), *a priori* erosion rate of  $0.46 \pm 0.23$   
403 km/Myr (slightly lower than that of the reference model) and a time interval length of 1.5 Ma. The  
404 combination of these *a priori* parameters result in a major increase in erosion rate to 0.55-0.6  
405 km/Myr at 6 Ma, which is 1.5 Myr latter than that of the reference model (7.5 Ma). The subtle  
406 differences from the reference model mainly result from the time interval length used in these  
407 models. Comparing the misfit values, the new model produces slightly better fits than the reference  
408 model, with the *a posteriori* misfit values of 1.81 and 0.11 for the observed age and geothermal  
409 data.

410

#### 411 9.2 Himalayan Dharladar range transect

412 AFT and ZHe data from the Dharladar range in the northwestern Himalayas, reported in  
413 the publications by Deeken et al. (2011) and Thiede et al. (2017) are used as an example for regions  
414 of young cooling ages and fast exhumation. The samples were collected in an elevation range  
415 between 1.5 and 4.5 km, covering a topographic relief of 3 km within a spatial distance of  $\sim 15$  km  
416 on the hanging wall of the main central thrust of the Himalayan fold-thrust-belt (Deeken et al.,  
417 2011; Thiede et al., 2017). AER slope regression of ZHe and AFT ages performed in Deeken et al.  
418 (2011) produced apparent erosion rates of  $\sim 2.8$  km/Myr and  $\sim 0.2$  km/Myr for the time intervals  
419 6.4–14.5 Ma and 1.7–3.7 Ma, respectively, implying a potential increase in erosion rates at  $\sim 3.7$ –  
420 6.4 Ma. Using geothermal gradients of 25–45 °C/km, time-averaged erosion rates were estimated  
421 as 0.8–2.0 km/Myr since 3.7 Ma (Deeken et al., 2011).

422 The modelling of the Dharladar range data uses a modern geothermal gradient constraint  
423 of  $45 \pm 8$  °C/km (Deeken et al., 2011). The relatively large uncertainty is assigned for the  
424 geothermal gradient, because of the absence of direct geothermal measurements in the study area.

425 Our exhumation inversion for the AER data using the stepwise modeling guideline yields relatively  
426 slow rates of 0.1-0.6 km/Myr and fast rates of 1.2-1.6 km/Myr before and after  $\sim$ 3 Ma, respectively  
427 (Fig. 10b). The abrupt increase of exhumation rates at  $\sim$ 3 Ma is generally consistent with the  
428 estimates from the slope regression results of Deeken et al. (2011). However, the inverted  
429 exhumation rates since 3 Ma are significantly lower than the estimation from the AER slope ( $\sim$ 2.8  
430 km/Myr), which is likely due to the overestimation of exhumation of the AER slope due to  
431 topographic perturbation of isotherms. Such a perturbation is a function of exhumation rates: the  
432 higher the exhumation, the larger the perturbation (Glotzbach et al., 2015). The modelling yields  
433 a history of the geothermal gradient that gradually increases to a modern value of  $\sim$ 46  $^{\circ}$ C/km, close  
434 to the input value ( $45 \pm 8$   $^{\circ}$ C/km).

435

436 9.3 KTB borehole

437 The KTB borehole yields a large thermochronologic and geochronologic age data  
438 (Warnock and Zeitler, 1998; Stockli and Farley, 2004). Previous studies suggest the borehole are  
439 truncated by multiple faults, which offset the age-depth relationship (Wagner et al., 1997). Here  
440 we use the data at depths shallower than 1 km, where data are abundant and have linear relationship  
441 with depths.

442 The KTB apatite, zircon and titanite (U-Th)/He (AHe, ZHe and THe) and AFT age data  
443 vary largely between 85-50 Ma. These clustered ages have been interpreted as indicating a late  
444 Cretaceous phase of exhumation, followed by slow exhumation (Wagner et al., 1997; Stockli and  
445 Farley, 2004), as also shown by previous thermal history reconstructions based on k-feldspar  
446  $^{40}$ Ar/ $^{39}$ Ar data (Warnock and Zeitler, 1998).

447 Our modeling, using the AER data and a modern geothermal gradient of  $27.5 \pm 2.8$  °C/km  
448 (Clauser et al., 1997), shows that elevated exhumation rates (0.1-0.13 km/Myr) between 80-50 Ma,  
449 followed by slower exhumation rates of ~0.04 km/Myr (Fig. 10c), are similar to previous estimates  
450 (Wagner et al., 1997; Warnock and Zeitler, 1998; Stockli and Farley, 2004). Associated with  
451 changes in exhumation, geothermal gradient gradually decreases from the peak values at 70-60  
452 Ma to a value of ~28 °C/km at the present-day.

453

#### 454 **10. Conclusion**

455 The *a priori* information has important effects on the inversion results using the least-  
456 squares inversion method. Our study demonstrates the importance of geothermal gradient and the  
457 *a priori* exhumation rate in estimating the exhumation history from the thermochronology data.  
458 To take into account the geothermal data into the exhumation history inversion, we outlined a  
459 stepwise inversion method that first searches for the appropriate initial geothermal gradient, which  
460 is then used in the modelling searching for the *a priori* exhumation rate. Our modelling guideline  
461 produces exhumation history and geothermal gradient that provide reasonable fits for both the  
462 observed AER and modern geothermal data, as tested by datasets of both synthetic models and  
463 natural samples. The code and data used in this work are available in GITHUB  
464 ([https://github.com/yuntao-github/A2E\\_app](https://github.com/yuntao-github/A2E_app)).

465

#### 466 **Code availability**

467 The code used in this work are available in GITHUB ([https://github.com/yuntao-github/A2E\\_app](https://github.com/yuntao-github/A2E_app)).

468

#### 469 **Data availability**

470 The data used in this work are available in GITHUB ([https://github.com/yuntao-github/A2E\\_app](https://github.com/yuntao-github/A2E_app)).

471

472 **Author contribution**

473 Yuntao Tian: Conceptualization, Methodology, Software, Data curation, Visualization,

474 Investigation, Writing- Original draft preparation. Lili Pan: Visualization, Writing- Reviewing and

475 Editing. Guihong Zhang and Xinbo Yao: Writing- Reviewing and Editing.

476

477 **Competing interests**

478 The contact author has declared that none of the authors has any competing interests.

479

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484

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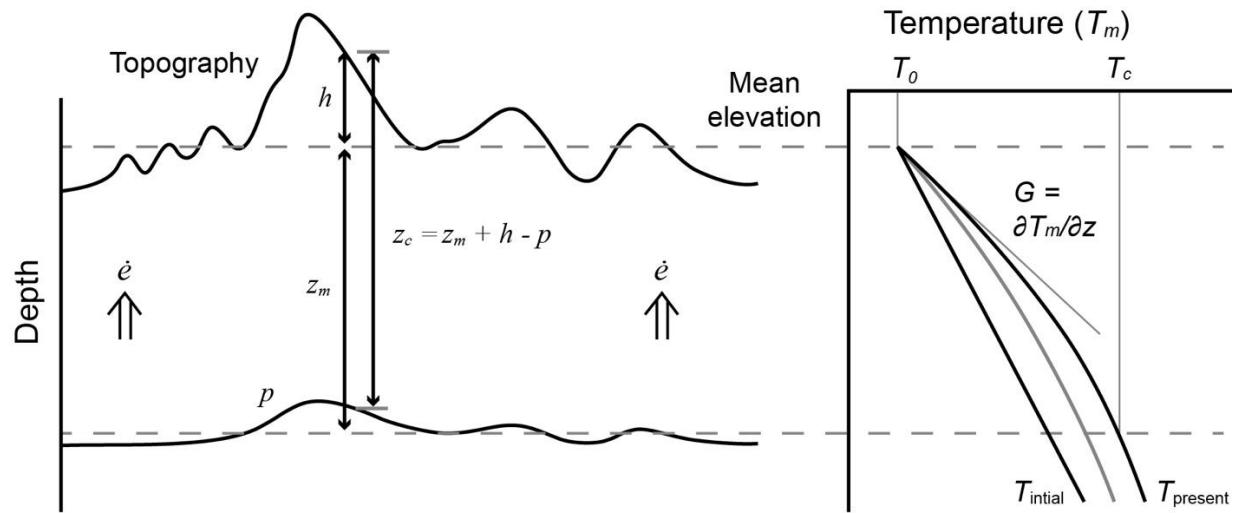
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626 **Figures captions:**

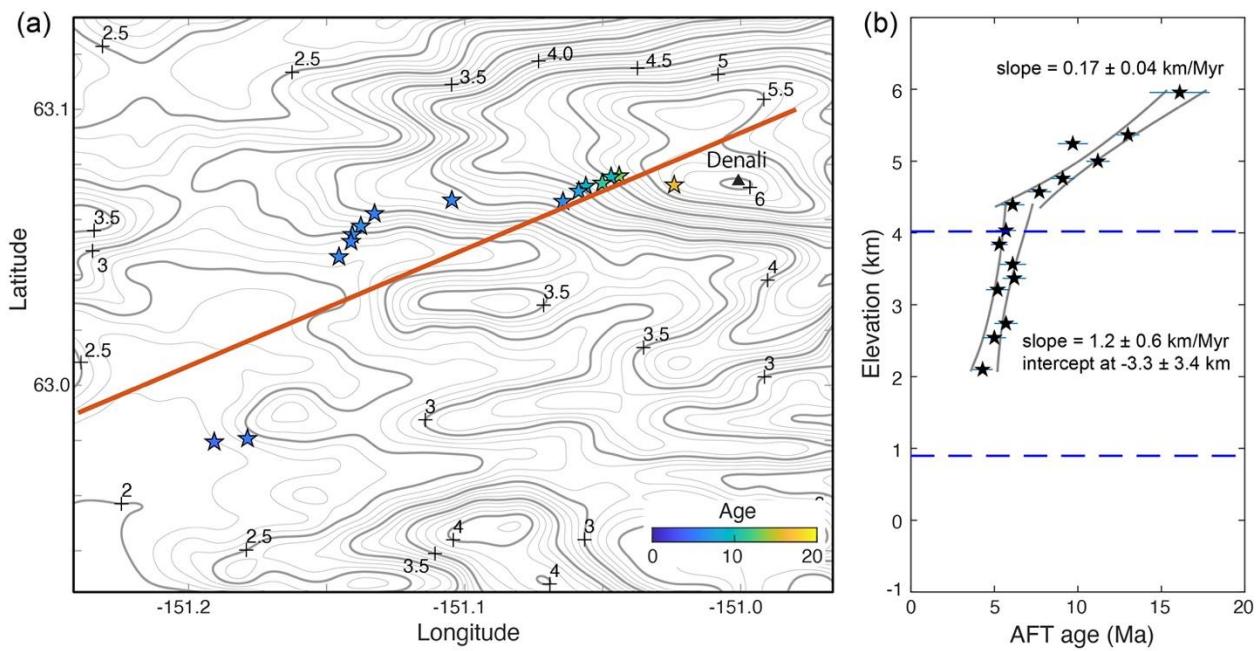
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628 Figure 1. Schematics showing the relationship among closure depth ( $z_c$ ), topography and its  
629 perturbation ( $p$ ). The parameter  $h$  denotes the difference between the sample and the mean  
630 elevation, and  $z_m$  the depth of the closure temperature ( $T_c$ , the lower dashed line) derived from  
631 the mean elevation (upper dashed line) and intial temperature field ( $T_{initial}$ ) and exhumation  
632 history ( $\dot{e}$ ).

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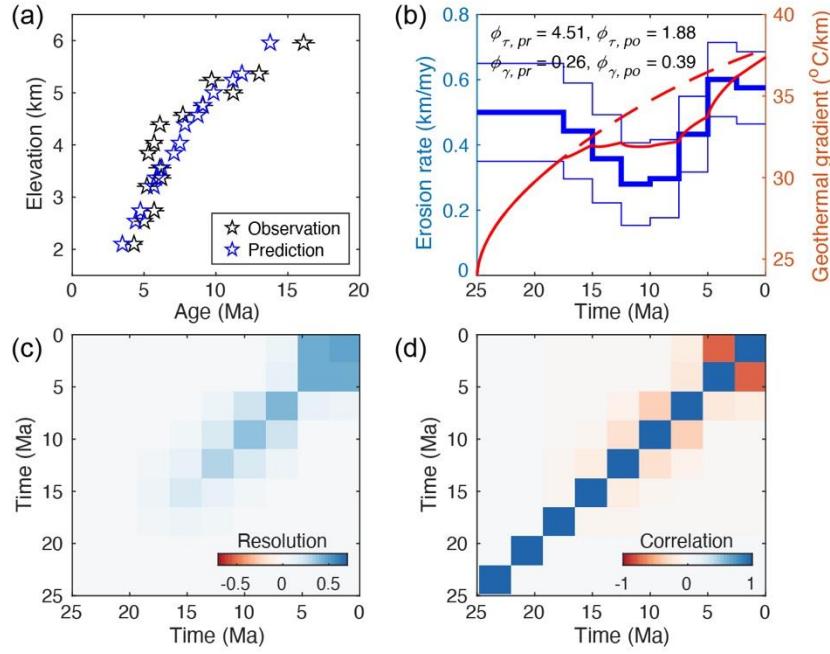
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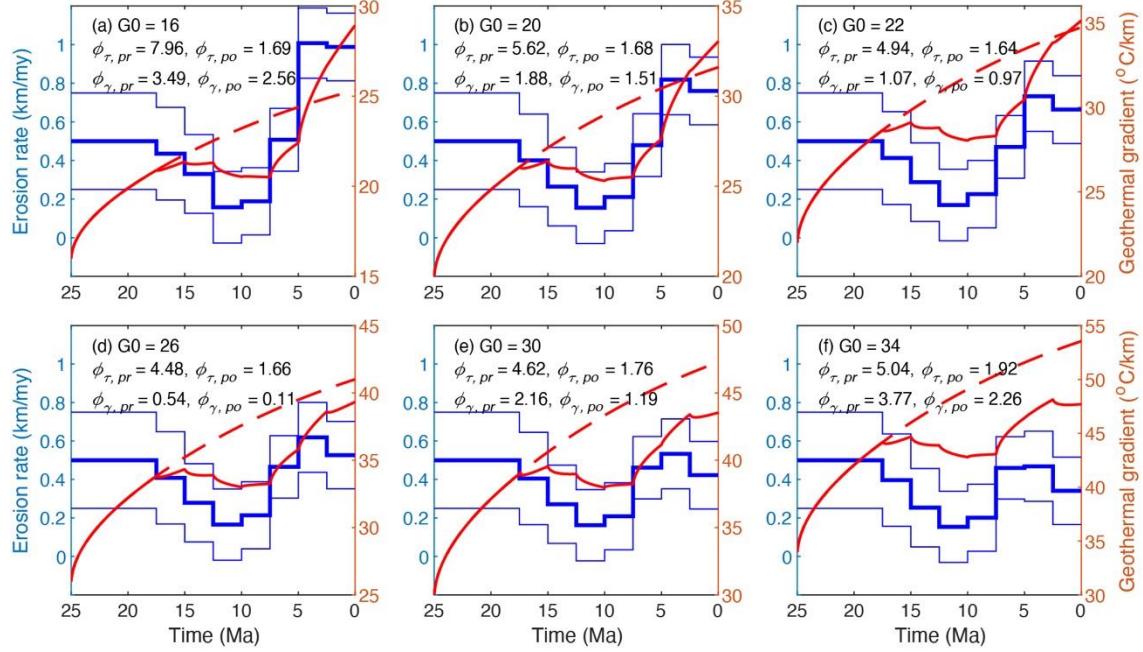
636 Figure 2. (a) Distribution of AFT age data (pentagons, colored by age values) over the elevation  
 637 contour map computed using the SRTM30 data of the Denali massif in Alaska. AFT data  
 638 sourced from Fitzgerald et al. (1995). (b) AER and the slope fitting results using isoplotR  
 639 (Vermeesch, 2018). AER fitting of ages older than 6.7 Ma yields a slope of  $0.17 \pm 0.04$  km/Myr;  
 640 whereas the fitting of ages between 6.5 Ma and 4.3 Ma produces a slope of  $1.2 \pm 0.6$  km/Myr  
 641 and an intercept at  $-3.3 \pm 3.4$  km. The upper and lower dashed lines denote the mean elevation  
 642 (4.02 km) and the depth of the nominal closure temperature (110 °C), calculated using the  
 643 modern geothermal gradient (38.9 °C/km) and the surface temperature (-12 °C).

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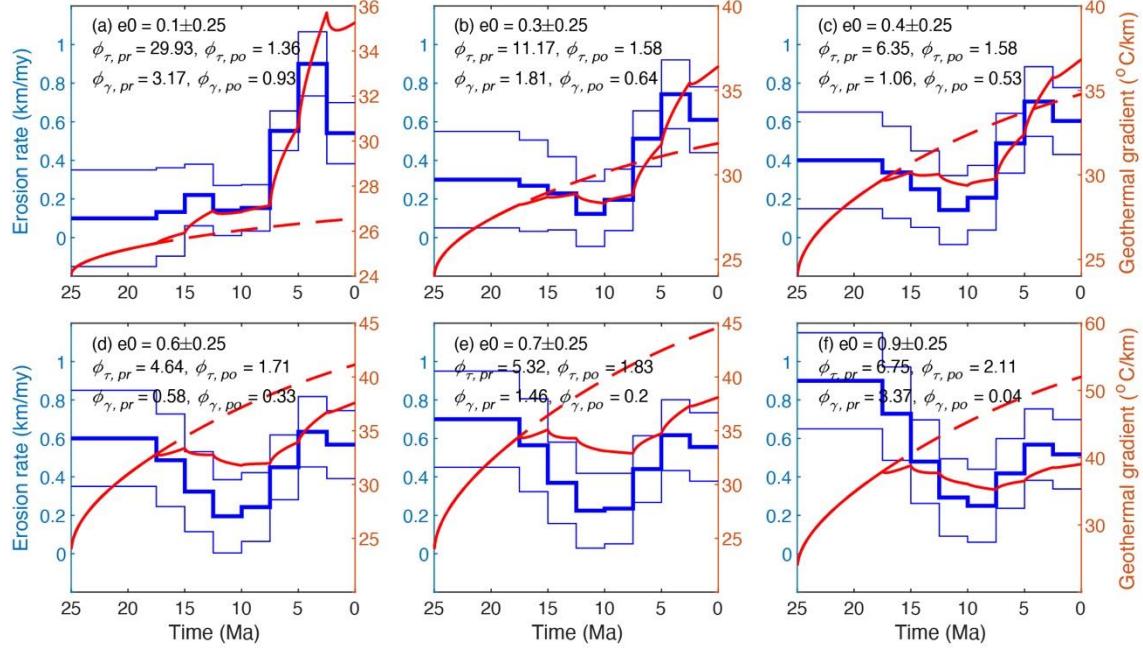
646 Figure 3. Inputs and outputs of the reference model for the Denali AFT. (a) Comparison between  
 647 the observed (in black) and predicted (in blue) AER. (b) The *a posterior* exhumation history  
 648 generated by the reference model. Thick and thin lines are the mean and one standard deviation  
 649 of the inverted exhumation history. The red dash and solid lines are the history of the geothermal  
 650 gradients, predicted by the *a priori* and *a posterior* models, respectively. (c) and (d) Plots of the  
 651 resolution and correlation matrix.



652

653 Figure 4. Histories of exhumation and geothermal gradients, predicted by models using different  
 654 initial geothermal gradients between 18 °C/km and 34 °C/km. The blue thick and thin lines are  
 655 the mean and one standard deviation of the inverted exhumation history. The red dash and solid  
 656 lines are the history of the geothermal gradients, predicted by the *a priori* and *a posteriori*  
 657 models, respectively. Except for the initial geothermal gradient, other parameters are the same as  
 658 the reference model. Comparing to the reference model which used an initial geothermal gradient  
 659 of 24 °C/km (Fig. 3), models using a lower initial geothermal gradient yield relatively higher  
 660 exhumation rates (panels a-c), whereas those using a higher gradient produce lower exhumation  
 661 rates (panels d-f).

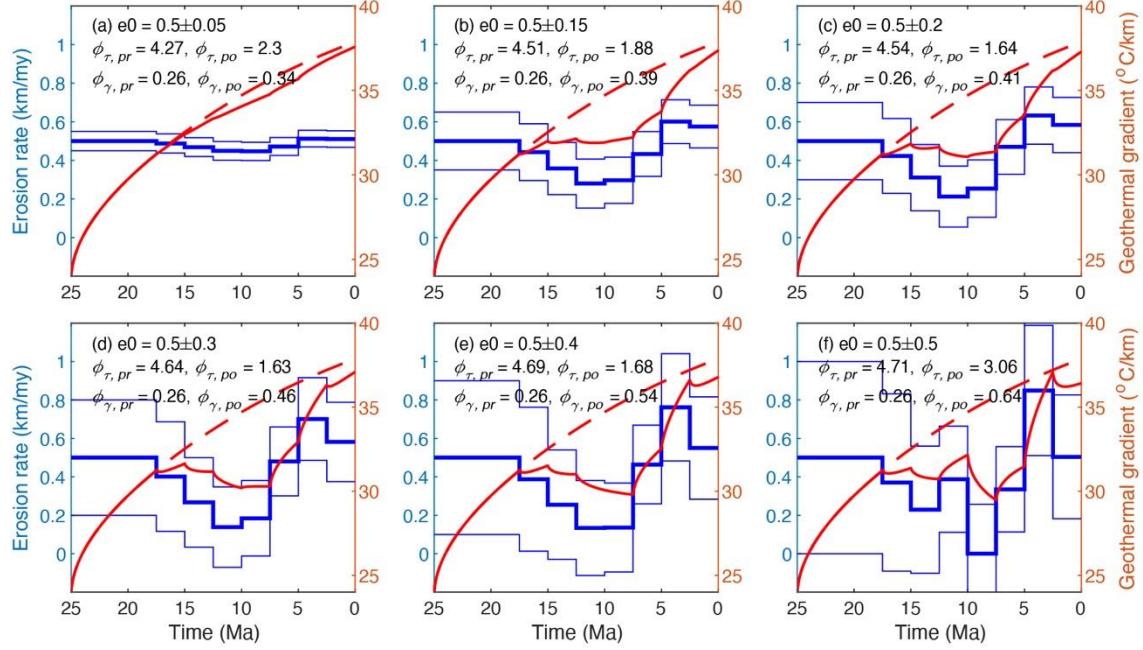
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664 Figure 5. Histories of exhumation and geothermal gradients, predicted by models using different  
 665 *a priori* mean values of the exhumation rates, ranging from 0.1 km/Myr to 0.9 km/Myr. Other  
 666 parameters are the same as the reference model. For explanation of the plotted lines, see Figure  
 667 4. Comparing to the reference model which used *a priori* mean exhumation of 0.5 km/Myr (Fig.  
 668 3), models using a lower *a priori* exhumation yield relatively higher exhumation rates for the last  
 669 three stages (7.5 - 0 Ma) (panels a-c), whereas those using a higher *a priori* exhumation produce  
 670 lower exhumation rates for the last three stages (panels d-f).

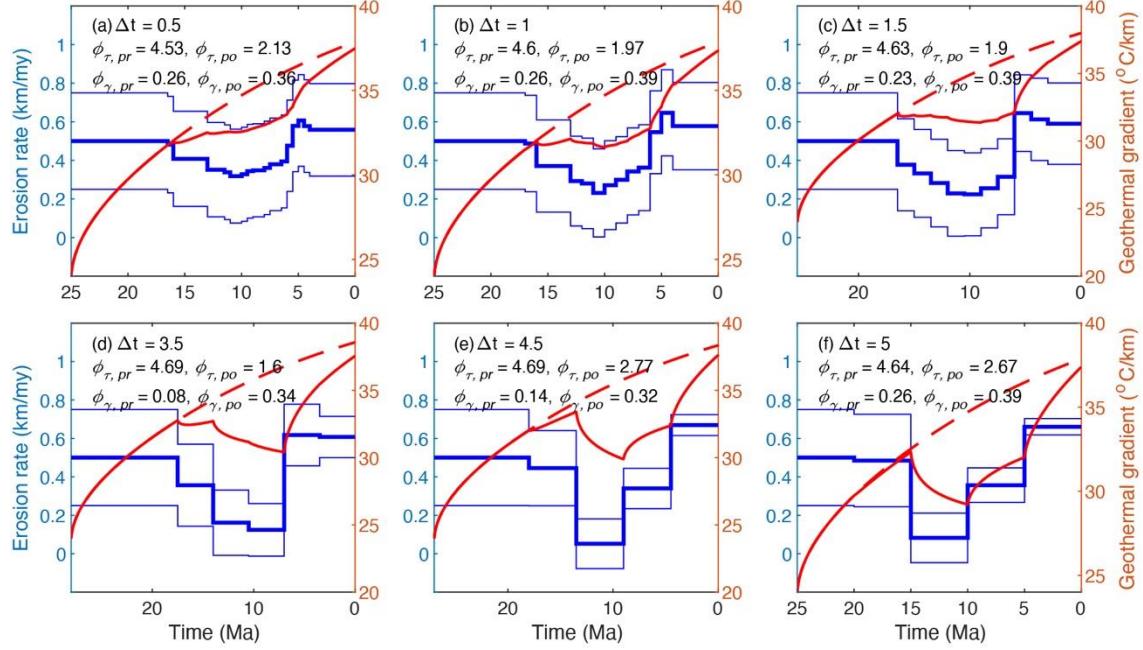
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672

673 Figure 6. Histories of exhumation and geothermal gradients, predicted by models using different  
 674 *a priori* variance values (between 0.05 km/Myr and 0.5 km/Myr) of the exhumation rates (0.5  
 675 km/ Myr). Other parameters are the same as the reference model. For explanation of the plotted  
 676 lines, see Figure 4. Comparing to the reference model which used *a priori* variance of the  
 677 exhumation (0.25 km/Myr) (Fig. 3), models using a lower *a priori* variance yield limited  
 678 variations and uncertainties in exhumation (panels a-c), whereas those using a higher *a priori*  
 679 variance produce larger variations and uncertainties (panels d-f).

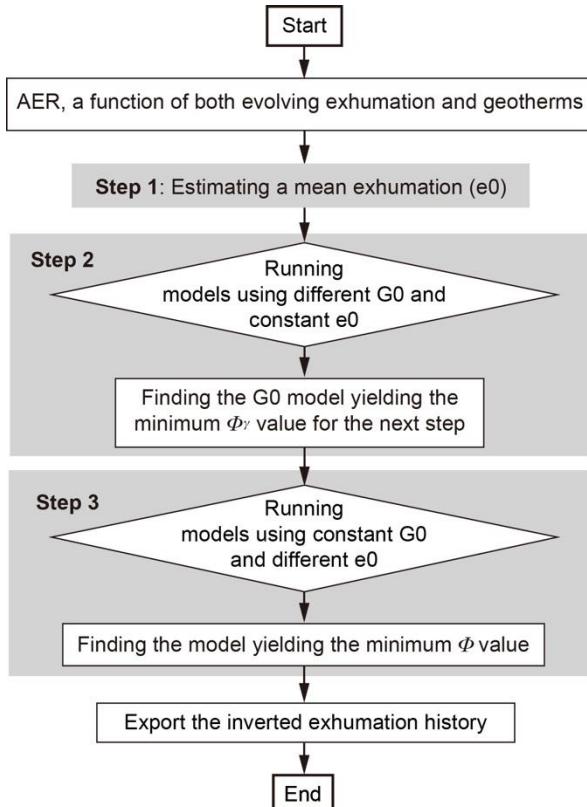
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682 Figure 7. Histories of exhumation and geothermal gradients, predicted by models using different  
 683 time interval lengths. Other parameters are the same as the reference model. For explanation of  
 684 the plotted lines, see Figure 4. Comparing to the reference model which used a time interval  
 685 length of 2.5 Ma (Fig. 3), models using smaller time interval lengths yield lower variations in  
 686 exhumation (panels a-c) than other using larger time interval lengths (panels d-f).

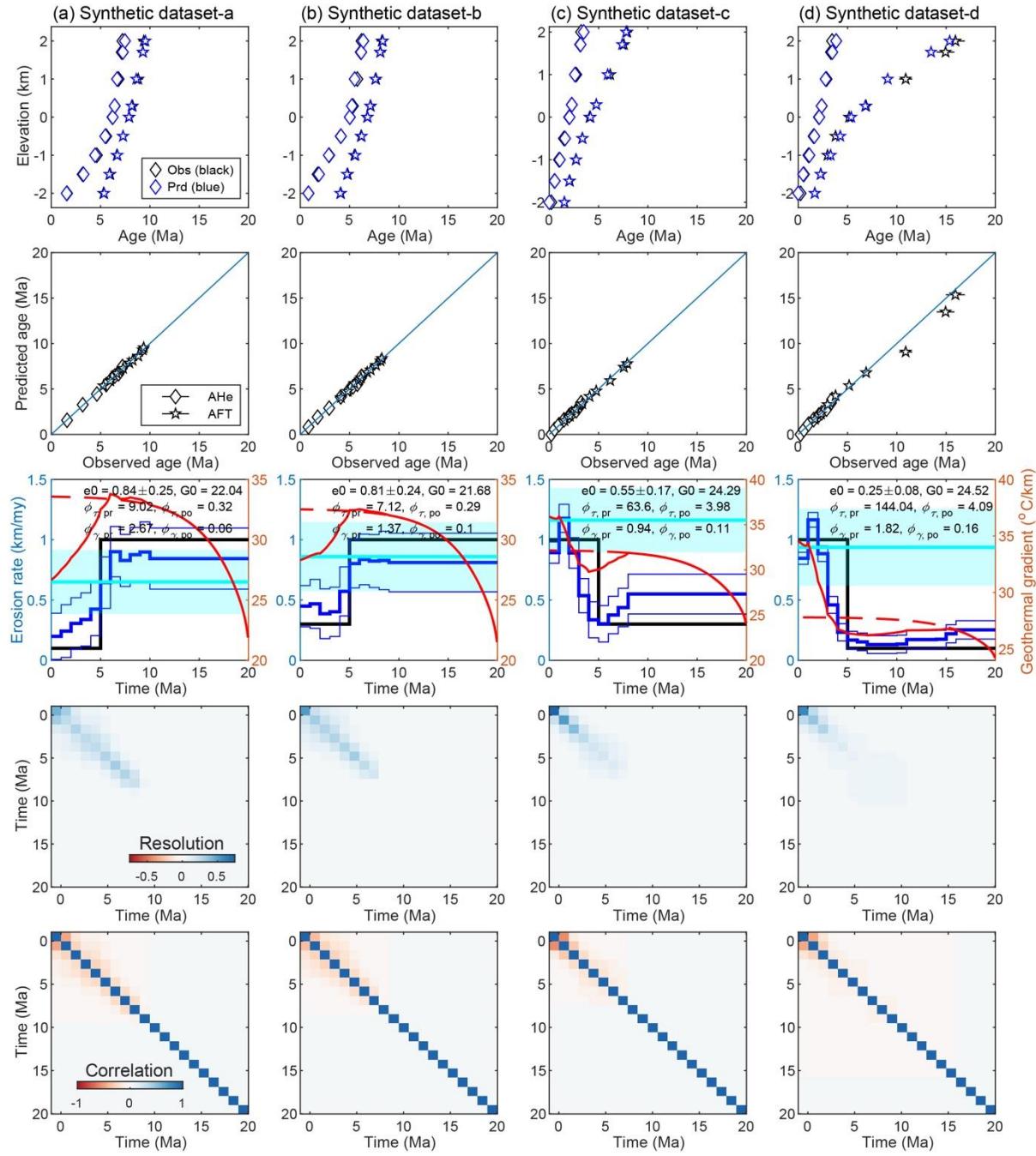
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689 Figure 8. Flow chat of a stepwise modeling method, which includes three main steps. The first  
 690 step estimates a mean exhumation rate ( $e_0$ ) using the nominal closure temperatures, modern  
 691 geothermal gradient and sample ages. The mean rate is used in the second step which runs a set  
 692 of models using different initial geothermal gradients for optimizing the initial geothermal  
 693 model. The third step runs a set of models using different *a priori* exhumation rates, which is  
 694 generated around the mean rate, and the optimized initial geothermal model by the second step,  
 695 to find the best model that yields the minimum misfit to both age data and modern geothermal  
 696 gradient.

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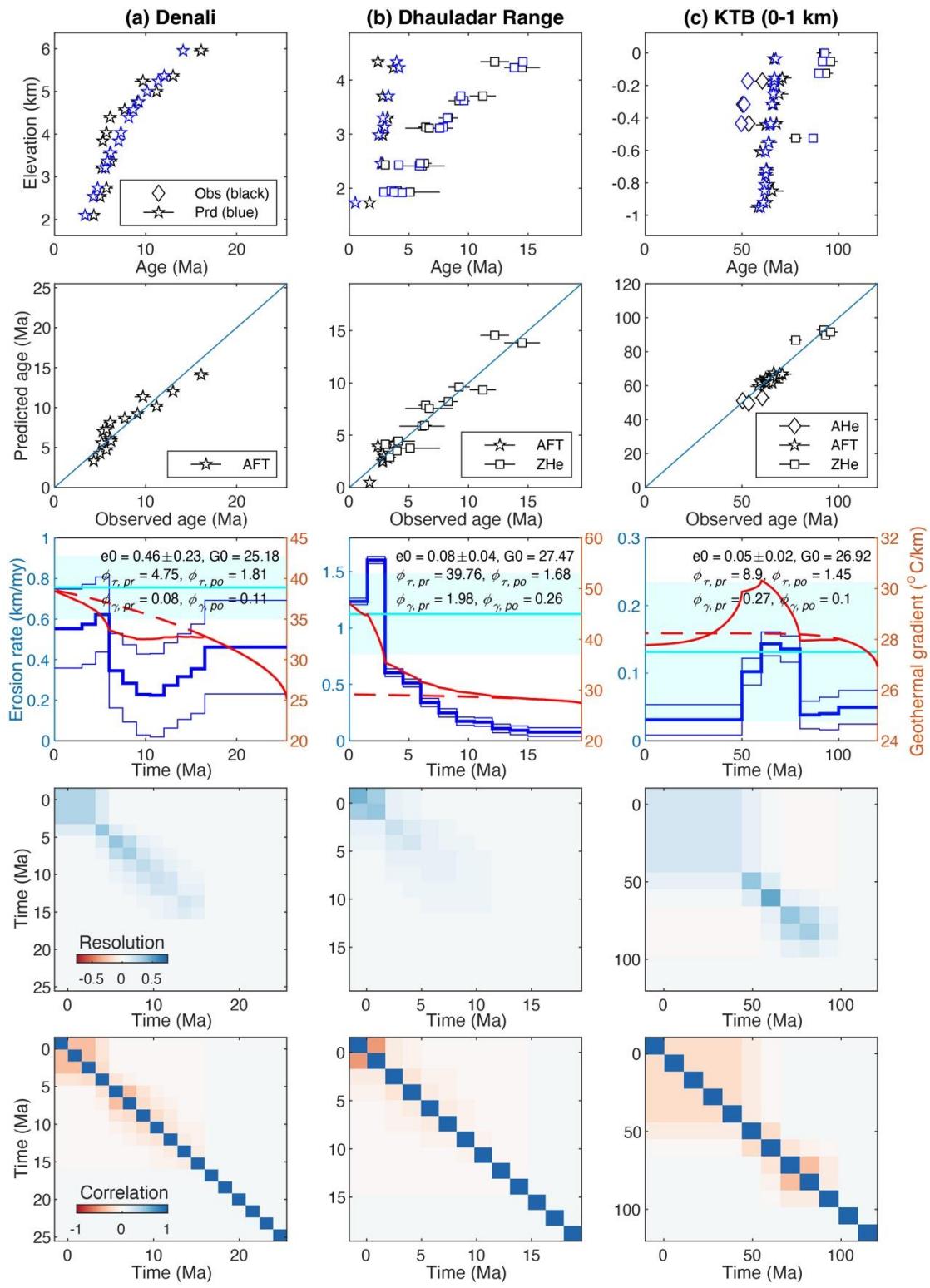


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699 Figure 9. The best-fit model for the synthetic dataset-a, -b, -c and -d using the modeling method  
700 shown in figure 8. First row: Comparison between the observed (in black) and predicted (in blue)  
701 AER. Second row: plots of observed and modeled ages. Third row: Histories of exhumation and  
702 geothermal gradients. The black line marks the “true” exhumation history used for simulating the  
703 age dataset, whereas the blue thick and thin lines are the mean and one standard deviation of the

704 inverted exhumation. The red dash and solid lines are the history of the geothermal gradients,  
705 predicted by the *a priori* and *a posterior* models, respectively, whereas the cyan line and polygon  
706 denotes the modern geothermal gradient. Fourth and bottom row: Plots of the resolution and  
707 correlation matrix.

708



709

710 Figure 10. The best-fit model for the Denali (a), Dhanladar range (b) and upper KTB (c)  
711 transects, using the modeling method shown in figure 8. See Fig. 8 for panel interpretations.