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Supplementary Materials for:
Thermal history modeling techniques and interpretation strategies: Applications using HeFTy
Kendra E Murray, Andrea L Stevens Goddard, Alyssa L Abbey, Mark Wildman

The Supplementary Materials for this manuscript include the following:

1. **A HeFTy modeling tutorial**
   This tutorial accompanies and expands upon the manuscript section entitled “Forward and Inverse Modeling of Synthetic Data: Exploring Data Uniqueness and Model Resolution”.

2. **Table S1:** Path 5 inputs, settings, and boundary conditions for thermal history model simulations

3. **Table S2:** Deep time example: inputs, settings, and boundary conditions for thermal history model simulations

4. **Figure S1**: Deep-time example, Ar-only model results annotated to illustrate the determination of exploration box bounds in He-only models (e.g., Fig. 7B).

5. **Table S3:** Data for path family example

6. **Table S4:** Path family example: inputs, settings, and boundary conditions for thermal history model simulations

HeFTy Modeling Tutorial
Building understanding of low-temperature thermochronometer behavior using HeFTy

This activity was designed to accompany the text of Murray et al. (2022) *Thermal History Modeling Techniques and Interpretation Strategies: Applications Using HeFTy* using HeFTy v.1.9.3. It was inspired by Wolf et al. (1998). We recommend reading the section of Murray et al. (2022) entitled, "Forward and Inverse Modeling of Synthetic Data: Exploring Data Uniqueness and Model Resolution". All references to this activity should cite Murray et al. (2022).

PART I: Forward Modeling

Why Forward Modeling?

Forward models predict cooling ages (ZFT, ZHe, AFT, AHe) and/or track lengths (FT) given a single specific tT history input by the user. These predictions are useful for a wide range of applications, including:

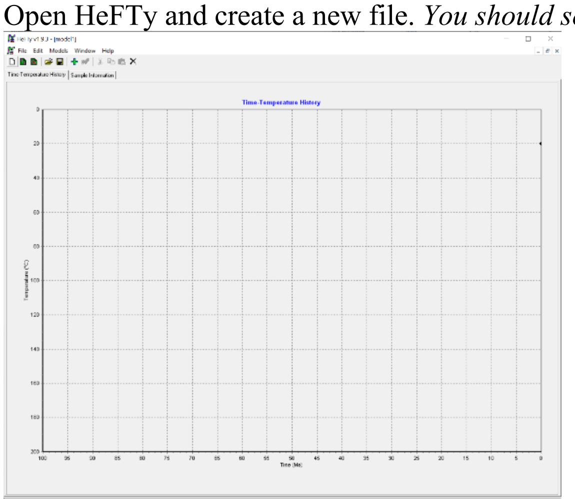
- comparing predicted data to measured data in order to:
  - systematically test specific hypothesized cooling histories
  - eliminate geologic scenarios that predict thermochronometric ages that are inconsistent with observations
- research planning, because the user can, for example:
  - test whether hypothetical rock tT histories can actually be distinguished from each other using thermochronology
  - evaluate how specific parameters (such as grain size and composition in the He system) or multi-chronometer approaches may more clearly constrain tT histories
  - explore the consequences of choosing to use one set of published kinetics over another during thermal history modeling.
- learning and teaching thermochronology, because exploring hypothetical thermal histories and the cooling ages is an excellent way build intuition about thermochronometer behavior

I.A. Forward model a single He age

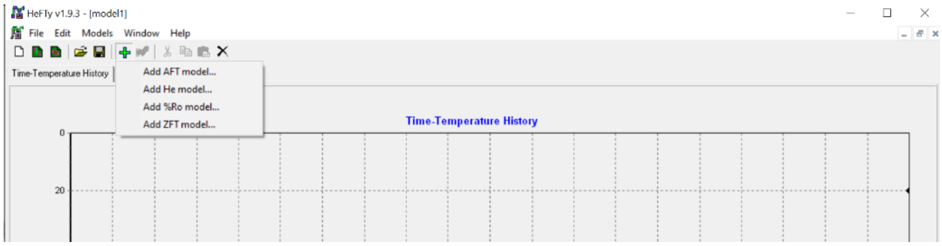
Objective: Create a single apatite crystal in HeFTy and predict its He age using 6 different tT paths.

<u>Step-by-step instructions to set up this model and start exploring forward modeling.</u>

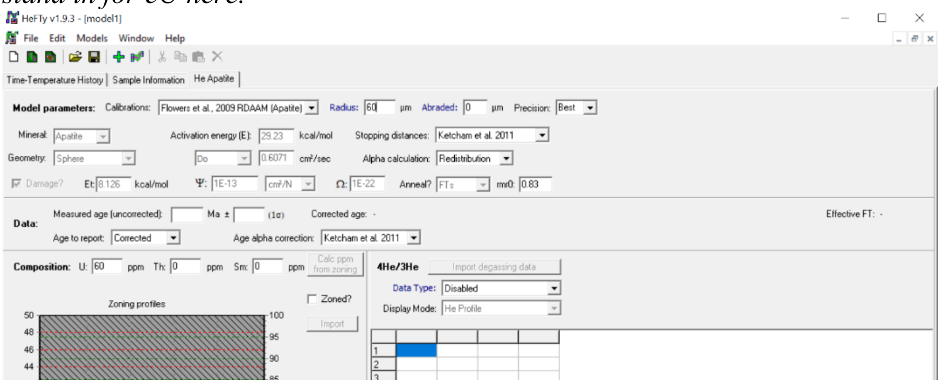
1. Open HeFTy and create a new file. *You should see a blank Time-Temperature History plot.*



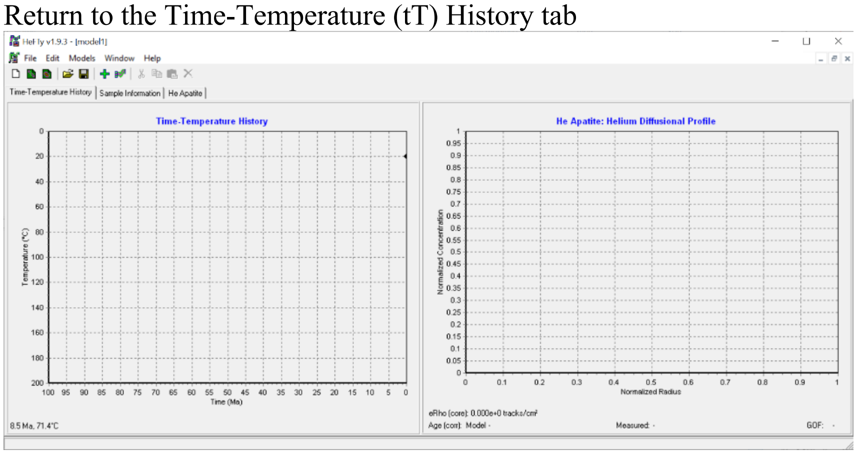
2. Create a new He model.



3. Adjust inputs in the He Apatite tab to create our single 60 µm radius, 60 ppm eU grain.
   a. Select Flowers et al., 2009 kinetics
   b. Choose 60 µm radius
   c. Input grain composition U= 60; Th = 0, Sm = 0. *For simplicity, we are just using U as a stand in for eU here.*

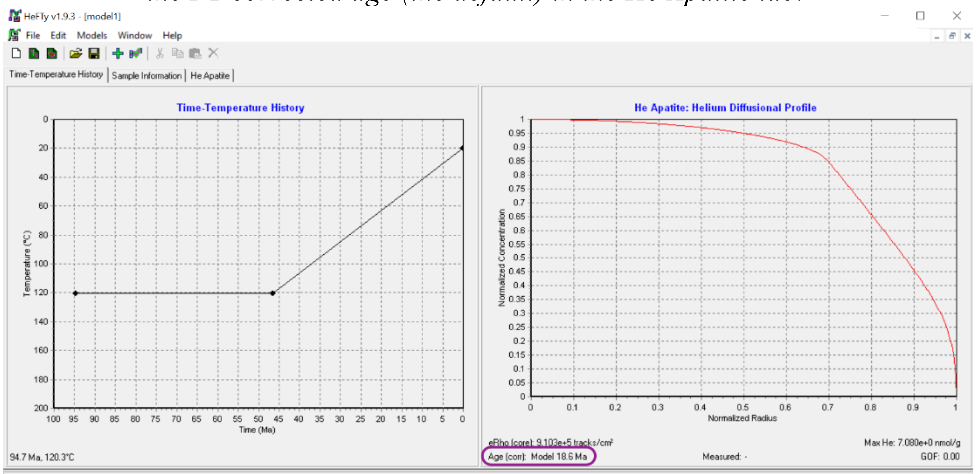


4. Explore how different tT histories impact this single crystal's age
   a. Return to the Time-Temperature (tT) History tab



   b. Click twice in the tT history panel to create some points (nodes) that will link together to form a thermal history. *You will see the panel with the AHe data populated with predicted (modeled) He age reported in the lower left corner and a diffusion profile plot. Also note that:*

- *The diffusion profile dominates the user interface but is not used when you're just working with routinely collected (bulk) He analyses, because that does not involve measuring diffusion profiles (or zonation of any kind).*
- *The predicted age is reported as the "model" age because we asked HeFTy to report the FT corrected age (the default) in the He Apatite tab.*



c. In the tT History panel, click and drag existing nodes to adjust their position or click anywhere in tT space to create additional nodes that shape the tT history. *The predicted age (and diffusion profile) will adjust dynamically..*

d. Try some other ways to adjust the nodes in the tT history window
- Right click on a node for options to erase it or type in a specific t and T
- Right click on tT space for other options, including deleting all nodes.
- Double click on the x- or y-axis to adjust the axis dimensions.
- You can also import a tT path from a text file (see user manual for info about the text file format needed).

<u>Exercise #1: Predict a single AHe age for 6 different tT histories.</u>
Overview: The table below provides the tT information for 6 different thermal histories. Use HeFTy's tT tab to forward model each thermal history and record the predicted AHe age in the last row of the table.

Path #	**1**		**2**		**3**		**4**		**5**		**6**	
	time	*temp*	*time*	*temp*	*time*	*temp*	*time*	*temp*	*time*	*temp*	*time*	*temp*
	40	200	100	145	100	90	100	90	100	5	100	20
	39.9	5	0	5	20	60	75	70	5	82.5	41	20
	0	5			19.9	5	29.5	70	0	5	40.5	200
					0	5	0	5			40	5
											0	5
Predicted AHe age:												

Questions:

1. For each tT path, describe what is happening at 40 Ma (ex: cooling rate relative to sample cooling history, heating, is it the start of cooling, the end of cooling, etc). In each case, is the He age telling you about a cooling "event"?

2. Is there something that all these paths have in common that causes them to yield a 40 Ma age?

3. All of these paths (except Path 1) start at 100 Ma. What are we *assuming* is true about the geologic history of this apatite grain by designing the model in this way?

Additional activities for Part I.A

1) Change the eU or grain size of the apatite crystal.
   a) What impact does this have on the He age predicted for each path?
   b) Describe why this change happens, based on your understanding of how eU or grain size control apatite He ages.
2) Add another chronometer (for example, AFT) tab to your forward model.
   a) Add the predicted AFT age to your table of predicted ages.
   b) What is the relationship between the AFT age and the AHe age? Does this make sense, given your understanding of these two systems? Explain.
3) Start the model prior to 100 Ma, at various times and temperatures, but otherwise keep each path the same. In other words, explore the consequences if this apatite existed before 100 Ma.
   a) Under what circumstances does a pre-100 Ma history impact the measured AHe age?
   b) Using your understanding of the AHe system, explain why.
4) Combine #2 and #3 above and explore the relative sensitivity of two systems to a longer history.
5) Find 6 similar paths that also all yield 40 Ma ages for another thermochronometer (AFT, ZHe).
   a) What is different from the 6 AHe paths? Similar? Why?
      What would the apatite He ages be for each path?

I.B. Forward modelling trends: examples from AHe age-eU trend and AFT track lengths

Objective: Create a hypothetical sample with 6 apatite grains identical in size (60μm) that span a large U-Th-Sm (eU) compositional range (given below) and an AFT age and track length distribution. Then, forward model the 6 *tT* paths from Exercise #1 and document the AHe and AFT ages that result.

First you will need to create the following files:

- **HeFTy file with six single grain AHe tabs and one AFT tab**
  1. *Open a new model in HeFTy.*
  2. *Create 6 He apatite models (6 tabs).*
     a. *eU of 10, 30, 60, 90, 150, 300 ppm, respectively (use U)*
     b. *All grains 60 μm radius*
     c. *All grains RDAAM kinetics of Flowers et al., 2009*
     d. *Report the corrected age to the user interface.*
     e. *You should see 6 windows added to the tT history tab, one for each grain.*

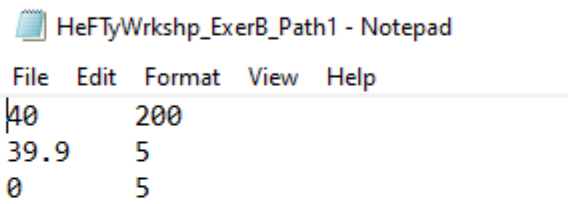
  3. *Create an AFT model (tab 7)*

a. 5.5M C-axis projection
b. Model c-axis projected lengths

4. Save your file.

- **Text files of the t-T history of Paths 1-6**

  1. For each Path 1-6 described in Exercise 1, create a text file with time in the first column and temperature in the second column. An example (screenshot) of the textfile for Path 1 is provided below.



HeFTyWrkshp_ExerB_Path1 - Notepad

File Edit Format View Help

```
40      200
39.9    5
0       5
```

- **Excel File**

  1. Create an Excel file that enables you to record the individual AHe ages and AFT age and lengths for each of the six thermal history Paths 1-6 (example of what these tables might look like below)

IDENTIFYING TRENDS

Apatite (U-Th)/He Grains	*eu (ppm)*	Path 1 *(Ma)*	Path 2 *(Ma)*	Path 3 *(Ma)*	Path 4 *(Ma)*	Path 5 *(Ma)*	Path 6 *(Ma)*
	10						
	30						
	60						
	90						
	150						
	300						

**enter data in yellow cells*

	Path 1	Path 2	Path 3	Path 4	Path 5	Path 6
AFT Model Age						
Mean Track Lengths						

**enter data in yellow cells*

Exercise #2: Predict age-eU patterns and AFT track lengths

Overview: Use HeFTy in the forward sense to predict the age-eU trends and AFT track length distributions that would result from the 6 different *tT* paths in Exercise #1. Make an age-eU plot of the results. Then, answer the questions that follow. *Note: We are using a much wider range of apatite eU compositions (10-300 ppm) than is commonly dated in a single sample.*

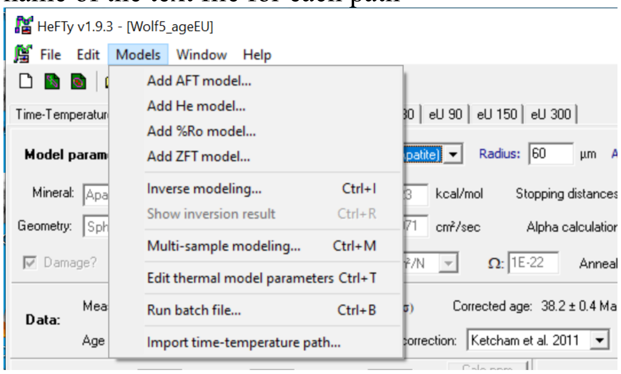
1. Open the HeFTy file that you created for this exercise. This file should include the following data:

   6 He apatite models (6 tabs - 1 tab per grain).
   a. eU of 10, 30, 60, 90, 150, 300 ppm, respectively (see U value)
   b. All grains 60 µm radius
   c. All grains RDAAM kinetics of Flowers et al., 2009

   AFT model (tab 7)
   a. 5.5M C-axis projection
   b. Model c-axis projected lengths

2. Open the Excel spreadsheet that you created. This sheet will create an age-eU plot of the data you will generate.

3. In HeFTy, input each tT path one at a time and transcribe the predicted ages and lengths into your spreadsheet. Let's practice importing *tT* paths from a text file, rather than manually creating each path in the *tT* window.
    a. Under the Models menu, choose "Import time-temperature path…" and navigate to the name of the text file for each path



    b. As before, the predicted age of each sample can be read off the lower left hand corner of each grain's panel in the Time-Temperature tab. *You may need to adjust the sizes of the panels so you can see this information.*
    c. Read off each predicted age and manually enter the age into your spreadsheet in the AHe. *Yep, this part is tedious.*
    d. Read off each predicted AFT age and mean track length and enter this into the tab AFT length trends. Take a screenshot of the AFT length distribution and plop that into your spreadsheet as well, to capture the results.

4. Repeat this process for each Path.

5. Create a scatter plot in Excel to plot age-eU for each individual plot. Plot all age-eU trends on the same scatter plot. It is standard to plot eU on the x-axis and the predicted age on the y-axis.

6. On your spreadsheet, quantify the AHe age variability that results from each tT history. *There is no one "right" way to do this, but using a clear, quantitative metric is important for describing a He dataset and deciding what to do next. The following is after Flowers et al., 2008, who used a 20% cut-off to distinguish between "variable" and "reproducible" samples.*
    a. Calculate the mean AHe age for each tT history.
    b. Calculate the standard deviation for each tT history.
    c. Calculate the % standard deviation of the mean age. *In other words, if the mean age is 56 Ma and the standard deviation is 15 Ma, the % s.d. is 27%. Most He thermochronologists would consider this a "variable" dataset that requires one to understand/demonstrate the principal source of this age variability in order to interpret the data. See also Flowers and Kelley (2011).*

Questions.

1. Describe the He age variability and age-eU patterns produced by each tT Path. *When describing age-eU, avoid the term "correlation" and stick to descriptive terms that paint a picture without implying a statistical assessment of the relationship between age and eU—you are making a qualitative assessment here, which for a real dataset would then lead into further quantitative assessment.*

2. Which tT histories result in “reproducible” He ages? “Variable” He ages?

3. WHY? Use your understanding of partial-retention and radiation damage accumulation and annealing behavior in the apatite He system to hypothesize/interpret why each tT path produces the trend that it does.

4. So, in general, what “ingredients” or conditions are necessary to produce a significant age-eU trend in an AHe dataset?

5. Which age-eU patterns are sufficiently distinctive from each other visually that you think you could resolve the difference between the tT histories using the age-eU trend alone? *We’ll test your ideas in Exercise #5.*

6. Describe the shapes and mean track lengths of predicted AFT track lengths for Path 1 (rapid cooling), Path 2 (steady cooling), and Path 4 (retention at PAZ temperatures). How can each of these data sets be used?

7. Identify two sets of paths for which trends in AFT data clearly distinguish between two possible cooling histories, but AHe data is not as clear. Vice versa? Discuss how this observation might influence what types of data you collect for an unknown dataset.

Additional activities for Part I.B.

1) Explore grain size (Rs) effects on AHe age instead of eU.
   a) Use a eU of 60 ppm, vary grain sizes from Rs = 30-120 μm (or your preference)
   b) Make age-Rs plot and calculate age variability that results from each tT path.
   c) What kind of age-Rs trends does grain size generate? How does this compare to eU?
   d) Does grain size have a larger or smaller influence on He age than [eU]?
   e) How big a range of apatite grain sizes would you need to pick from a real sample in order to produce an obvious age-Rs trend? How does the tT history impact the answer to this question?
2) Create a suite of AHe crystals that has variability in *both* Rs and eU. *This is the most common situation in real datasets. HeFTy can easily model both sources of age variability together, and both of these pieces of information are collected during routine (U-Th)/He analysis. However, these situations can result in data that appear highly scattered on bivariate plots. See Flowers and Kelley, 2011.*
   a) Demonstrate your understanding of Rs and eU effects by building a suite of crystals that produce a negative-slope relationship between age and eU for paths 4 and 5.
   b) How much grain size variability is necessary for grain size to be “more important” than eU? How does the tT history impact the answer to this question?

PART II: Inverse Modeling

Why Inverse Modeling?

In HeFTy, an inverse model result is a family (or families) of tT paths; each individual tT path produces predicted ages that fit the input data, given the model set up. Such models are an efficient way to explore tT space. *So, how well can inverse models resolve the 'true' tT histories under ideal circumstances?* **Here we use the forward model paths Exercise #1, and the synthetic apatite He age-eU trends we generated from the forward models of these paths in Exercise #2, to explore this question.**

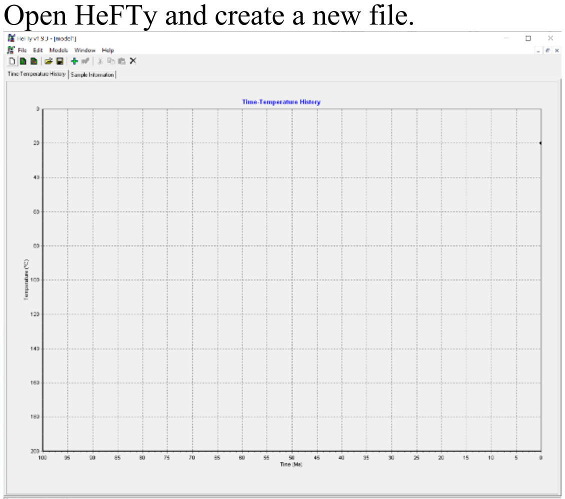
II.A. Inverse modeling a single AHe age

Objective: Set up an inverse model for the single AHe age that we forward modeled in Part 1A (Exercise 1). Design the model such that it finds good fits to Paths 1-6, which we know all yield this same ~40 Ma AHe age.

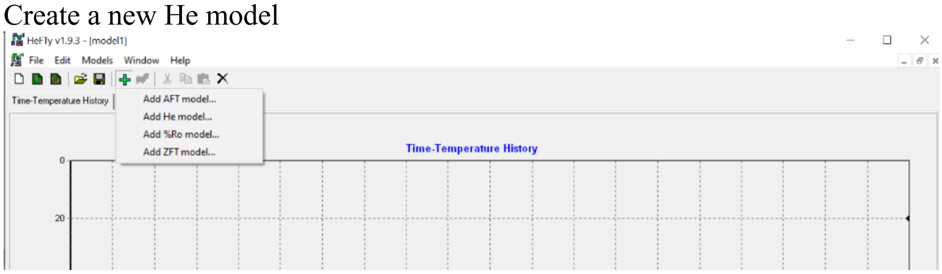
Files Needed: none, build your own in HeFTy

Step-by-step instructions for building an inverse model in HeFTy.

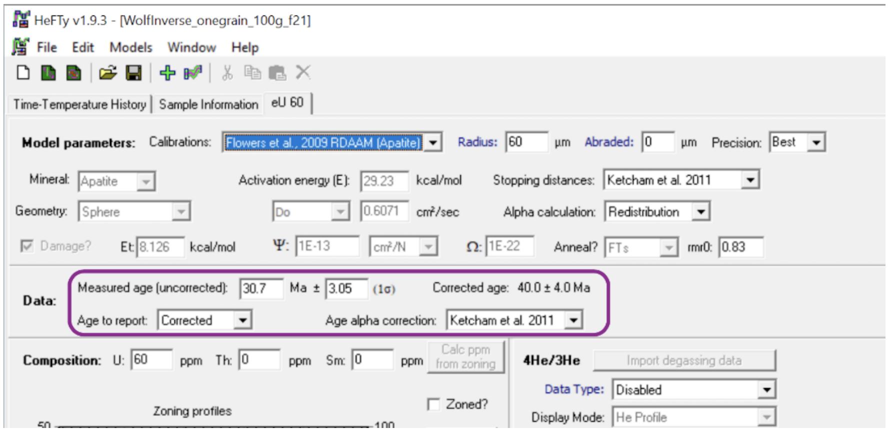
1. Open HeFTy and create a new file.



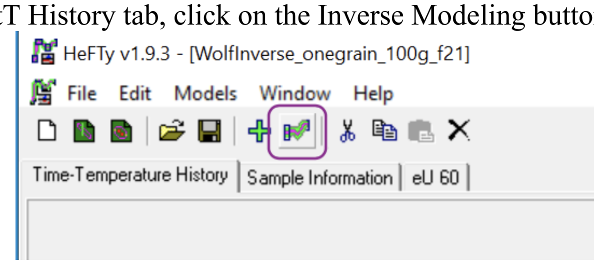
2. Create a new He model



3. Adjust inputs in the He Apatite tab to create our single 60 µm radius, 60 ppm eU grain.
    a. Select Flowers et al., 2009 kinetics
    b. Choose 60 µm radius
    c. Input grain composition U= 60; Th = 0, Sm = 0
    d. Input an uncorrected age of 30.7 Ma, with 10% 1-sigma error (i.e., 3.0 Myr); you should see that HeFTy corrects this age to 40 +/- 4 Ma. *This is the only difference from the set-up in Part A. You could also include an age in Part A; this would otherwise not change the forward modeling exercises because observed ages are only used by HeFTy in inverse modeling.*

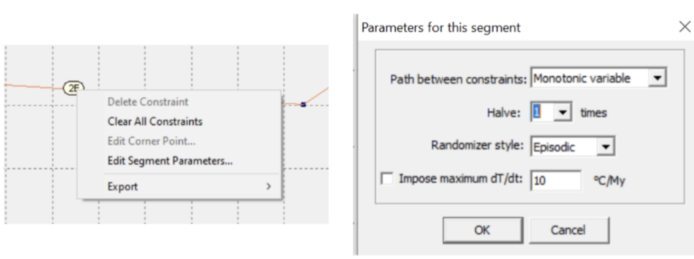


4. Set up the Time-Temperature space you want the model to explore. *Our intention here is to set up a model that explores 100 Ma of tT space relevant to AHe ages as* *__generically__* *as possible, i.e., with no assumptions of style of cooling, monotonicity of tT history, or starting at high or low temperature. This lets the data itself dominate the model result (to the extent to which that is possible).*
   a. In the Sample Information tab, enter a present-day temperature of 5 +/- 5 ˚C.
   b. In the tT History tab, click on the Inverse Modeling button



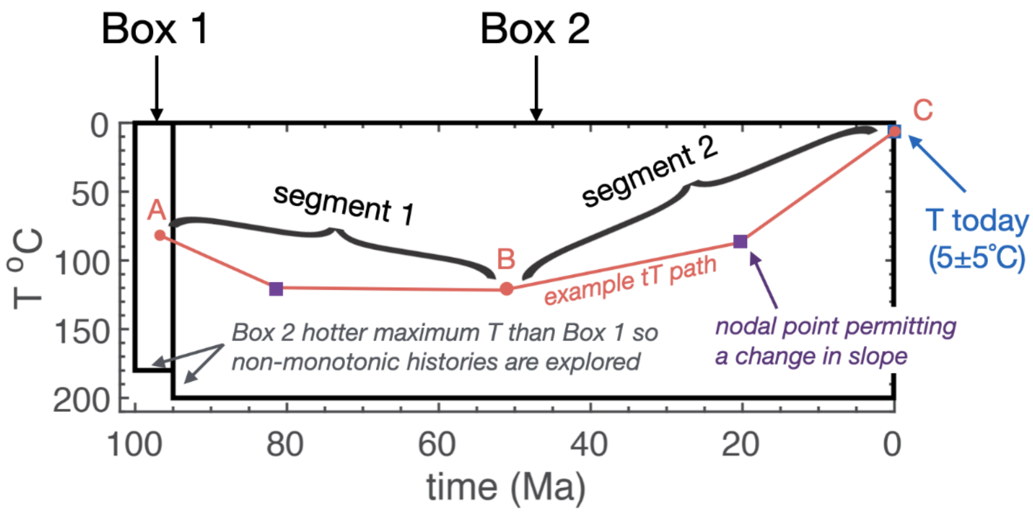
   c. Double click on the plot axes to adjust them, so you see 100-0 Ma and 0-200˚C. *This can be tricky, you have double-click just right on the axes to bring up a dialog box.*

5. Create two constraint boxes that generically explore this tT space.
   a. __Box 1, Initial condition__: Click in tT space to create an initial condition constraint box T = 0-180˚C; time = 100-95 Ma. *Right click on the box's corners..*
   b. __Box 2, Explore a wide range of tT paths between 100 Ma and today__. Click in tT space to create an "exploration" box that spans T=0-200˚C and time = 95-0.1 Ma. *Right click on the box's corners.*
   c. __Ask HeFTy to explore monotonic and non-monotonic histories__ between each constraint by right clicking on the code for the segment parameters and selecting "monotonic variable" and halve 1 time. The code should then read "1Ev".



   d. Save the file to save your model set-up.

You have three constraints (initial, exploration, final T today) so there are two segments (see Figure below). The spacing of the segments and the nodes is randomized, but point A must be in Box 1 and point C must be at t = 0 Ma, T = 5±5˚C. In this example, point B can be anywhere in Box 2.

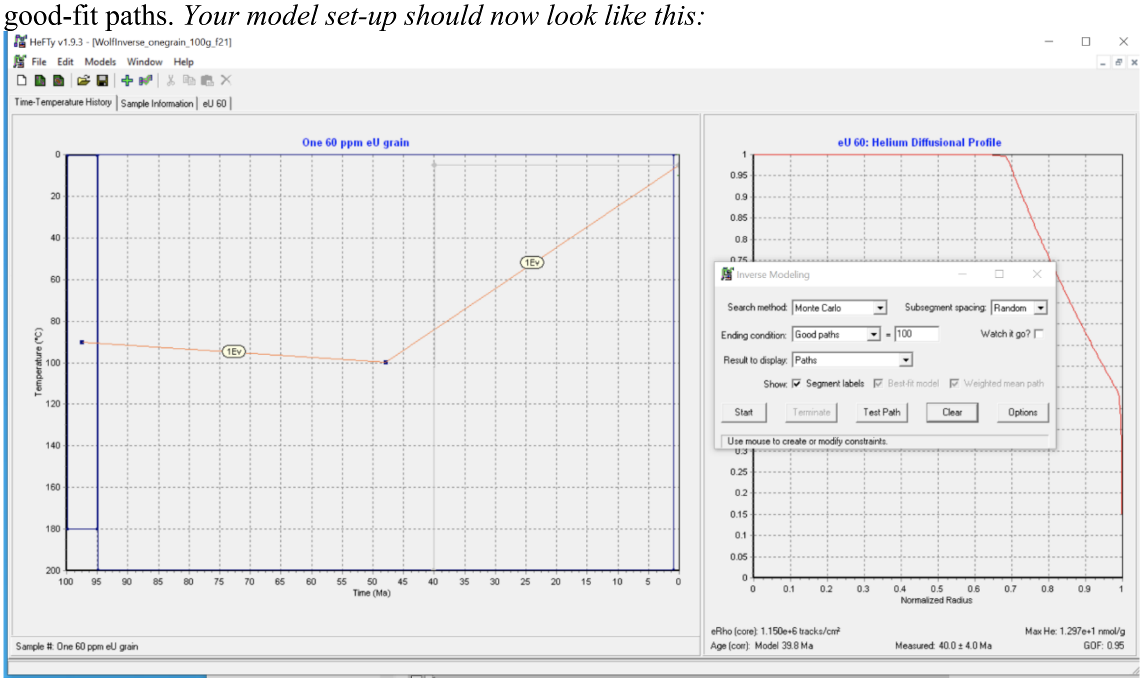


Exercise #3: Inverse model a single AHe age

***Overview**:* Use HeFTy in the inverse sense to find the range of tT paths that could produce our single 40 Ma AHe age from Exercise #1. *Use the Inverse Modeling pop-up window.*

1. Click the "Test Path" button several times to see examples of the individual tT paths that will be attempted. *This is a great way to double-check that you are exploring the types of histories you intend to.*

2. Adjust the "Ending condition" to "Good paths" and "100" to run the model until it finds 100 good-fit paths. *Your model set-up should now look like this:*



3. Click “Start” to run the model until it finds 100 good-fit paths. *The “watch it go” option can be useful to double check that the paths are behaving as intended, but it slows the computing time.*

4. Now that you have an inverse model result, explore how the user interface visualizes the results using options in the Inverse Modeling window.
    a. View results as paths, path envelopes, and constraint points.
    b. Turn on and off the best fit model and weighted mean path.

5. Export the results.
    a. Right click on the tT window and select “Export…”
    b. Save as PDF. Open this file in a PDF viewer.
    c. Save as Text file. Open this file in Excel and examine.

Questions. *Examine the result as HeFTy presents it in tT space; or, you can create your own plots using the exported data file.*

1. What do all the good and acceptable tT paths have in common?

2. Is the weighted mean path geologically meaningful? Why or why not?

3. Are all of the forward model paths from Exercise #1 represented in this inversion result? Should we expect them to? Why or why not?

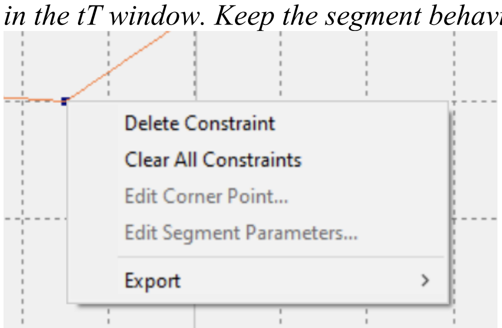
4. Is the Best Fit Model statistically better than the other good- and acceptable- fit models? *(Answering this question requires the HeFTy user manual and/or Ketcham et al., 2015).*

<u>Exercise #4: The role of the exploration box, Box 2.</u>
Overview*:* Remove the exploration box (Box 2) and run the inverse model from Exercise #3 again, in order to learn about tT path behavior in HeFTy inversions.

1. Make a copy of your one-AHe-age HeFTy file (Save As ---> new file name).

2. Clear the Exercise #3 inversion by clicking the “Clear” button on the Inverse Modeling panel.

3. Right click on the center of Box 2 (blue dot) and select “Delete Constraint”. *If you accidentally selected Clear All Constraints, either close this file without saving it and reopen, or rebuild Box 1 in the tT window. Keep the segment behavior “1Ev”.*



4. Run this modified model to find 100 good-fit paths, as before.

Questions.

1. Compare and contrast the model results to those from Exercise #3.

2. Does adding more nodal points change the model result? (E.g., change segment parameters to 3Ev and run the model again). If so, how?

3. What is the value of "exploration boxes" like Box 2?

Additional activities for Part II.A.

1) Change the constraint boxes or segment parameters and see how the model result changes as a result.
   a) Add more halve points (nodes) to one or both segments.
   b) Impose a maximum dT/dt.
   c) Change the high T constraints on Boxes 1 and 2.
   d) Change where in time Box 1 ends and Box 2 begins.
   e) Change the randomizer style or subsegment spacing.
   f) Change how the path behaves between constraints.
2) Run the model until 1000 good-fit paths. Does this change the model result in a useful way? Why or why not?
3) Change assumed error on the He age.
4) There are many other variables to play with here...these are perhaps even more useful to explore using the model results from Exercise #5.

II.B. Inverse modeling an age-eU trend

Objective: Use the age-eU trends generated in Exercise #2 as data in 6 identically set-up thermal history models, to test how well inverse models can resolve the 'true' tT history of a sample under ideal conditions.

To complete this exercise, you will need to create six new HeFTy files for Paths 1-6 with the synthetic AHe single grain data generated for each in Exercise 2 (it will be helpful to consult your Excel table). All synthetic data needs to be entered manually into HeFTy following the procedures described in Part 2A "Step-by-step instructions for building an inverse model in HeFTy".

Each HeFTy file (one for each Path) will have 6 He apatite models (6 tabs - 1 tab per grain).

a. *eU of 10, 30, 60, 90, 150, 300 ppm, respectively (see U value)*
b. *Synthetic age recorded for respective eU values of 10 – 300 ppm*
c. *All grains 60 μm radius*
d. *All grains RDAAM kinetics of Flowers et al., 2009*

<u>Exercise #5: Inverse model the 6 age-eU trends we generated with the forward models in Exercise #2.</u>

Overview: Run one inversion for each synthetic age-eU trend, using identical model set-ups (the constraint boxes in all models are the same as Exercise #4). Examine the inversion results for these "perfect" data and develop your intuition for how well inversion models may (or may not) resolve a 'true' thermal history—and why.

1. Inverse model Path 1.
   a. Open the Path 1 HeFTy file.

b. If needed, adjust the size of the user interface windows so you can see the tT plot well.
c. Click on the Inverse Modeling button.
d. Run the model to find 100 good-fit paths.
e. Once the model run is complete, save the file.
f. Take a screenshot of the tT plot and paste it to a working document, so you have a quick view of this model result. *We find it useful to also capture the file name (in the upper left part of the window) and the Inverse Modeling window in this screenshot, for easier referencing later).*

2. Run the other 5 files in the same manner. Paste screenshots in the same working document so you can make visual comparisons and answer the questions that follow.
    a. <u>Special instructions for Path 5</u>: run for 100,000 attempted paths instead of 100 good-fit paths. *This model takes a while to run - that is ok. See discussion about why Path 5 takes so long to run in the text of the manuscript.*

Reflection Questions: *For each, always ask yourself <u>why</u> the inversion is yielding the result you see, based on your understanding of thermochronology.*

1. Compare and contrast inversion results from Path 1 and Path 6. Are these thermal histories resolvable from each other given these data and model set up?

2. Compare and contrast the inversion results from Path 3 and Path 4. Are these thermal histories resolvable from each other given these data and model set up?

3. Which inversion result(s) are most similar to the model result from Exercise #3, and why?

4. Which inversion result(s) are the most distinctive (narrowest, most tightly constrained), and why?

5. Which model took the most time to run, and why? What does this tell you about the data + model design?

Additional activities for Part II.B.

1) What is the sensitivity of the model results to individual grain ages? *We rarely get such a big range of eU from a single rock sample, and many labs only date 3-4 grains per sample…*
    a) Ex: remove the youngest/lowest eU grain(s), run model again
    b) Ex: remove the oldest/highest eU grain(s), run model again
    c) Ex: remove a grain at middle eU compositions that changes the 'shape' of the age-eU trend, run model again
2) What is the sensitivity of the model results to how the constraint boxes are configured and the paths between them behave? Here are suggestions to get you started. *For some tT histories, this really matters. Understanding how the box configuration is controlling the shape of the attempted paths and therefore the model results is critical.*
    a) Ex: Narrow a constraint box in some way that reflects some hypothetical geologic knowledge of a particular tT path. For example, narrow Box 1 in Path 5 model to restrict starting T to cold, near-surface conditions. What is different about the model run and result?
    b) Ex: remove Box 2 from Path 5 model.
    c) Ex: change the path behavior from '1Ev' to

i) 1E
ii) 2Ev

3) What is the sensitivity of the model results to the % error assigned to each input age? Change the errors from 10% to 20% and rerun each model. *When using the RDAAM in HeFTy for real datasets with age-eU trends, most workers bin data by eU and input representative grains that capture the first-order age-eU trend. Part of this process involves assigning a reasonable error on each representative grain age—HeFTy can help you explore how much that error assumption matters.*
4) What is the sensitivity of the model results to the choice of kinetic model?

TABLE S1. PATH 5 INPUTS, SETTINGS, AND BOUNDARY CONDITIONS FOR THERMAL HISTORY MODEL SIMULATIONS.

1. Thermochronologic data

samples and data used in inverse models

AHe data

Data Treatment, Uncertainties, Other Relevant Constraints

Treatment:	Six single (synthetic) grains
eU (ppm):	10, 30, 60, 90, 150, and 300 ppm
eU zonation:	None.
He dates (Ma):	Synthetic dates predicted by eU, Rs, and Path 5
Error (Ma) applied in modeling:	10% of single grain age
r (µm):	60 µm size assigned to each synthetic grain

2. Additional Constraints

All models use a 0 Ma (modern) T = 5°C ± 5°C

Assumption	***Explanation (see also Figure 4)***	***data source***
Unknown Geologic Context (Fig. 3H)		
Box 1: 100 -95 Ma; 0-180°C	Designed to sample wide range of monotonic and non-moonotonic cooling	
Box 2: 95 - 0 Ma; 0 - 200°C	histories between 100 - 0 Ma and 200-0°C	this study, Table 1
Surface Starting Condition (Fig. 4A)		
Box 1: 100 -95 Ma; 0-20°C	Surface condtions at 100 - 95 Ma from a geologic observation	
Box 2: 95 - 0 Ma; 0 - 200°C	Designed to sample wide range of monotonic and non-monotonic	this study, Table 1
Attempt to Increase Model Efficiency by Narrowing Box 2 Temperature (Fig. 4B)		
Box 1: 100 -95 Ma; 0-180°C	Surface condtions at 100 - 95 Ma from a geologic observation	
Box 2: 95 - 0 Ma; 0 - 100°C	Attempt to more efficiently search model space, supported by 96 Ma grain	this study, Table 1
Early Surface + Model Efficiency (Fig. 4C)		
Box 1: 100 -95 Ma; 0-20°C	Surface condtions at 100 - 95 Ma from a geologic observation	
Box 2: 95 - 0 Ma; 0 - 100°C	Attempt to more efficiently search model space, supported by 96 Ma grain	this study, Table 1
Early Surface + Model Efficiency Relaxed (Fig. 4D)		
Box 1: 100 -95 Ma; 0-20°C	Surface condtions at 100 - 95 Ma from a geologic observation	
Box 2: 95 - 0 Ma; 0 - 130°C	Attempt to more efficiently search model space, supported by 96 Ma grain, but don't want possible paths to touch bounding constraint box	this study, Table 1

3. System and model specific parameters

Inverse models

He kinetic model: RDAAM (Flowers et al., 2009)
Statistical fitting criteria: HeFTy default values (Ketcham et al., 2009)
Modeling code: HeFTy v. 1.9.3.
Model inputs: Six single synthetic grains from known tT history
Model outputs: Good and acceptable tT paths and path envelopes.
Segment Parameters: 1Ev, 1Ev

Table S2: DEEP TIME EXAMPLE: INPUTS, SETTINGS, AND BOUNDARY CONDITIONS FOR THERMAL HISTORY MODEL SIMULATIONS

1. Thermochronologic data

Samples and data used in models.
These data are from Boulder Canyon (Boulder County, Colorado). See data sources for sample location information.

Model	**AHe data** *(Murray et al, 2022)*	**ZHe data** *(Murray et al, 2022)*	**Ar Hbl data** *(Shaw et al., 1999)*	**Ar Bt data** *(Shaw et al., 1999)*
Ar-only	n/a	n/a	R30416-2	R30416-2, R30416-3
He-only	13BC-A, 13BC-B, 13BC-C	13BC-A, 13BC-B, 13BC-C	n/a	n/a

Data treatment, uncertainties, and other relevant constraints

(U-Th)/He data

Samples together form a zircon He age-[*eU*] trend qualitatively consistent with the coevolution of radiation damage and He diffusivity in zircon. We jointly modeled three samples 13BC-A, 13BC-B, 13BC-C (in a joint model named '13BC-ABC') to investigate what thermal histories would produce this full age-[*eU*] trend. These three samples were collected within ~200 m elevation and 2.5 km spatially and have reproducible apatite He ages of 58 ± 4.3 Ma. This supports the assumption we make when jointly modeling them: they have a shared thermal history and therefore the difference between the cooling ages is a function of radiation damage as well as grain size and composition.

^{40}Ar/^{39}Ar data

Shaw et al. (1999) report integrated and plateau ^{40}Ar/^{39}Ar ages for two samples in the Boulder Canyon area close to the zircon He samples: R30416-2 and R30416-3. We use these ages as data in the 'Ar-only' *tT* models.

Data input and uncertainties

One hornblende and one biotite ^{40}Ar/^{39}Ar age were used in our 'Ar only' model. We input the average and standard deviation of the plateau and integrated hornblende ^{40}Ar/^{39}Ar ages from sample R30416-2. We input the average and standard deviation of the plateau and integrated biotite ^{40}Ar/^{39}Ar ages from samples R30416-2 and R30416-3 together as a single data input. The grain size was set to 150 µm.

Two apatite and five zircon He inputs were used in the preferred He model, see data input values in table below. A HeFTy model can accommodate no more than 7 ages total. Therefore, to input zircon He age data into HeFTy, we grouped the He ages by [*eU*] composition in order to calculate 5 synthetic grains with representative He age, [*U*], [*Th*], and grain size (*Rs*, equivalent spherical radius). These representative synthetic grains were the model inputs. Ages were grouped to capture the observed first-order age-[*eU*] trend and emphasize the observed ages at the lowest and highest amounts of [*eU*] and radiation damage. For this dataset, the [*eU*] bins used to calculate the synthetic grains are: <500 ppm; 500-700 ppm; 700-1000 ppm; 1000-1200 ppm; and >2000 ppm. The two high-[*eU*] bins define the width of the ~70 Ma age 'pediment' in this age-[*eU*] trend (Guenthner, 2021). Five ZHe grains with [*eU*] 1200-2000 sit within this age pediment but were not used to calculate a synthetic grain.

Apatite He ages in all samples are invariant with [*eU*]. For models of 13BC-ABC, the 14 apatite He ages are invariant over a large range of [*eU*] (~2-70 ppm), and this lack of an age-[*eU*] trend is significant. Therefore, we input two synthetic grains to represent the low-[*eU*] and high-[*eU*] apatite grains.

Uncertainties on synthetic grain ages input into HeFTy were the % standard deviation (s.d.) on the mean bin age if this s.d. was >20% and otherwise 10 or 20%.

HeFTy data input values

model ID	Input grain *Z, A, H, or B, #*	Uncorrected age *Ma*	Uncertainty *Myr or %*	Rs *µm*	[U] *ppm*	[Th] *ppm*	[Sm] *ppm*
Ar only	H1	1449	7 Myr	150	n/a	n/a	n/a
	B1	1351	22 Myr	150	n/a	n/a	n/a
13BC-ABC	Z1	368.9	38 %	54	352	125	0
	Z2	154.5	35 %	48	581	220	0
	Z3	92.9	36 %	48	782	264	0
	Z4	56.3	22 %	54	1292	489	0
	Z5	54.7	20 %	62	2144	850	0
	A1	43	10 %	46	7	19	243
	A2	47	10 %	56	48	43	272

2. Additional geologic information

#	*Assumption*	*Explanation and data source*
1	Emplacement of Boulder Creek batholith	The Boulder Creek batholith is 1714.4 ± 4.6 Ma (Premo and Fanning, 2000).
2	**exploration box**	The hornblende $^{40}Ar/^{39}Ar$ age supports cooling below 450˚C between 1500 and 1400 Ma (Fig. S1). Otherwise, this time is unconstrained, so we use this box to explore a range of monotonic and non-monotonic histories.
3	**exploration box**	The biotite $^{40}Ar/^{39}Ar$ age supports cooling to T <250˚C by 1275 Ma (Fig. S1). Otherwise, this time is unconstrained, so we use this box to explore a range of monotonic and non-monotonic histories.
4	Tavakaiv quartzite injectite formation	Quartzite dikes and other clastic bodies hosted in the crystalline rocks of the Boulder Creek area crop out near Arapahoe Pass near our Range Interior samples. The sand bodies in the Southern Front Range are interpreted to have resulted from the forceful injection of unlithified Neoproterozoic sands deposited on a proto-Great Unconformity into the crystalline basement rocks (Siddoway and Gehrels, 2014; Jensen et al., 2018; Flowers et al., 2020). We conservatively interpret this constraint, using it to place the bedrock sampled within ~2 km (~60 ˚C) of a proto-Great Unconformity at the paleosurface during the time of Tava emplacement.
5	**exploration box**	The post-Tava time is unconstrained by the rock record, so we use this box to explore a range of monotonic and non-monotonic histories with peak T limited to <285˚C (Fig. S1).
6	Great Unconformity	The presence of Cambrian strata on basement rock throughout the region, combined with a lack of preservation of Neoproterozoic strata, suggest that samples returned to within ~60 ˚C (~2 km) of the surface by ca. 500 Ma.
7	Paleozoic burial	Paleozoic strata are preserved throughout the Southern Rockies and record the net deposition of no more than a few hundred meters of strata during this time (Tweto, 1979; Siddoway et al., 2013). We allow for burial up to T of 100 ˚C through the Paleozoic, which is the equivalent of at least ~1 km burial with a 30 ˚C/km geothermal gradient plus a 10˚C surface temperature.

8	Ancestral Rocky Mountains uplift and erosion	This event removed pre-Pennsylvanian strata from the study area and much of the surrounding region, re-establishing the Great Unconformity, or a similar surface, as the late Paleozoic land surface in this part of the Front Range. We use the timing of this orogeny from Leary et al. (2017).
9	Mesozoic burial	Pennsylvanian-Cretaceous strata preserved in the Denver Basin near Boulder give constraints on Mesozoic deposition (Wells, 1967; Weimer and Ray, 1997). By 87 Ma, the Great Unconformity was buried by ~400-700 m. For simplicity and to improve model efficiency, we model Mesozoic burial as gradual and monotonic at a maximum rate of 0.2 ˚C / My i.e., <40 ˚C burial heating between ~300 Ma and ~85 Ma.
10	Niobrara Formation	From 87-82 Ma, the Niobrara Formation records ~240 m of deposition, bringing the total maximum burial depth of the Great Unconformity in the study area to ~950 m. Therefore, by the end of Niobrara deposition ca. 82 Ma, the Great Unconformity surface was no hotter than ~40 ˚C (30 ˚C geotherm +10 ˚C surface T) and the rocks that we sampled were no more than ~2 km (60 ˚C) warmer.
11	Pierre Shale and timing of peak T prior to Laramide	Late Cretaceous peak burial depth, and we assume T_P, occurred after the deposition of the Pierre Shale (82-68 Ma). The Pierre Shale is ~2500 m thick in the Boulder area (Scott and Cobban, 1965). Age control on the Pierre is known in detail from ammonite biozones (Kauffman, 1977).
12	Modern surface T	Modern mean annual temperature from Nederland, Co (http://www.usclimatedata.com/climate/nederland/colorado/united-states/usco0652/2017/1, 1.85 ˚C, 2511 m) adjusted for sample elevation using a temperature lapse rate of -6.5 ˚C/km (Pepin and Losleben, 2002; Minder et al., 2010) 13BC-ABC: 3.5 ± 2.5 ˚C.

Constraints and model path characteristics in Ar-only models

#	Max time Ma	Min time Ma	Max T ˚C	Min T ˚C	Model path characteristics HeFTy code
1	1750	1700	800	750	2Ev
4	700	650	60	0	1E
5	650	540	285	0	1E
6	540	500	60	0	0G
7	330	320	100	0	0E
8	320	280	60	0	0G/0.2
9	No constraint box				
10	87	82	110	30	0E
11	70	40	285	100	2E
12	today		-		-

Constraints and model path characteristics in He models

#	Max time Ma	Min time Ma	Max T ˚C	Min T ˚C	Model path characteristics HeFTy code
1	1750	1700	800	750	1Ev
2	1500	1400	500	450	1Ev
3	1475	1275	250	0	1Ev
4	700	650	60	0	1E
5	650	540	285	0	1E
6	540	500	60	0	0G
7	330	320	100	0	0E
8	320	280	60	0	0G/0.2
9	No constraint box				
10	87	82	110	30	0E

11	70	40	285	100	2E
12	today		Varies by sample		-

3. System- and model-specific parameters

Modeling software:	HeFTy v. 1.9.3
Biotite $^{40}Ar/^{39}Ar$ kinetics:	E_a = 47.1 kcal/mol; D_0 = 0.075 cm^2/s (McDougall and Harrison, 1999)
Hornblende $^{40}Ar/^{39}Ar$ kinetics:	E_a = 64 kcal/mol; D_0 = 0.06 cm^2/s (McDougall and Harrison, 1999)
Apatite He kinetic model:	RDAAM (Flowers et al., 2009); precision 'good; stopping distances 'Ketcham et al., 2011'; alpha calculation 'redistribution'; age alpha-correction 'Ketcham et al., 2011'
Zircon He kinetic model:	RDAAM (Guenthner et al., 2013); precision 'good; stopping distances 'Ketcham et al., 2011'; alpha calculation 'redistribution'; age alpha-correction 'Ketcham et al., 2011'
Statistical fitting criteria:	HeFTy default values (Ketcham et al., 2009)
Number of *t-T* paths attempted:	The number required to return 100 good-fit paths, typically 10^5 – 10^6 paths
t-T path characteristics:	The Monte Carlo search method with random subsegment spacing was used.

Table S2 References:

Flowers, R.M., Ketcham, R.A., Shuster, D.L., and Farley, K.A., 2009, Apatite (U–Th)/He thermochronometry using a radiation damage accumulation and annealing model: Geochimica et Cosmochimica Acta, v. 73, p. 2347–2365, doi:10.1016/j.gca.2009.01.015.

Flowers, R.M., Macdonald, F.A., Siddoway, C.S., and Havranek, R., 2020, Diachronous development of Great Unconformities before Neoproterozoic Snowball Earth: Proc Natl Acad Sci USA, v. 117, p. 10172.

Guenthner, W.R., Reiners, P.W., Ketcham, R.A., Nasdala, L., and Giester, G., 2013, Helium diffusion in natural zircon: Radiation damage, anisotropy, and the interpretation of zircon (U-Th)/He thermochronology: American Journal Of Science, v. 313, no. 3, p. 145–198, doi: 10.2475/03.2013.01.

Jensen, J.L., Siddoway, C.S., Reiners, P.W., Ault, A.K., Thomson, S.N., and Steele-MacInnis, M., 2018, Single-crystal hematite (U–Th)/He dates and fluid inclusions document widespread Cryogenian sand injection in crystalline basement: Earth And Planetary Science Letters, v. 500, p. 145–155, doi: 10.1016/j.epsl.2018.08.021.

Kauffman, E.G., 1977, Geological and biological overview: Western Interior Cretaceous basin: The Mountain Geologist, v. 14, no. 3-4, p. 75–98.

Ketcham, R.A., Donelick, R.A., Balestrieri, M.L., and Zattin, M., 2009, Reproducibility of apatite fission-track length data and thermal history reconstruction: Earth and Planetary Science Letters, v. 284, p. 504–515, doi:10.1016/j.epsl.2009.05.015.

Leary, R.J., Umhoefer, P., Smith, M.E., and Riggs, N., 2017, A three-sided orogen: A new tectonic model for Ancestral Rocky Mountain uplift and basin development: Geology, v. 45, no. 8, p. 735–738, doi: 10.1130/G39041.1.

McDougall, I., and Harrison, T.M., 1999, Geochronology and Thermochronology by the $^{40}Ar/^{39}Ar$ Method: Oxford University Press, New York.

Minder, J.R., Mote, P.W., and Lundquist, J.D., 2010, Surface temperature lapse rates over complex terrain: Lessons from the Cascade Mountains: Journal of Geophysical Research, v. 115, no. D14, p. D14122–13, doi: 10.1029/2009JD013493.

Pepin, N., and Losleben, M., 2002, Climate change in the Colorado Rocky Mountains: free air versus surface temperature trends: International Journal of Climatology, v. 22, no. 3, p. 311–329, doi: 10.1002/joc.740.

Premo, W.R., and Fanning, C.M., 2000, SHRIMP U-Pb zircon ages for Big Creek gneiss, Wyoming and Boulder Creek batholith, Colorado Implications for timing of Paleoproterozoic accretion of the northern Colorado province: Rocky Mountain Geology, v. 35, no. 1, p. 31–50, doi: 10.2113/35.1.31.

Scott, G.R., and Cobban, W.A., 1965, Geologic and biostratigraphic map of the Pierre Shale between Jarre Creek and Loveland, Colorado: U.S. Geological Survey Numbered Series IMAP, no. 439, p. 1-4.

Siddoway, C., Myrow, P., and Fitz-Díaz, E., 2013, Strata, structures, and enduring enigmas: A 125th Anniversary appraisal of Colorado Springs geology, *in* Classic Concepts and New Directions: Exploring 125 Years of GSA Discoveries in the Rocky Mountain Region, Geological Society of America, p. 331–356.

Siddoway, C.S., and Gehrels, G.E., 2014, Basement-hosted sandstone injectites of Colorado: A vestige of the Neoproterozoic revealed through detrital zircon provenance analysis: Lithosphere, v. 6, no. 6, p. 403–408, doi: 10.1130/L390.1.

Shaw, C.A., Snee, L.W., Selverstone, J., and Reed, J.C., Jr, 1999, $^{40}Ar/^{39}Ar$ thermochronology of Mesoproterozoic metamorphism in the Colorado Front Range: The Journal of Geology, v. 107, no. 1, p. 49–67, doi: 10.1086/314335.

Tweto, O., 1979, Geologic Map of Colorado: Colorado Geological Survey Department of Natural Resources MI-16, scale 1:500,000, 1 sheet.

Weimer, R.J., and Ray, R.R., 1997, Laramide Mountain Flank Deformation and the Golden Fault Zone, Jefferson County, Colorado, *in* Bolyard, D.W. and Sonnenberg, S. A., eds., Geologic History of the Colorado Front Range, Rocky Mountain Association of Geologists, p. 49–64.

Wells, J.D., 1967, Geology of the Eldorado Springs Quadrangle, Boulder and Jefferson Counties, Colorado: U.S. Geologic Survey Report, no. 1221-D, p. D1-D85.

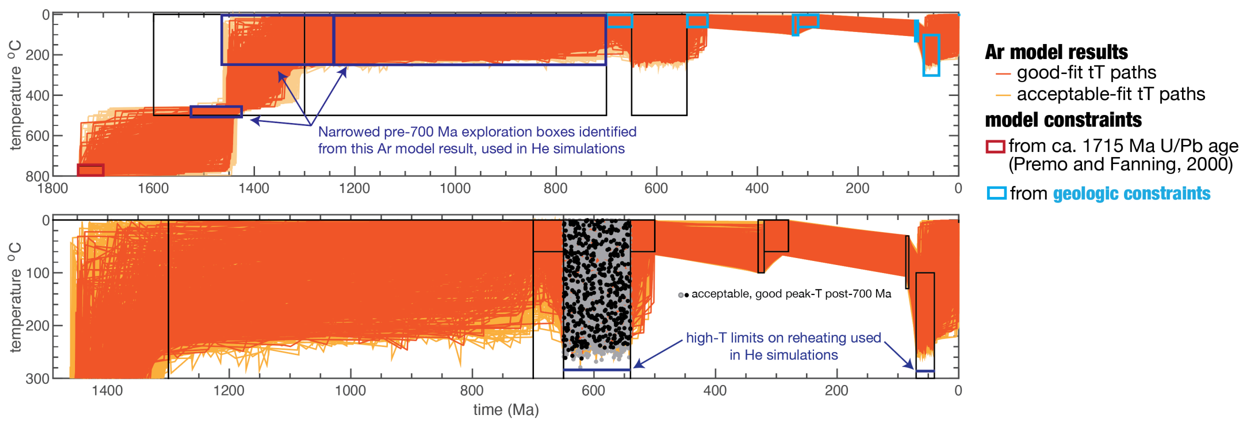


Figure S1. Results of Ar-only model of deep-time example, demonstrating how the temperature bounds on the He-only models (e.g., orange boxes in Figure 7B) were determined. These Ar-only models were run to find 500 good fit paths.

TABLE S3. DATA FOR PATH FAMILY EXAMPLE

(U-Th)/He Data Table

Sample Name	length 1 (mm)	width 1 (mm)	length 2 (mm)	width 2 (mm)	Rs (µm)	U (ppm)	±	Th (ppm)	±	Sm (ppm)	±	eU	Raw Date It (Ma)	±	Ft	Corrected Date (It) (Ma)	Analytic Unc. (Ma)2s
FPT17-55																	
AG_FPT17-55_zr1	125	62	122	51	33.65	1738.99	24.6	1046.47	19.49	0	0	1984.9	14.47	0.18	0.671	21.55	0.54
AG_FPT17-55_zr2	124	67	122	52	34.58	1782.48	17.41	1042.79	22.95	0	0	2027.5	20.41	0.19	0.679	30.02	0.54
AG_FPT17-55_zr4	155	68	154	60	39.38	1756.08	28.93	1044.74	275.23	1.47	2.95	2001.6	14.67	0.52	0.715	20.49	1.46

ZFT Data Table

Sample Name: FPT17-55		
Zeta Factor ± Error	144.1	4.1
Rho d (% Relative Error)	5.43E+05	1.52
N d	4305	
N s	***N i***	
234	157	
165	84	
210	158	
185	141	
152	113	
163	129	
169	149	
207	142	
168	149	
158	118	
117	104	
188	137	
194	146	
206	186	
226	185	
330	281	
247	195	
189	159	
253	210	
140	102	

TABLE S4. PATH FAMILY EXAMPLE: INPUTS, SETTINGS, AND BOUNDARY CONDITIONS FOR THERMAL HISTORY MODEL SIMULATIONS.

1. Thermochronologic data

samples and data used in inverse models

ZHe data

FPT17-55

ZFT data

FPT17-55

Data Treatment, Uncertainties, Other Relevant Constraints

ZHe data

Treatment: Each of the 3 grains was used as a separate constraint

eU (ppm): Measured U, Th, and Sm used for each grain

eU zonation: None.

He dates (Ma): Mean uncorrected He date of each sample used in data entry and corrected in HeFTy for α-ejection using Ketcham et al., 2011

Error (Ma) applied in modeling: 10% of single grain age

r (μm): Measured equivalent spherical radius for each grain

ZFT data

Treatment: 20 grains used in age calculation

2. Additional Constraints

Assumption	***Explanation***	***data source***
Geologic Constraints		
Near surface conditions (0-100°C) 160 - 130 Ma	Volcanic unit (~ 160 Ma) in depositional contact with overlying sedimentary unit (deposited 150 - 130 Ma)	Mueller et al., 2021
Greenschist grade conditions (300 - 400°C) 100 - 70 Ma	Greenschist grade metamorphism dated to 100 Ma and dike emplacement at 10 km depth dated to 70 Ma	Calderón et al., 2012; Mueller et al., 2021
Model Exploration Boxes		
70 - 50 Ma; 0 - 350°C 50-10 Ma; 0 - 350°C	Combination of exploration boxes allows, but does not require non-monotonic tT pathways	Ketcham, 2005

3. System and model specific parameters

Inverse models

He kinetic model: ZRDAAM (Guenthner et al., 2013)

ZFT kinetic model: Ketcham unpub.

Statistical fitting criteria: HeFTy default (Ketcham et al., 2009)

Modeling code: HeFTy v. 1.9.3.

Model inputs: Three single grain ZHe data, ZFT data based on 20 grain counts

Model outputs: Good and acceptable tT paths and path envelopes.

Segment Parameters: Monotonic variable paths between constraints, halved 2 times, with episodic randomization style

Number of tT paths: 66,607 (Model run until 100 good fit paths found)