Short course IV
Thermochronology and landform development (Pecube-GUI)

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with significant input from Maxime Bernard

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Thermo2025 Kanazawa

Short course presenters and contributors

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Isabel Wapenhans

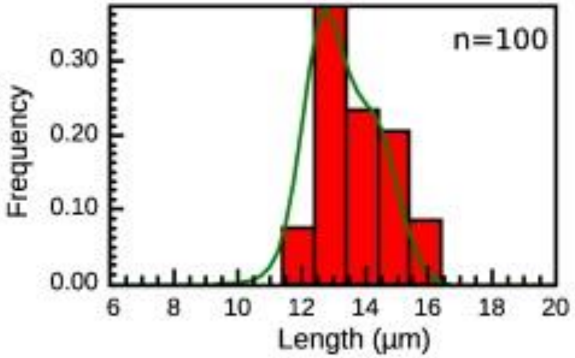
Maxime Bernard

Short course roadmap

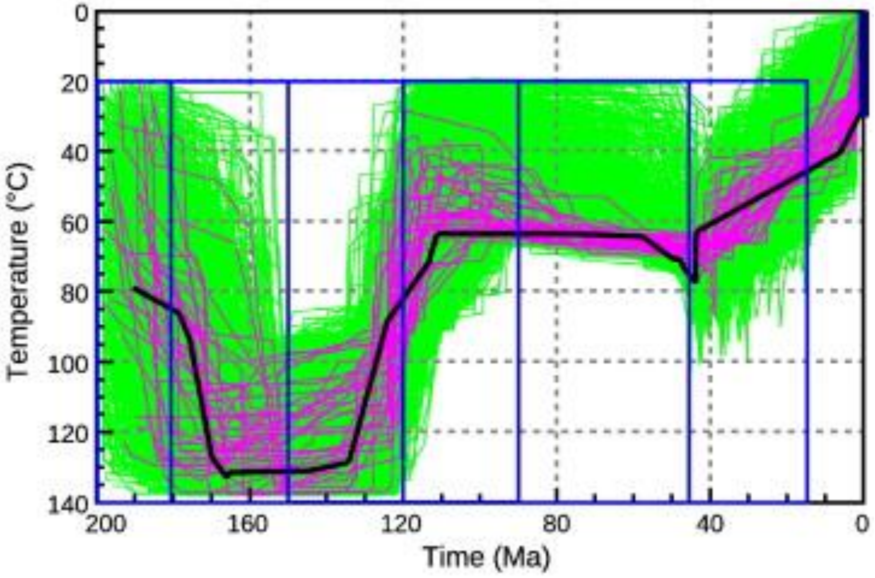
1. Pecube 1.01: Introduction to Pecube and Pecube-GUI (Peter)
2. Hands-on experience: running forward models in Pecube-GUI (Lingxiao)
3. Some notes on misfit (Peter)
4. Inverse modelling with Pecube / Pecube-GUI (Peter)
5. - if time permits – Inverse modelling exercise (Lingxiao)
6. Inverse modelling strategies and reporting inverse modelling results (Peter)

Thermochronology ⇒ thermal information

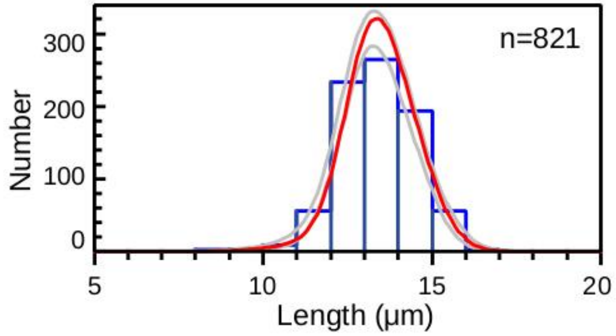
HeFTy



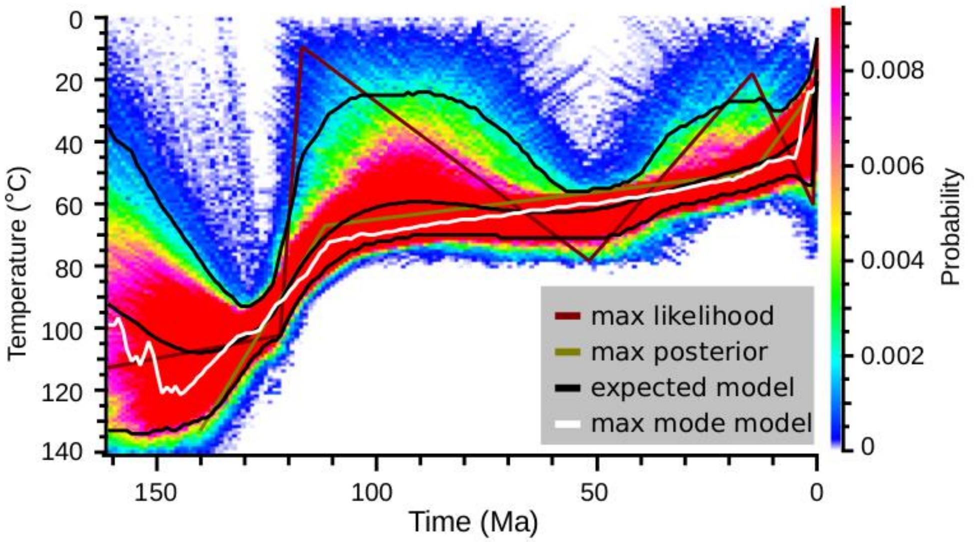
	MTL	AFT age	AHe age
Measured	13.4 ± 1.0	102 ± 7	55 ± 5
Modelled	13.3 ± 1.1	102	59



QTQt



	MTL	AFT age	AHe age
Measured	13.4 ± 1.2	102 ± 7	55 ± 5
Modelled	13.9 ± 0.9	102 ± 5	59 ± 4



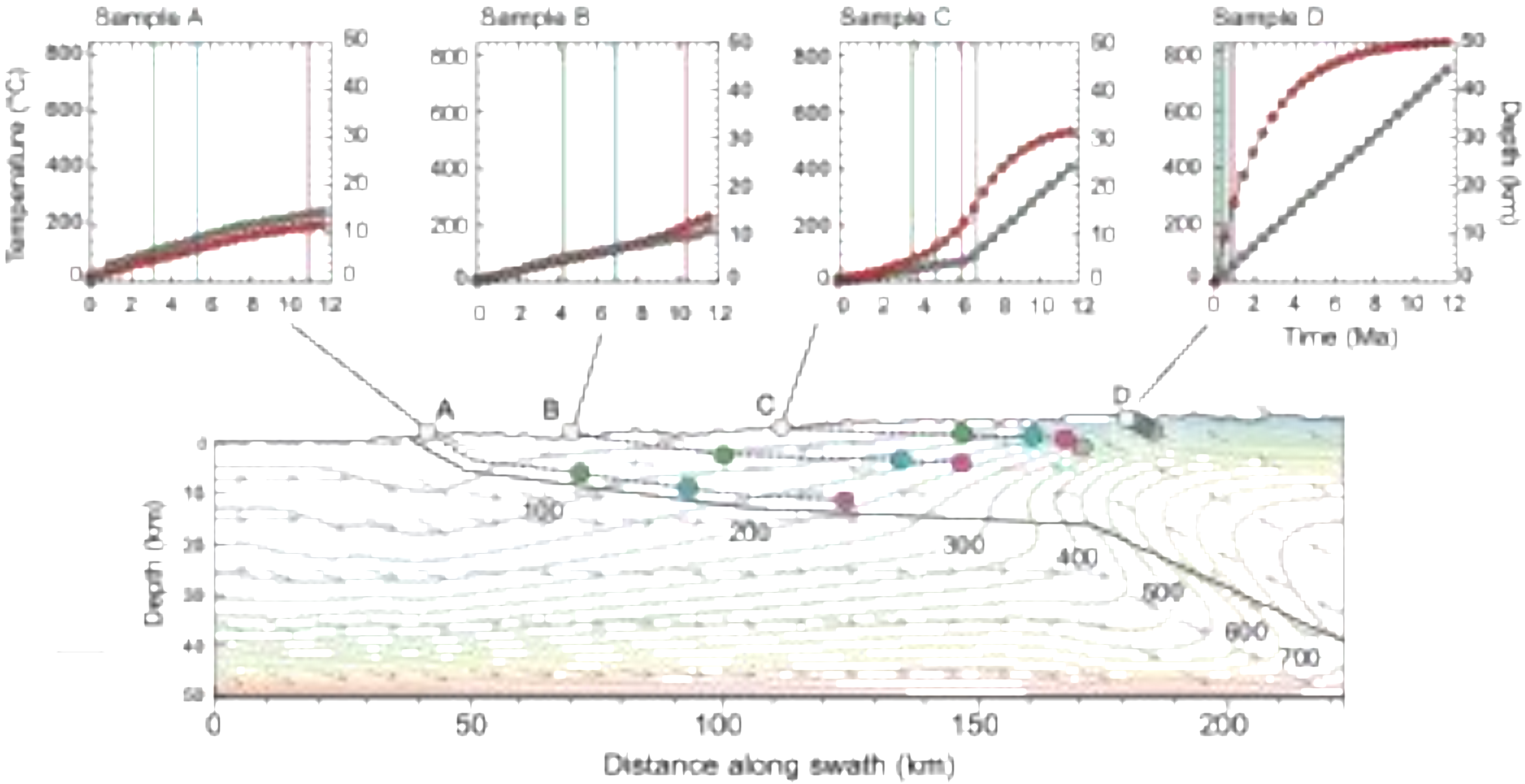
From Vermeesch & Tian, Earth Sci. Rev. 2014

Thermochronology ⇒ thermal information

But we are interested in kinematic information!

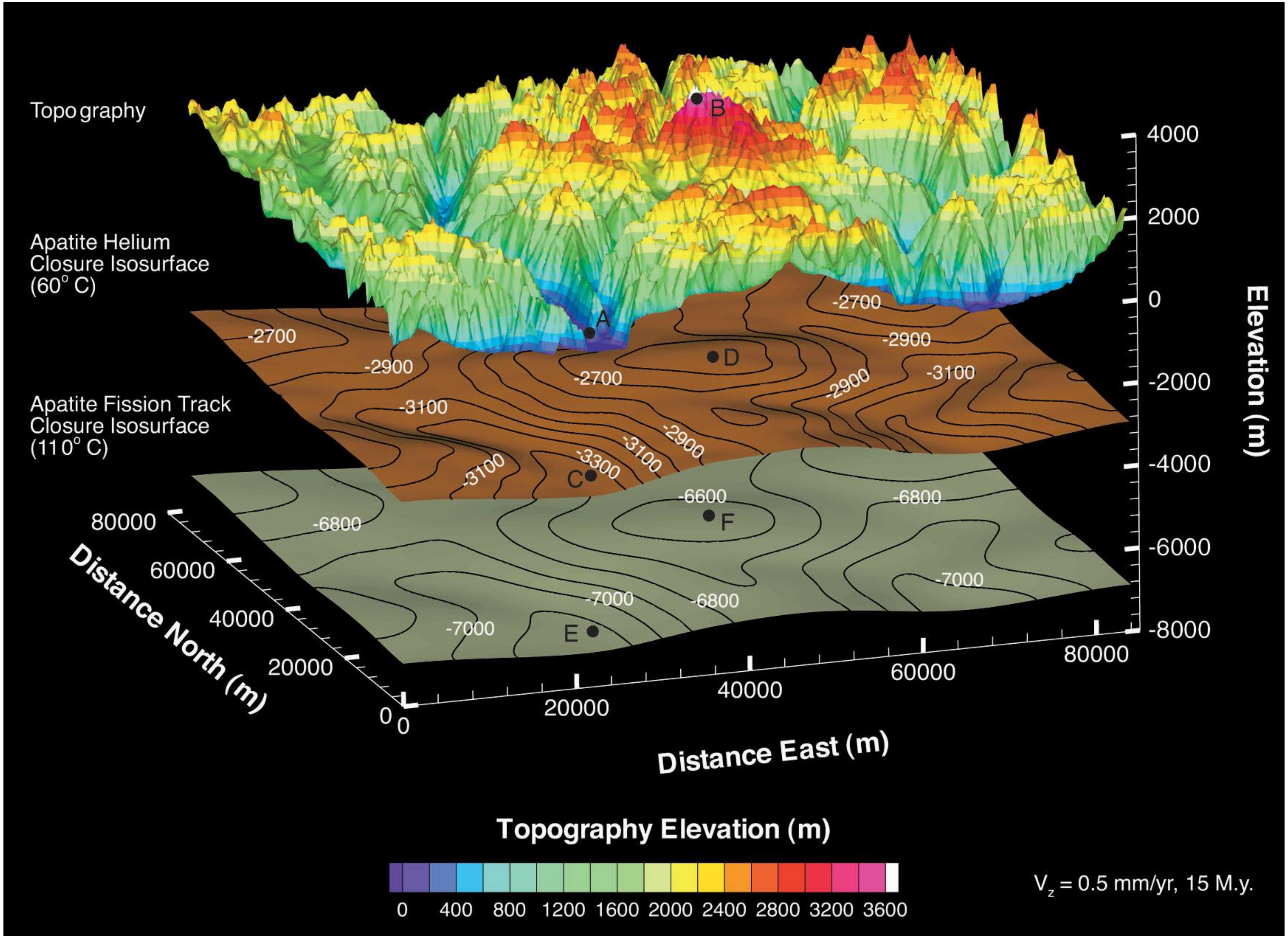
- When did exhumation occur, at what rate?
- At what time was this fault active?
- When did the current topography develop, what did it look like in the past?
- What does the pattern of thermochronology ages tell me about the tectonic history of this region?
- …

From thermal to kinematic reference frame



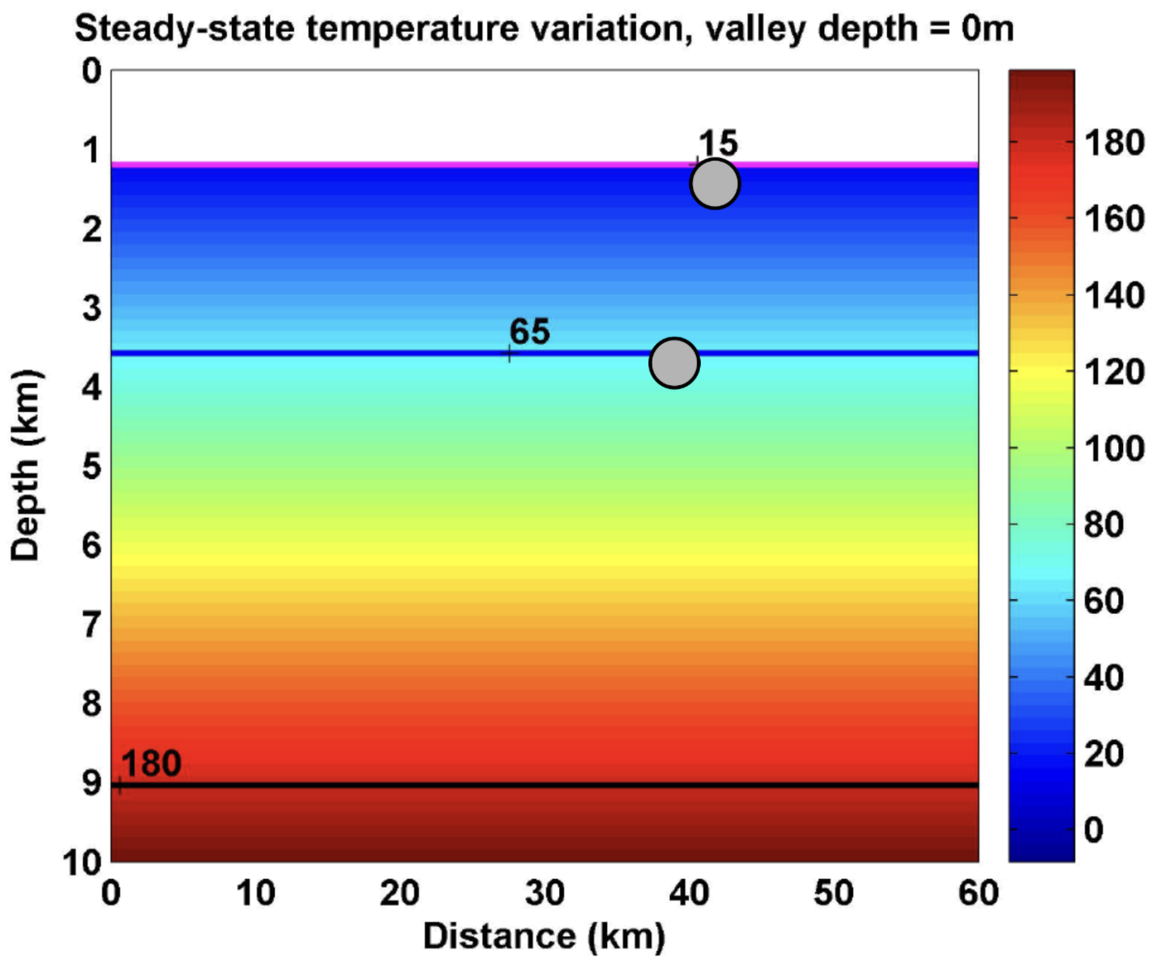
Modified from Coutand et al., JGR-SE 2014

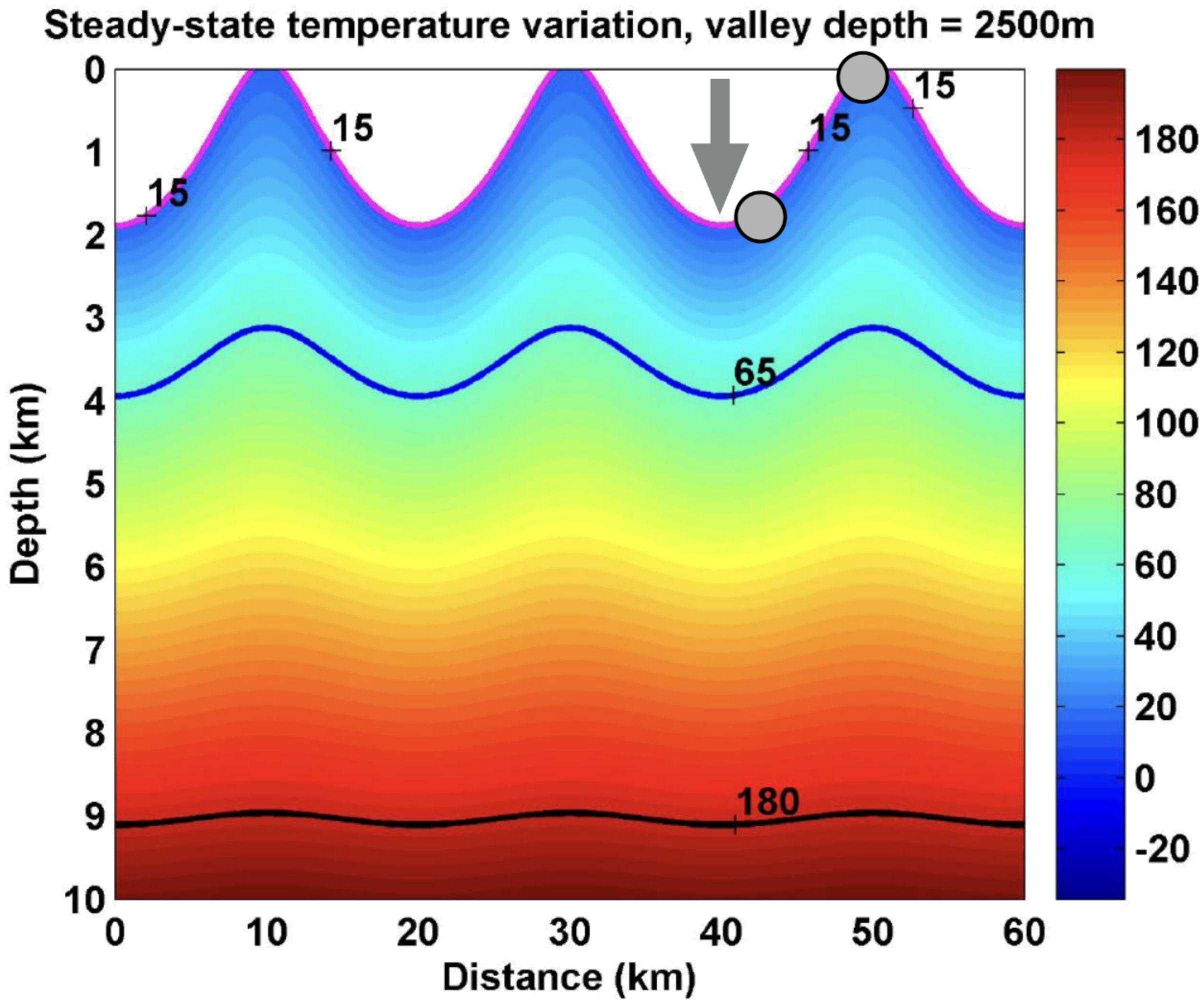
Effect of topography on isotherms



Ehlers & Farley, EPSL 2003

Using thermochronology to derive exhumation and relief histories





Using thermochronology to derive exhumation and relief histories

⇒ solving the 3D transient heat-transport equation

$$\frac{dT}{dt} = \kappa\,\nabla^2 T + v\nabla T + \frac{H}{\rho c} \qquad \nabla T = \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z}$$

Heat ***conduction*** (diffusion) — Heat ***advection*** — Heat ***production*** [K s^{-1}]

κ = Thermal diffusivity [m^2 s^{-1} / km^2 My^{-1}]

$\kappa = \frac{k}{\rho c}$; k = Thermal conductivity [W m^{-1} K^{-1}]

H = volumetric heat production [(μ)Wm^{-3}]

ρ = density [kg m^{-3}]

c = heat capacity [J kg^{-1} K^{-1}]

v = rock/particle velocity [m s^{-1}; km My^{-1}]

$v_{(x,y,z,t)} = v_{x(t)} + v_{y(t)} + v_{z(t)}$

Tectonics

Heat transport by conduction and advection

$$\frac{dT}{dt} = \kappa\,\nabla^2 T + v\nabla T + \frac{H}{\rho c}$$

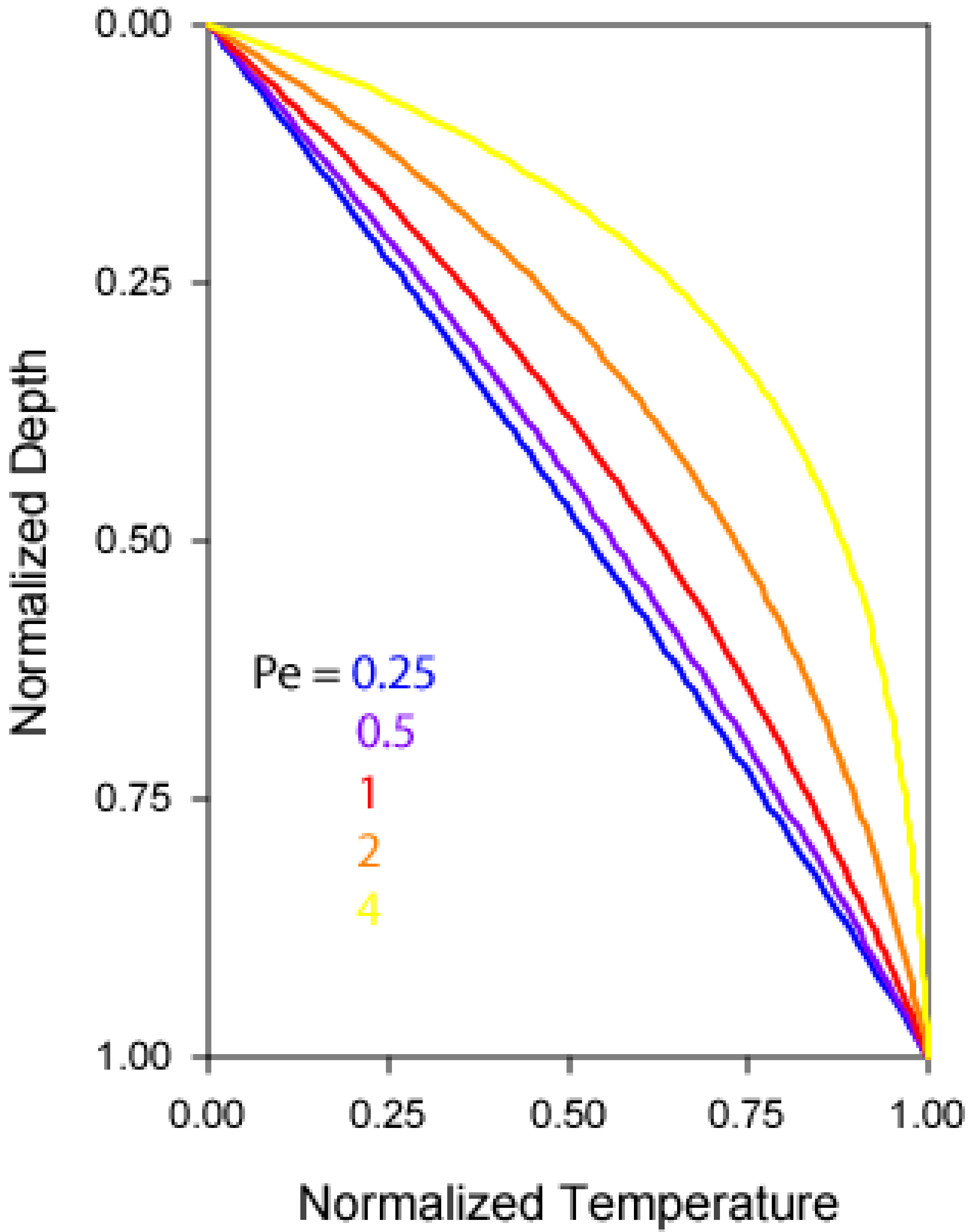
Characteristic timescales

L: “characteristic length” of system

conduction : $\tau_c = \frac{L^2}{\kappa}$

advection : $\tau_a = \frac{L}{v}$

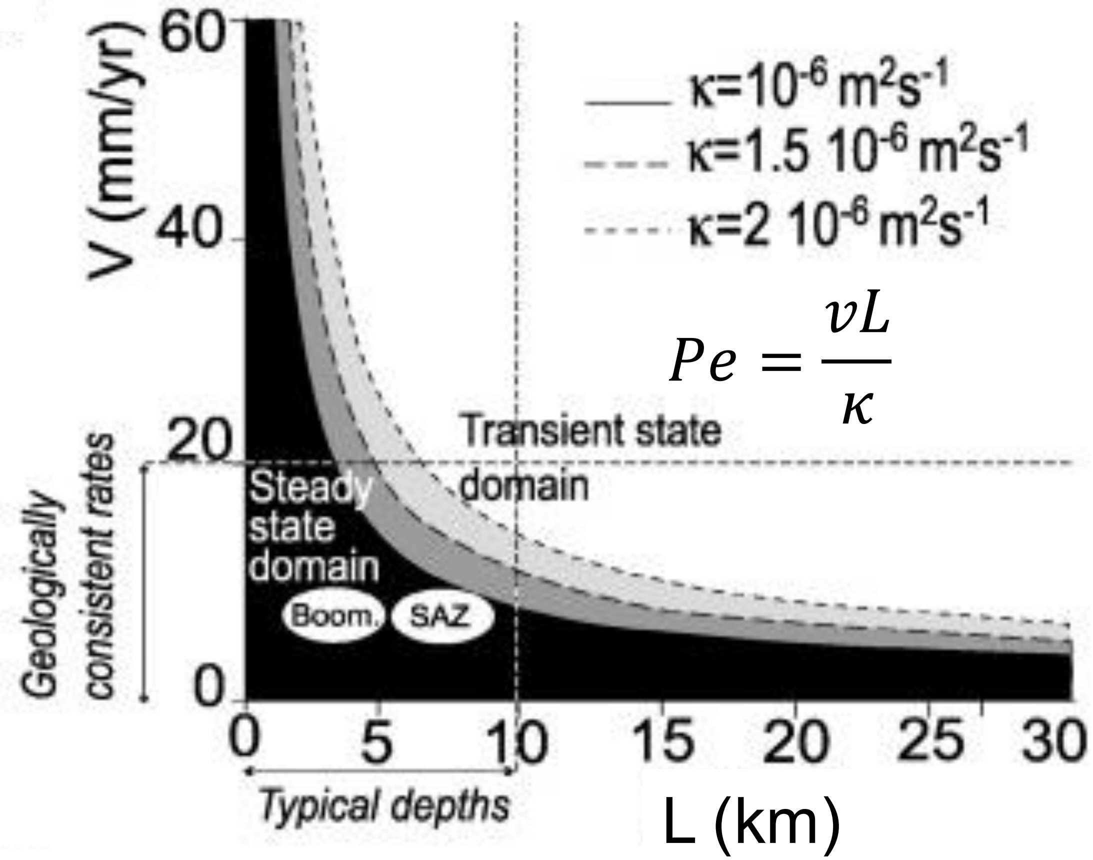
Péclet number: $Pe = \frac{\tau_c}{\tau_a} = \frac{vL}{\kappa}$



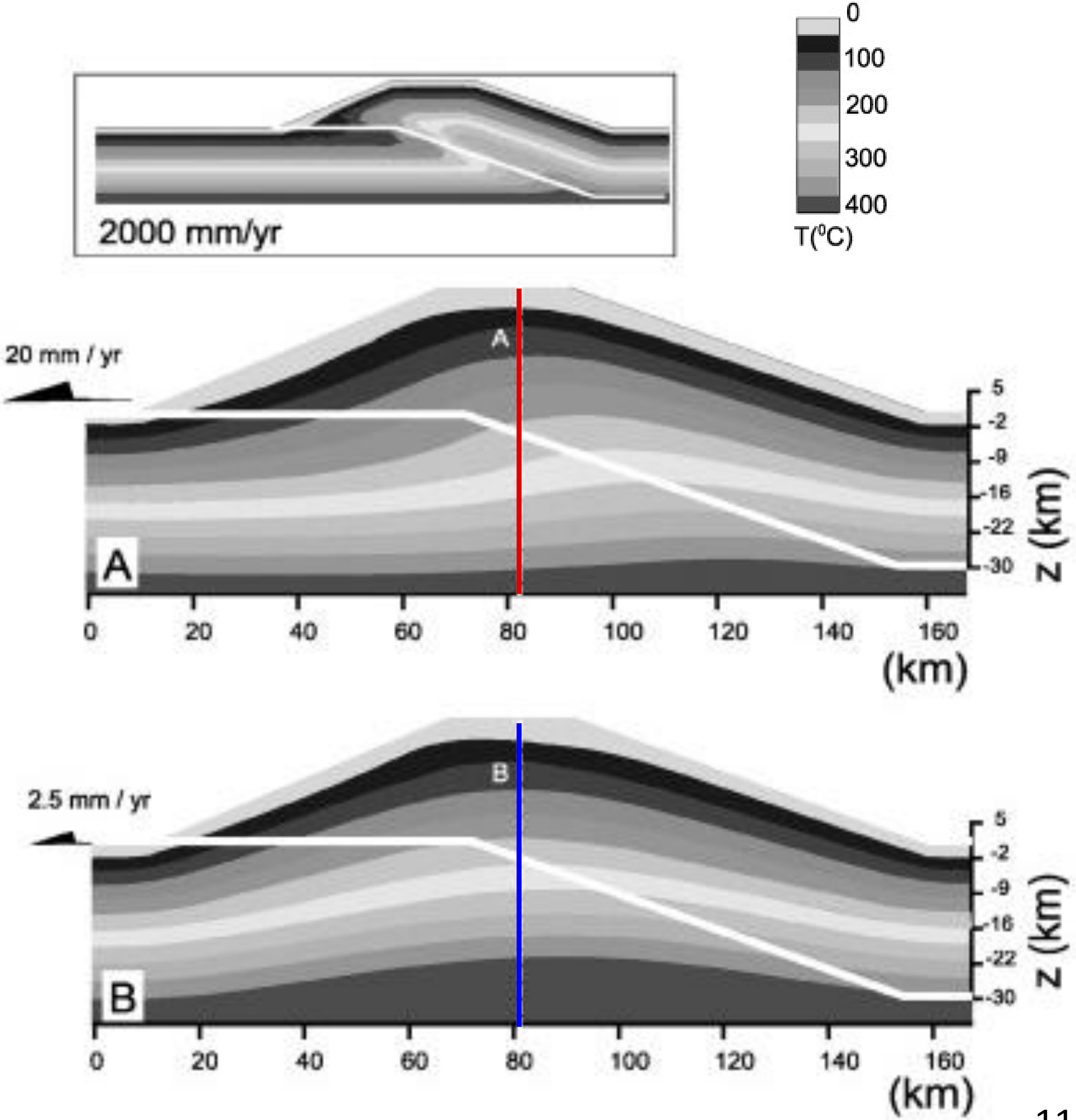
Analytical steady-state solution to 1D heat conduction-advection equation

$$T'_{(z')} = \frac{(1 - e^{-Pe\,z'})}{(1 - e^{-Pe})}$$

2D heat advection-conduction example: Thrusting



$$Pe = \frac{vL}{\kappa}$$



Husson & Moretti, Tectonophysics 2002

Using thermochronology to derive exhumation and relief histories

⇒ solving the 3D transient heat-transport equation

$$\frac{dT}{dt} = \kappa \nabla^2 T + v\nabla T + \frac{H}{\rho c}$$

$$\nabla T = \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} + \frac{\partial T}{\partial z}$$

Boundary conditions:

→ $T_{(z=L)} = T_L$

→ $T_0 = T_{(z=0)} - G\, h_{(x,y,t)}$

- $T_{(z=0)}$: Sea-level temperature
- G: Surface temperature gradient
- $h_{(x,y,t)}$: Surface evolution: *Geomorphic history*

$$E_{(x,y,t)} = \int_0^t v_{z\,(x,y,z,t)} - \Delta h_{(x,y,t)}$$

Exhumation = Rock uplift (*Tectonics*) − Surface change (*Geomorphology*)

What Pecube does

Input

- present-day topography (DEM)
- tectonic scenario ($v_{(x,\ y,\ z,\ t)}$)
- geomorphic scenario ($h_{(x,\ y,\ t)}$)
- (measured thermochronology data)

Output

- Predicted thermochronology data (ages, …) at surface; throughout model and/or at specific locations
- (misfit w.r.t. measured thermochronology data)

→ Run through tectonic/geomorphic scenario to calculate initial position of points ending up at the surface

→ Solve transient heat equation by time-stepping finite-element solution

→ Track temperature/time paths for particles ending up at the surface

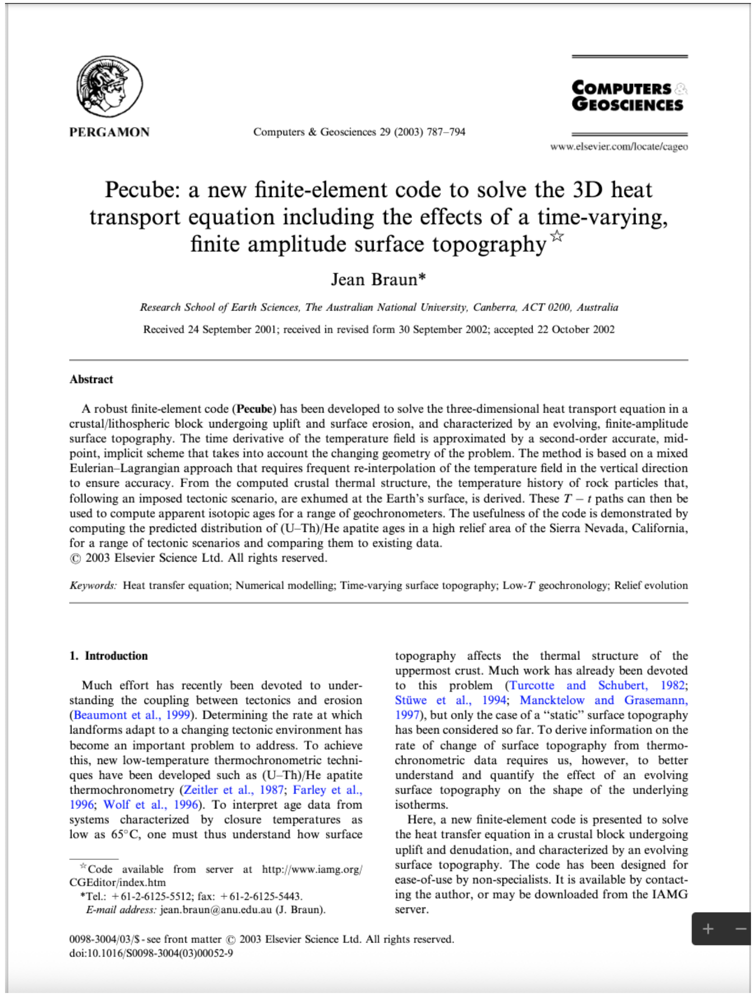
→ Use kinetic models to predict thermochronology data

→ (calculate misfit with measured thermochronology data)

When is Pecube useful?

- When you have rapid (and variable) exhumation rates so that $Pe > 1$ – for at least part of the history
- When you have lateral material transport
- When you have significant (and relatively rapid) changes in topography

Pecube v1



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Pecube: a new finite-element code to solve the 3D heat transport equation including the effects of a time-varying, finite amplitude surface topography☆

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Received 24 September 2001; received in revised form 30 September 2002; accepted 22 October 2002

Abstract

A robust finite-element code (**Pecube**) has been developed to solve the three-dimensional heat transport equation in a crustal/lithospheric block undergoing uplift and surface erosion, and characterized by an evolving, finite-amplitude surface topography. The time derivative of the temperature field is approximated by a second-order accurate, mid-point, implicit scheme that takes into account the changing geometry of the problem. The method is based on a mixed Eulerian–Lagrangian approach that requires frequent re-interpolation of the temperature field in the vertical direction to ensure accuracy. From the computed crustal thermal structure, the temperature history of rock particles that, following an imposed tectonic scenario, are exhumed at the Earth's surface, is derived. These $T-t$ paths can then be used to compute apparent isotopic ages for a range of geochronometers. The usefulness of the code is demonstrated by computing the predicted distribution of (U–Th)/He apatite ages in a high relief area of the Sierra Nevada, California, for a range of tectonic scenarios and comparing them to existing data.
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Keywords: Heat transfer equation; Numerical modelling; Time-varying surface topography; Low-*T* geochronology; Relief evolution

1. Introduction

Much effort has recently been devoted to understanding the coupling between tectonics and erosion (Beaumont et al., 1999). Determining the rate at which landforms adapt to a changing tectonic environment has become an important problem to address. To achieve this, new low-temperature thermochronometric techniques have been developed such as (U–Th)/He apatite thermochronometry (Zeitler et al., 1987; Farley et al., 1996; Wolf et al., 1996). To interpret age data from systems characterized by closure temperatures as low as 65°C, one must thus understand how surface topography affects the thermal structure of the uppermost crust. Much work has already been devoted to this problem (Turcotte and Schubert, 1982; Stüwe et al., 1994; Mancktelow and Grasemann, 1997), but only the case of a "static" surface topography has been considered so far. To derive information on the rate of change of surface topography from thermochronometric data requires us, however, to better understand and quantify the effect of an evolving surface topography on the shape of the underlying isotherms.

Here, a new finite-element code is presented to solve the heat transfer equation in a crustal block undergoing uplift and denudation, and characterized by an evolving surface topography. The code has been designed for ease-of-use by non-specialists. It is available by contacting the author, or may be downloaded from the IAMG server.

☆Code available from server at http://www.iamg.org/CGEditor/index.htm
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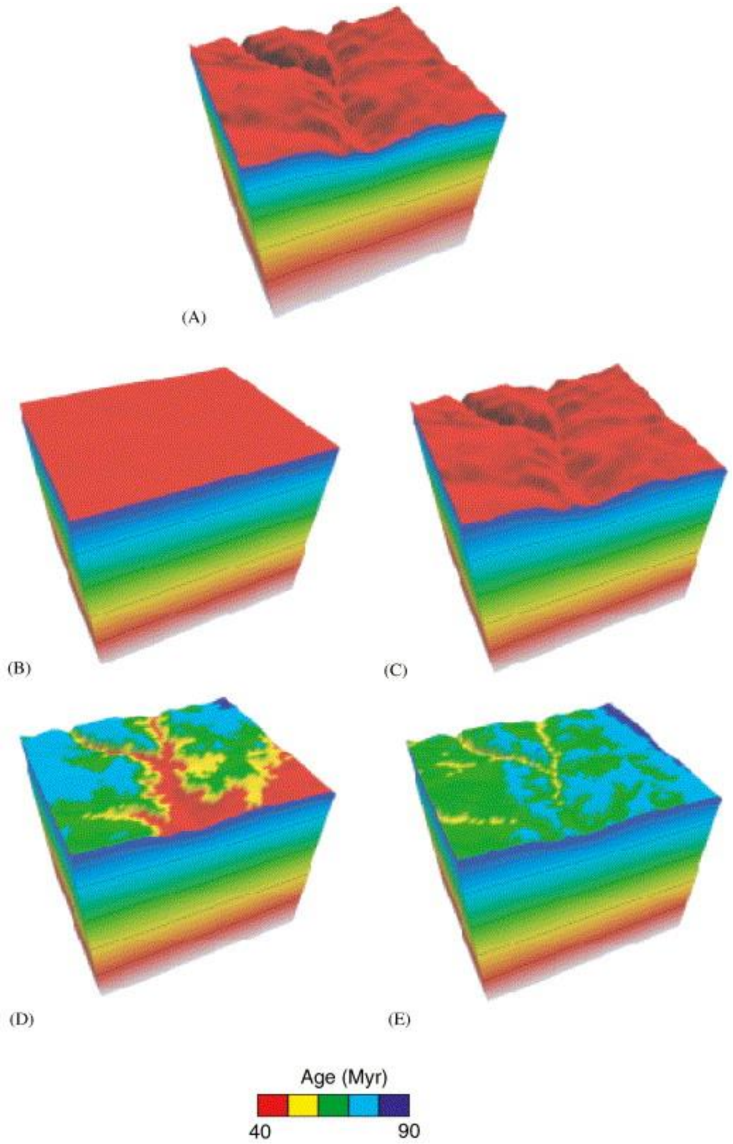
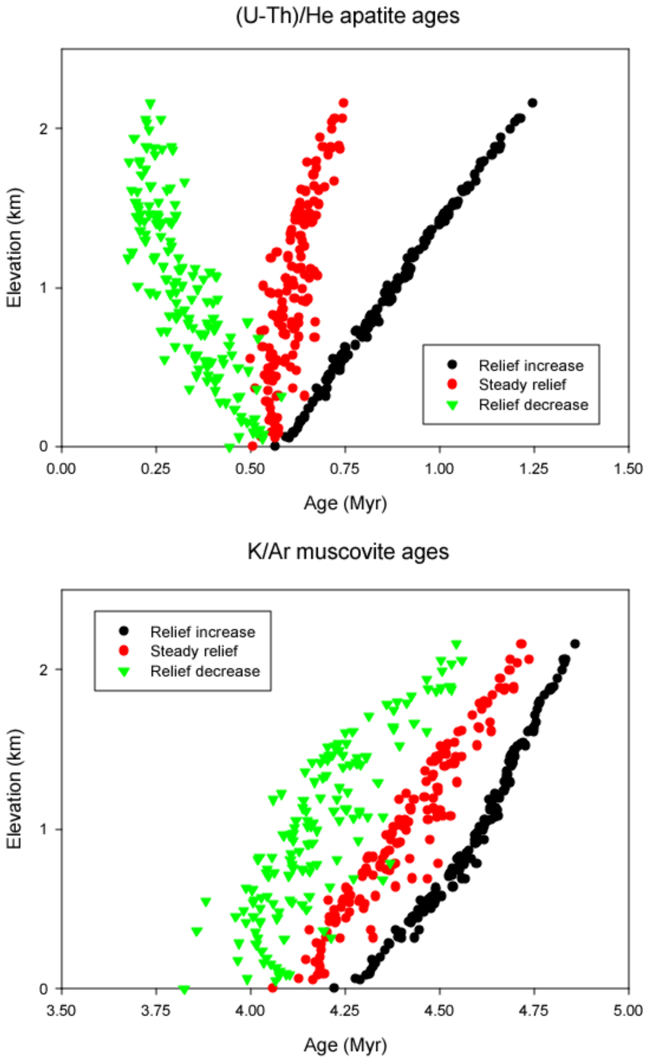
Braun, Comp. Geosci. 2003





After Braun, EPSL 2002

Pecube v2

Tectonophysics 524–525 (2012) 1–28

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Tectonophysics

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Review Article

Quantifying rates of landscape evolution and tectonic processes by thermochronology and numerical modeling of crustal heat transport using PECUBE

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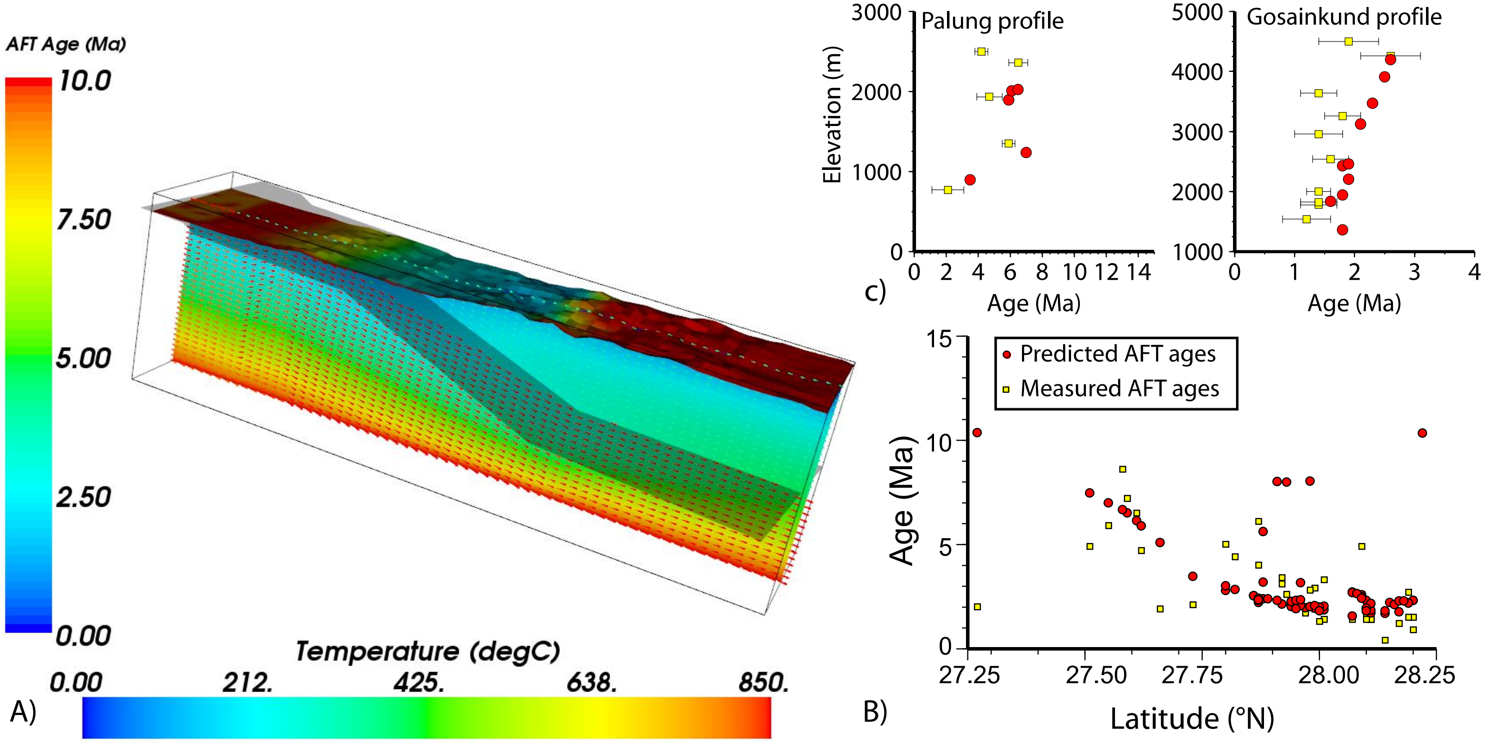
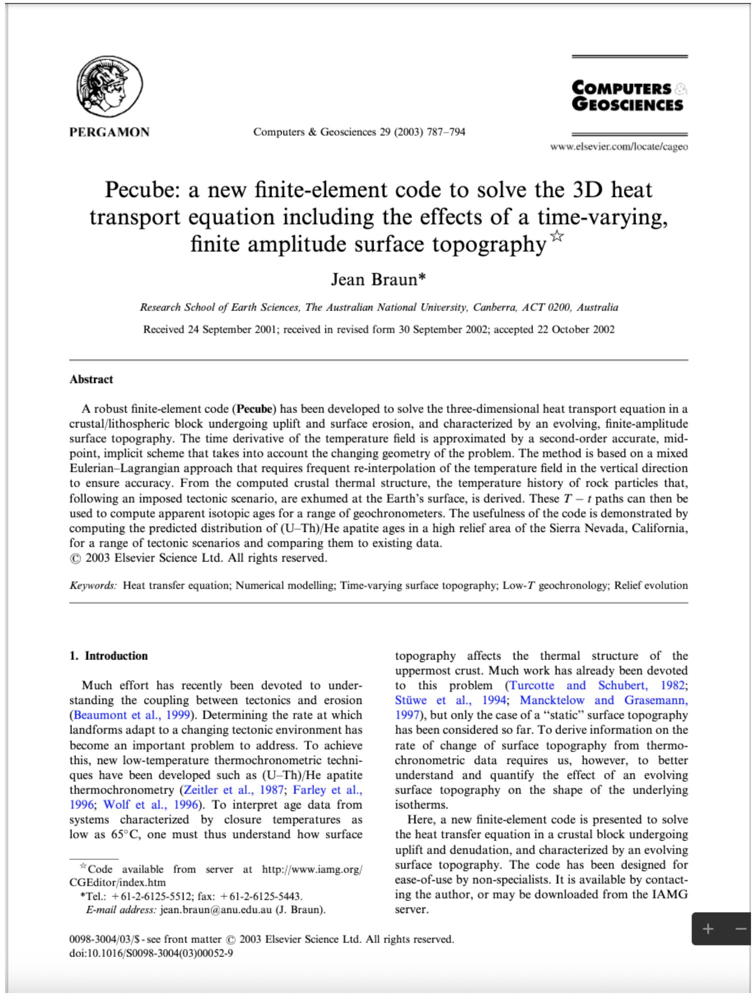
Braun et al., Tectonophysics 2012



Robert et al., Geology 2009

The Pecube “founding texts”



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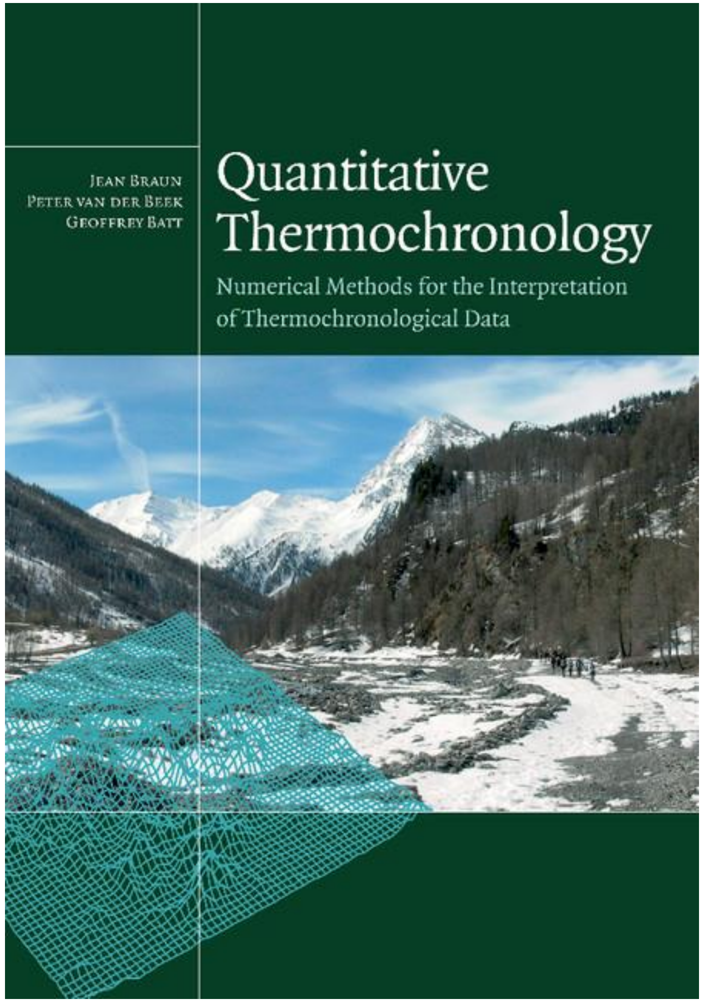

Braun, van der Beek & Batt, Quantitative Thermochronology, CUP 2006

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Braun et al., Tectonophysics 2012

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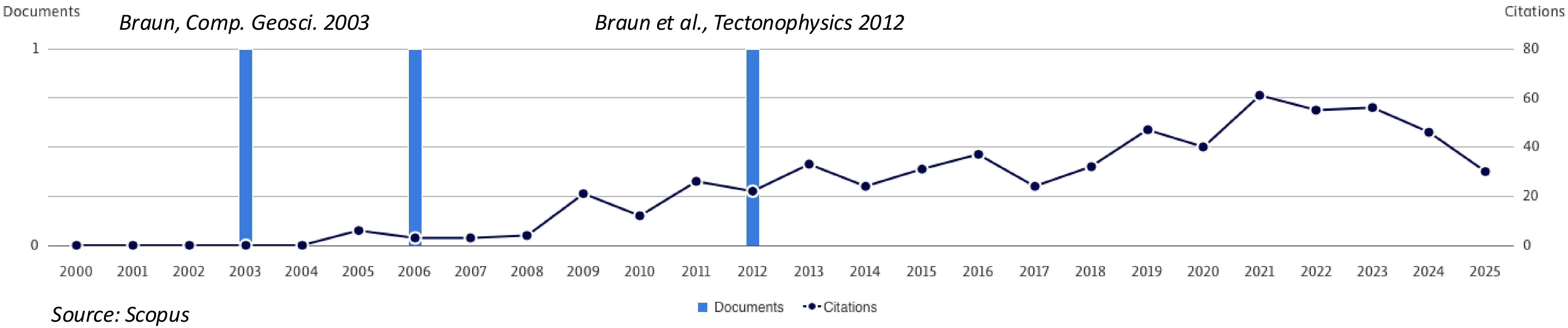
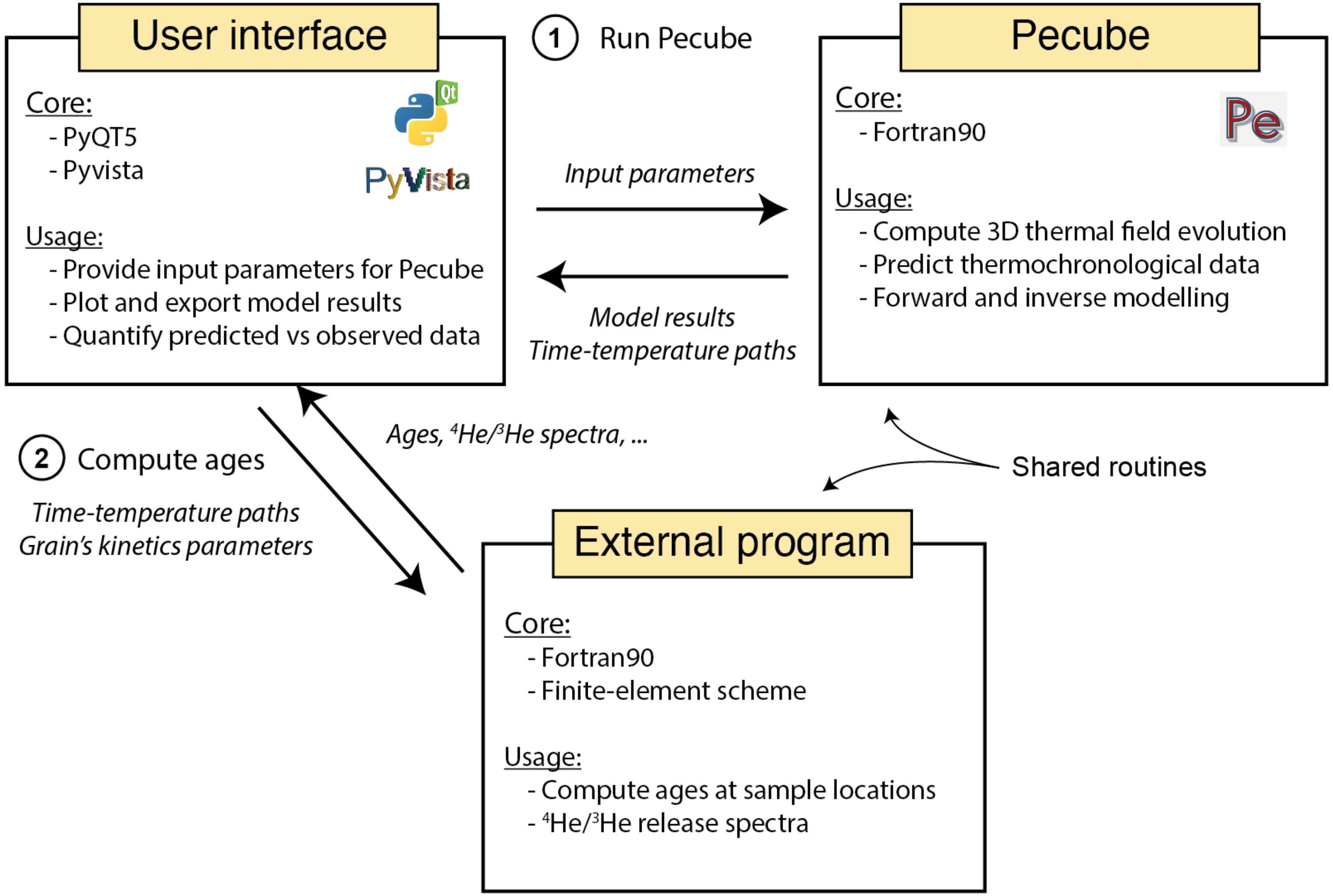


Source: Scopus

Challenges:
- Not very user friendly (complex input-file structure, non-intuitive units for input parameters, no prior verification of model setup);
- Need to develop pre- and post-processing tools;
- No multi-kinetic age-prediction models; no possibility of obtaining sample-specific thermochronometric predictions.

Pecube-GUI

- Python-based interface (PyQT5)
- Handles pre- and post-processing for Pecube
- Separated thermochronometric age predictions from Pecube core to provide more flexibility
- For Windows (≥ Windows 8) and MacOS (≥ 11)
- Online documentation available



Pecube-GUI versus most recent Pecube version

	Pecube v4	PecubeGUI
User interface	x	V
Sample-specific predictions	V	V
Grain-specific kinetics	x	V
Various kinetic models (AHe, ZHe, AFT, OSL)	V	V
Graphical output	x	V
Usage for teaching	x	V

Pecube-GUI website

PecubeGUI

What is PecubeGUI

PecubeGUI is a python-based program that uses PyQt5 to build the GUI. It is an open-source software distributed under the GNU license (soon released!)

The graphical user interface (GUI) aims to help any Pecube's user to set up their models with a user-friendly interface to provide the relevant input parameters. It also enables the users to directly plot the results within the interface, manipulate the characteristics of the plots, and export images. Finally, the PecubeGUI facilitates the coupling between Pecube and the glacial landscape evolution model iSOSIA (Egholm et al., 2011), by enabling the user to load iSOSIA output files, that can be read and used by Pecube. However, output files from other surface processes models can also be loaded.

PecubeGUI comes with a new version of Pecube that enables to predict (U-Th)/He ages on apatite for specific locations. It also includes some radiation damage models, alpha ejection distances, the possibility to set the characteristics of each grain (i.e., grain size, uranium and thorium concentration), and to predict 4He/3He profiles.

Visualization tools for PecubeGUI

PyPIVoT (PecubeGUI Visualization Tools) are a collection of newly developed Python- and Matlab-based visualization scripts designed to help users of PecubeGUI better their understanding of inversion parameter interdependence and the parameter space explored in inversion. PecubeGUI is a thermal-kinematic modelling software used in thermochronology.
[learn more]

Download PecubeGUI

PecubeGU-beta is now available!
Download from Zenodo

PecubeGUI works for MacOs > 11.0 (BigSur) and Windows. Please download the package that matches your chip (MacOS M1/M2 or Intel, Windows_exe)

PecubeGUI Documentation

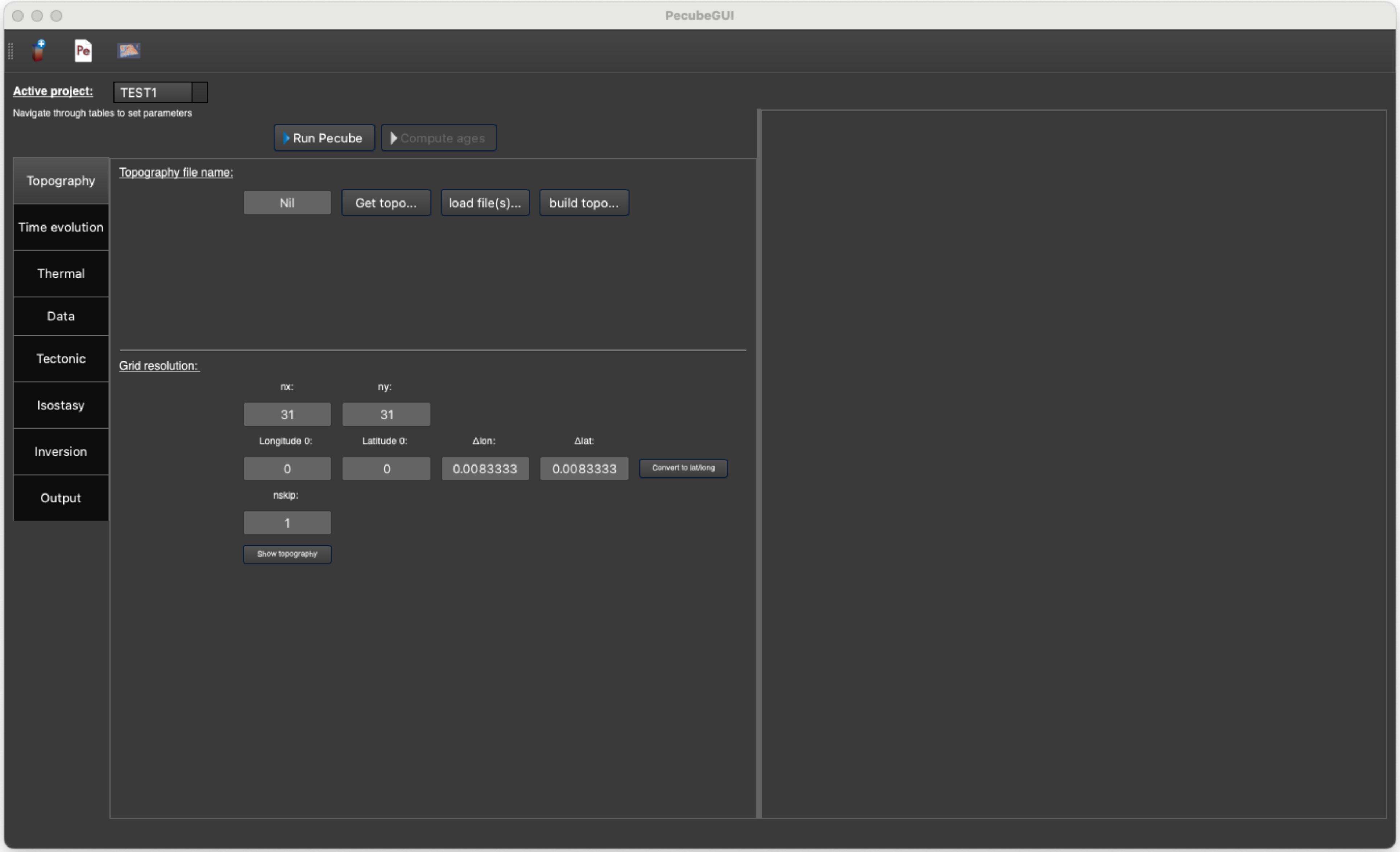
You can access the documentation, here: PecubeGUI – Documentation

Example input files

- Forward modelling (zip-file, 24 MB)
- Inversion (zip-file, 4,7 MB)

https://erc-cooler.eu/pecubegui/

Let’s try this!



Misfit

There are MANY different misfit (*objective*) functions / definitions of misfit …

The original version of Pecube used: $\phi = \frac{1}{N}\sqrt{\sum_{i=1}^{N}\frac{\left(\alpha_{i,mod}-\alpha_{i,dat}\right)^2}{\sigma_i^2}}$

Since Pecube v2 (2012) the χ^2-statistic is used:

$$\phi = \sum_{i=1}^{N}\left(\frac{\alpha_{i,mod} - \alpha_{i,dat}}{\sigma_i}\right)^2$$

ϕ = misfit
N = number of data
$\alpha_{i,mod}$ = modelled age of i^{th} datapoint
$\alpha_{i,dat}$ = observed age of i^{th} datapoint
σ_i = uncertainty of i^{th} datapoint

Misfit

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$\alpha_{i,dat}$ = observed age of i^{th} datapoint
σ_i = uncertainty of i^{th} datapoint
p = number of free parameters

Advantages of the χ^2-statistic $\phi = \sum_{i=1}^{N} \left(\frac{\alpha_{i,mod} - \alpha_{i,dat}}{\sigma_i}\right)^2$:

1. It can be easily transformed into the *reduced* χ^2-statistic:

$$\phi_r = \frac{1}{N-p-1} \sum_{i=1}^{N} \frac{(\alpha_{i,mod} - \alpha_{i,dat})^2}{\sigma_i^2}$$

Which gives insight into how well the data are fit: if $\phi_r < 1$ then all datapoints are fit to within 1σ error (if $\phi_r < 2$ then fit within 2σ, etc.)

Misfit

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N = number of data
$\alpha_{i,mod}$ = modelled age of i^{th} datapoint
$\alpha_{i,dat}$ = observed age of i^{th} datapoint
σ_i = uncertainty of i^{th} datapoint
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Advantages of the χ^2-statistic $\phi = \sum_{i=1}^{N}\left(\frac{\alpha_{i,mod}-\alpha_{i,dat}}{\sigma_i}\right)^2$:

1. It can be easily transformed into the *reduced* χ^2-statistic.

2. We can use it to calculate the *log-likelihood*:

$$\log(L) = -\sum_{i=1}^{N}\left[\frac{\ln(2\pi)}{2} + ln(\sigma_i) + 0.5\left(\frac{\alpha_{i,mod} - \alpha_{i,dat}}{\sigma_i}\right)^2\right]$$

3. Which can be used to calculate the *Bayesian Information Criterion*:

$$BIC = -2\log(L) + p\log(N)$$

The BIC informs us about the appropriate level of model complexity

Misfit

Objective functions / what we try to achieve:

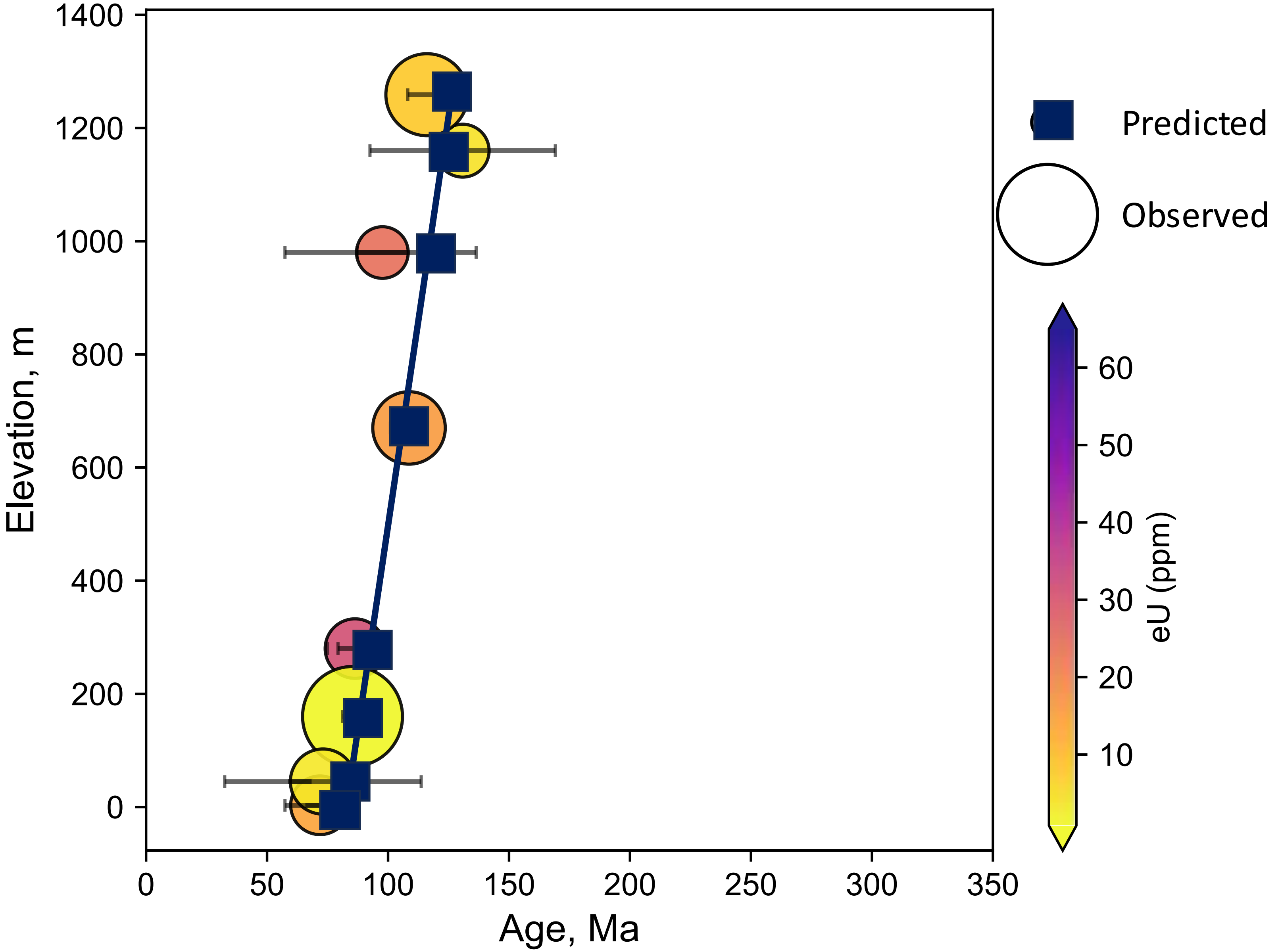
- *Minimise* the χ^2 / reduced χ^2
- *Maximise* the log-likelihood (note: $\log(L) < 0$ by definition)
- *Minimise* the BIC

Misfit

A simple case:

$\phi_r < 1$;
ϕ small;
$\log(L) \longrightarrow 0$

Good fit to data

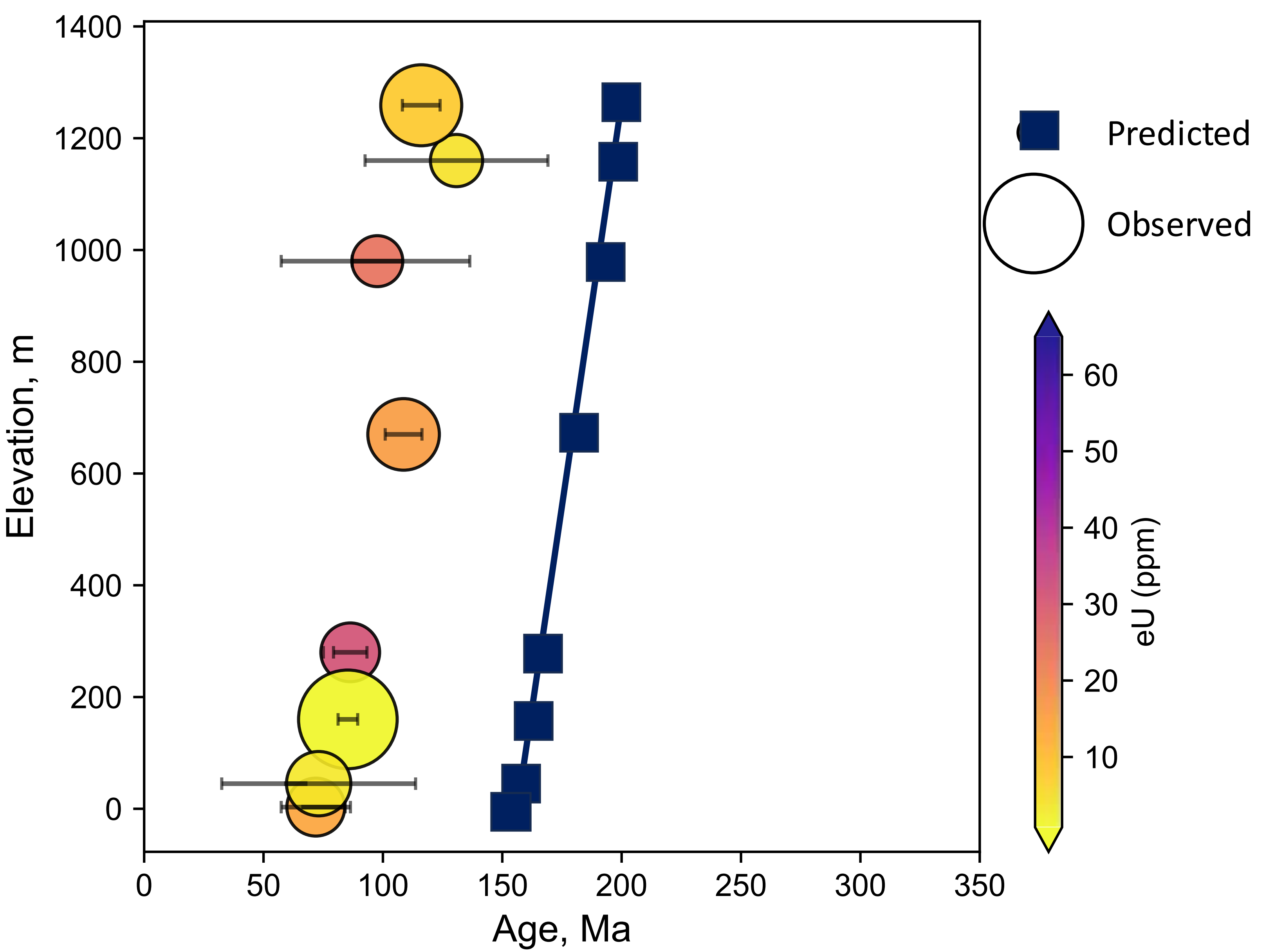


Misfit

A simple case:

$\phi_r > 1$;
ϕ large;
$\log(L) \ll 0$

Bad fit to data

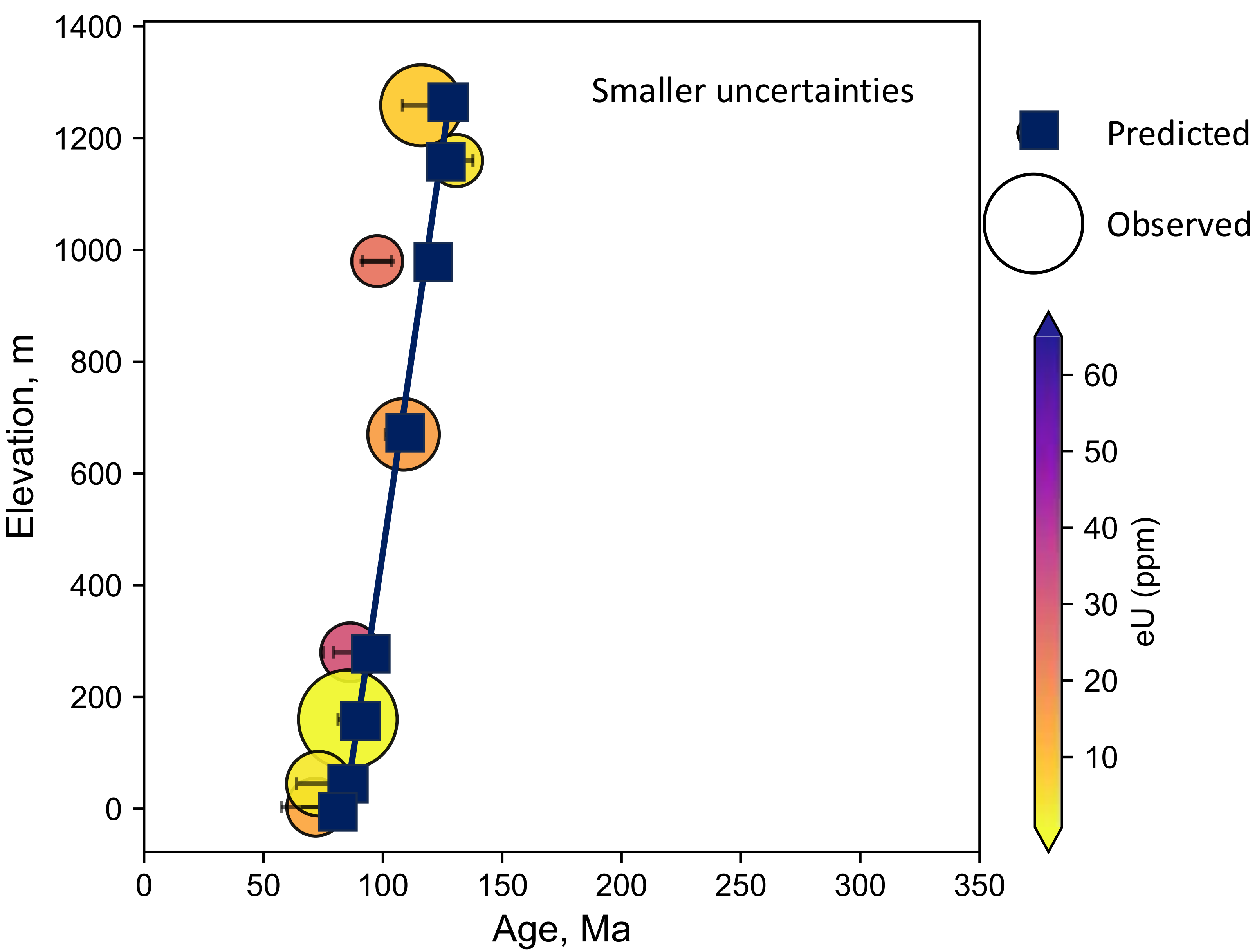


Misfit

But:

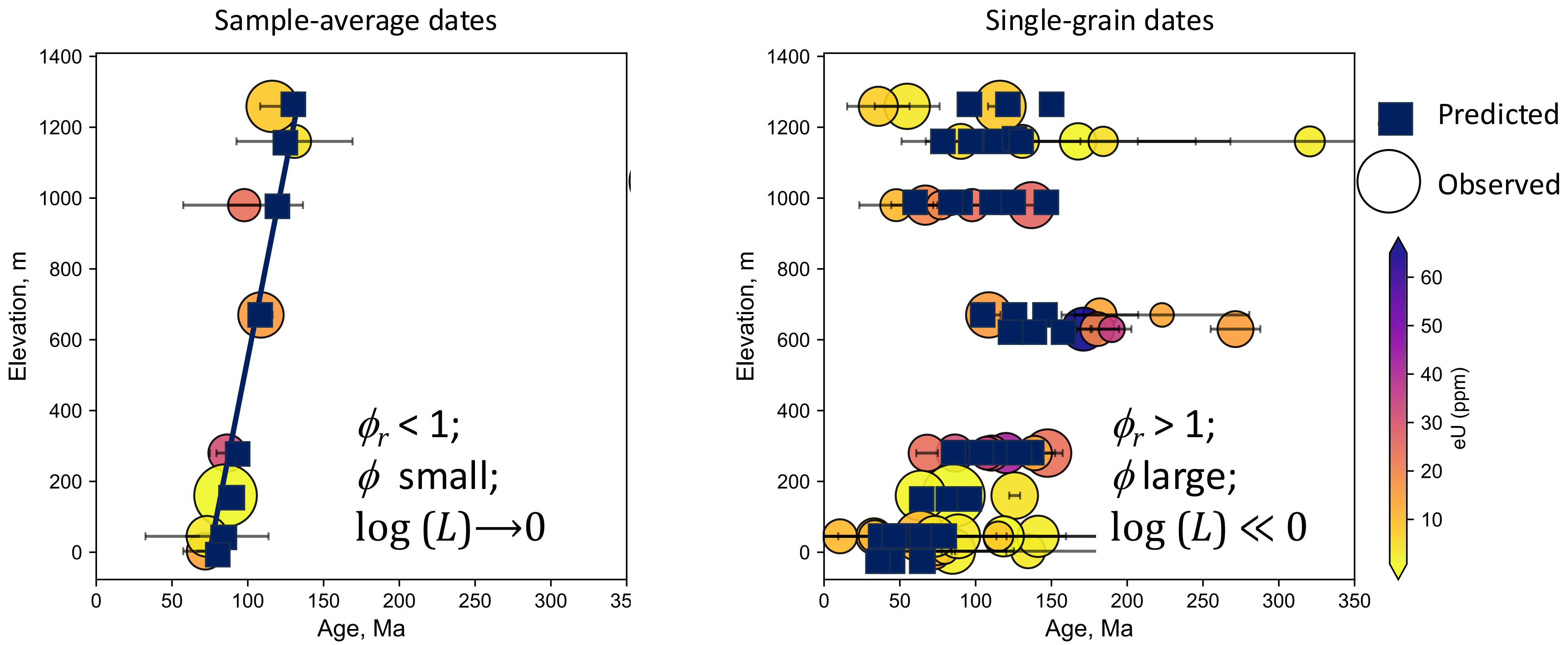
$\phi_r > 1$;
ϕ larger;
$\log(L) < 0$

Not such a good fit to data?



Misfit

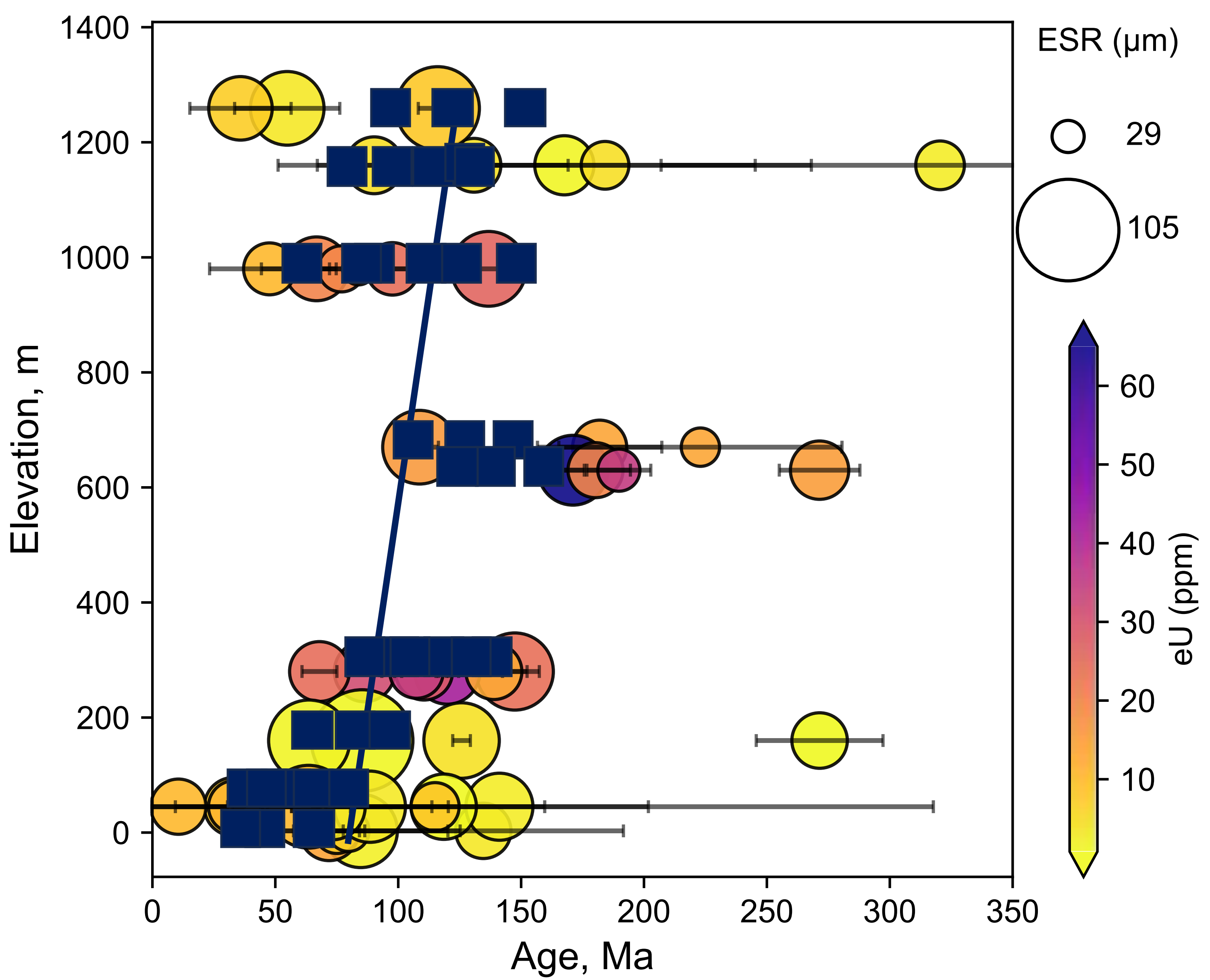
Working with sample-average versus single-grain data



Misfit

The role of outliers

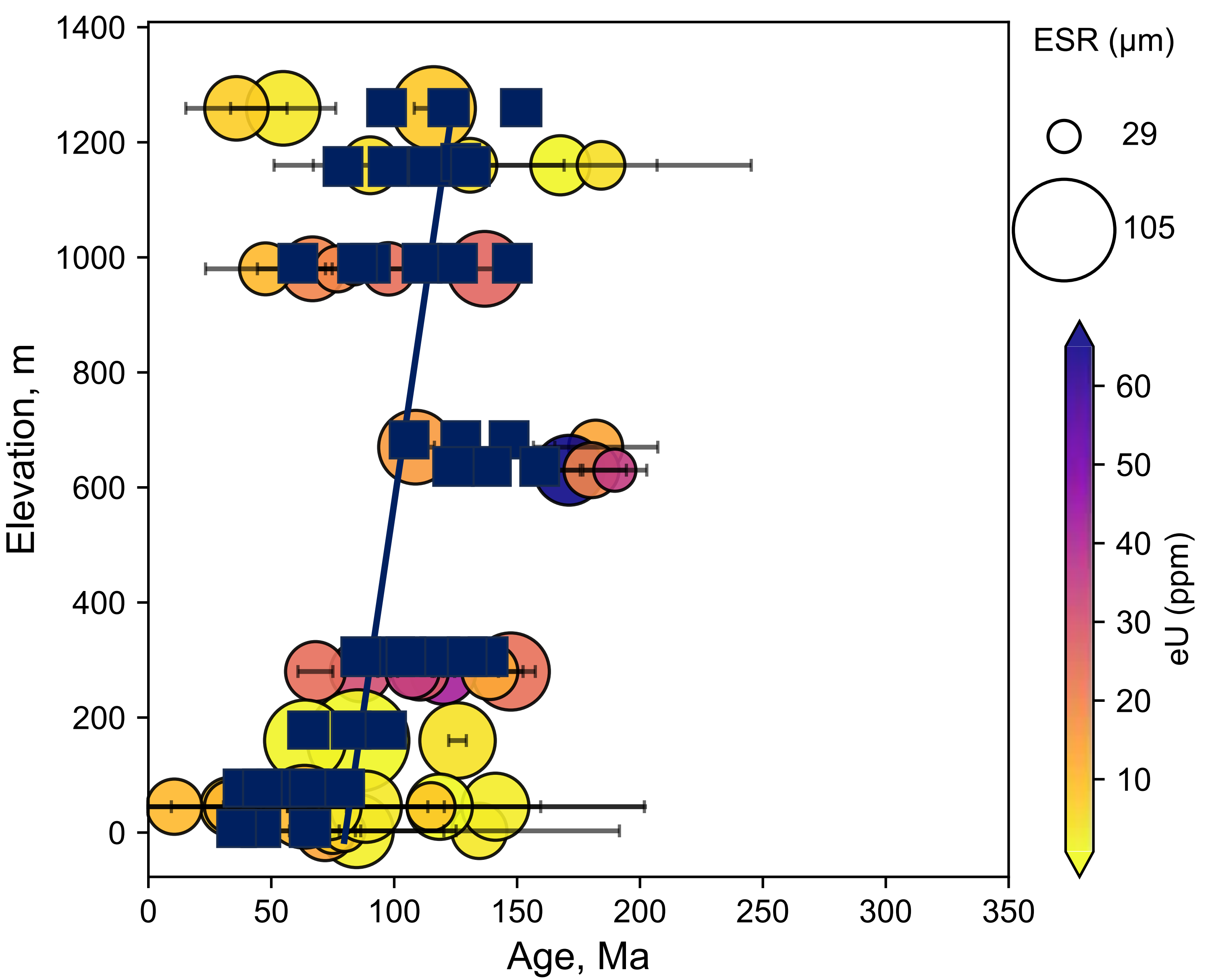
$\phi_r > 1$;
ϕ large;
$\log(L) \ll 0$



Misfit

The role of outliers

$\phi_r > 1$ but smaller;
ϕ smaller;
$\log(L) < 0$



Inversion in Pecube-GUI

Forward model: model $\longrightarrow$ data

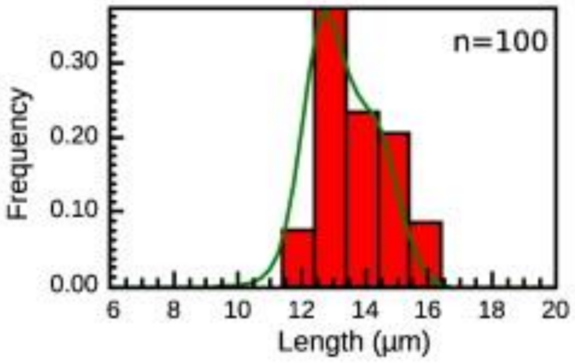
- Scenario testing;
- How well does this model fit my data?

Inverse model: data $\longrightarrow$ model

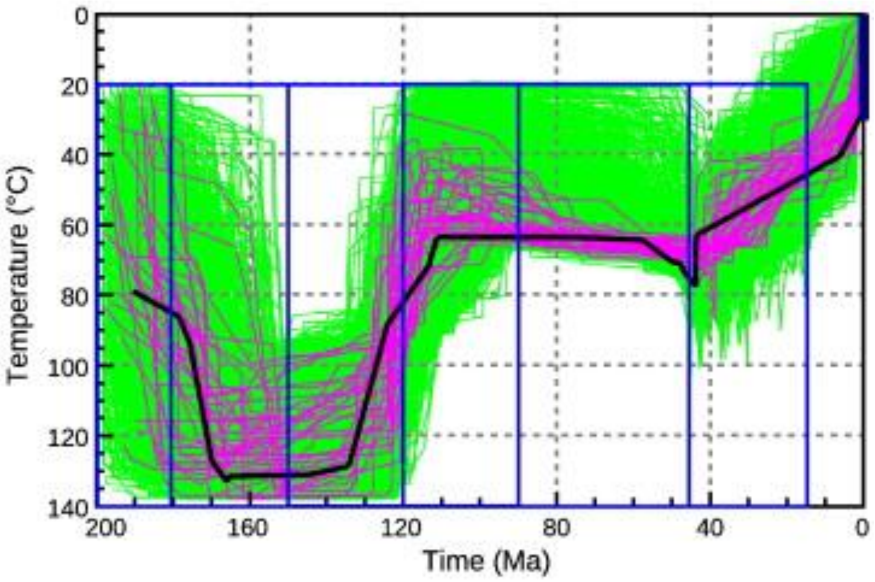
- What does the data say about my model?
- How well can the data resolve contrasting scenarios?

Thermal history models = inverse models

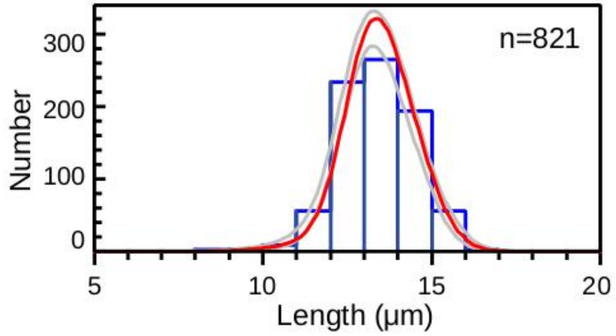
HeFTy



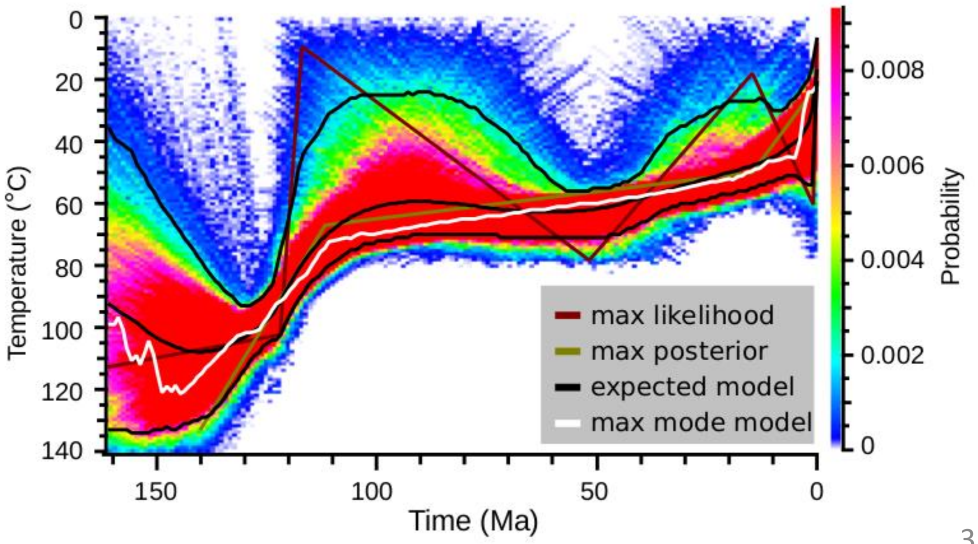
	MTL	AFT age	AHe age
Measured	13.4 ± 1.0	102 ± 7	55 ± 5
Modelled	13.3 ± 1.1	102	59



QTQt

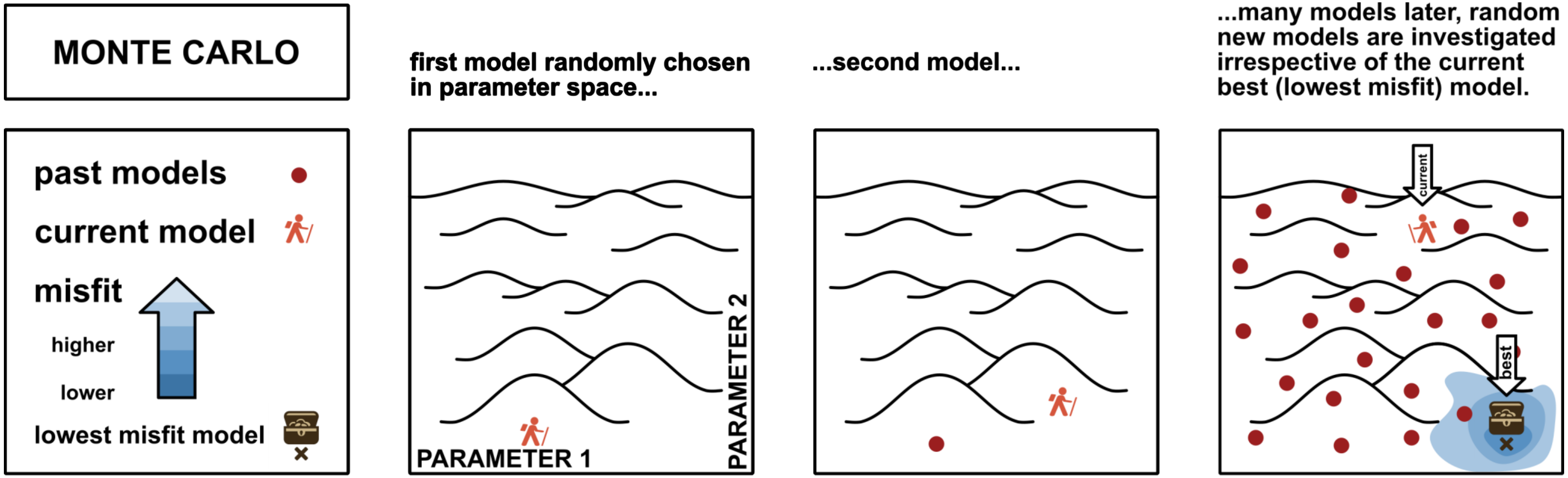


	MTL	AFT age	AHe age
Measured	13.4 ± 1.2	102 ± 7	55 ± 5
Modelled	13.9 ± 0.9	102 ± 5	59 ± 4

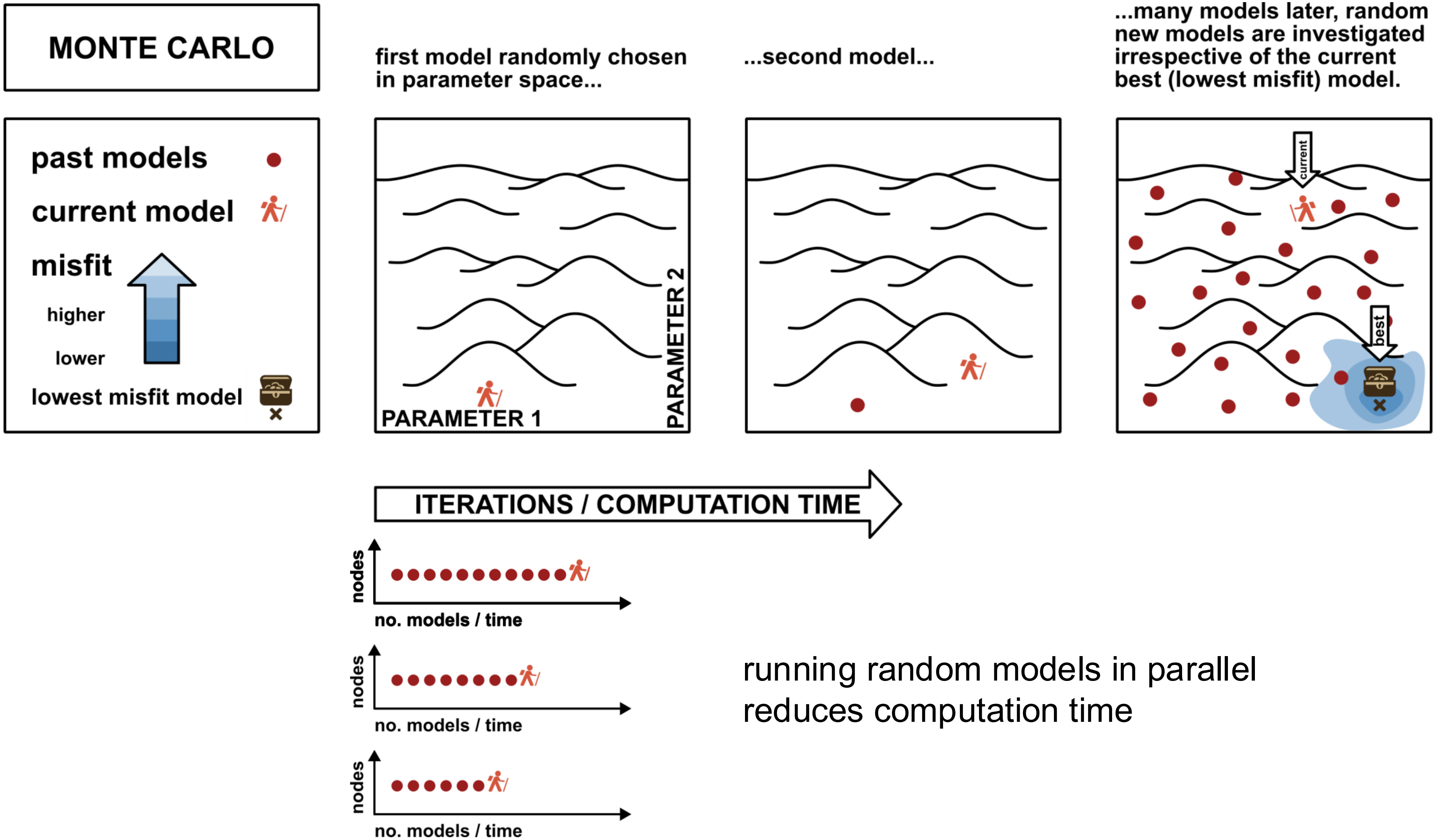


From Vermeesch & Tian, Earth Sci. Rev. 2014

Inverse modelling strategies

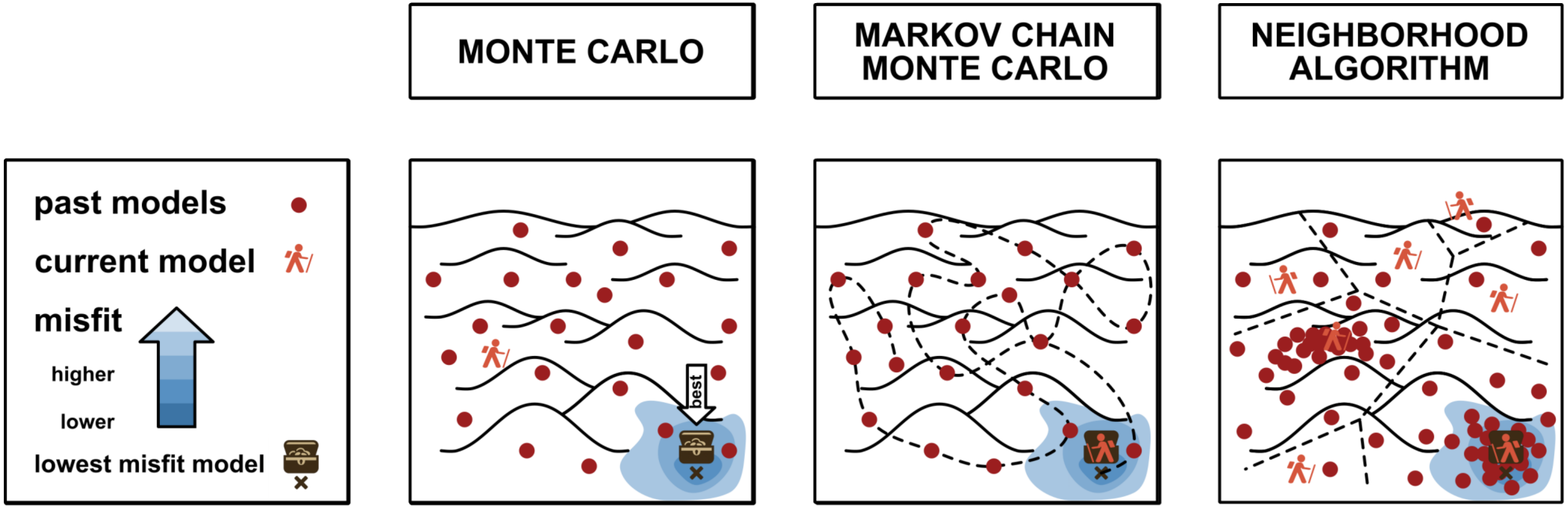


Inverse modelling strategies



running random models in parallel reduces computation time

Inverse modelling strategies



random

next step based on misfit of previous step

successful neighborhoods explored more

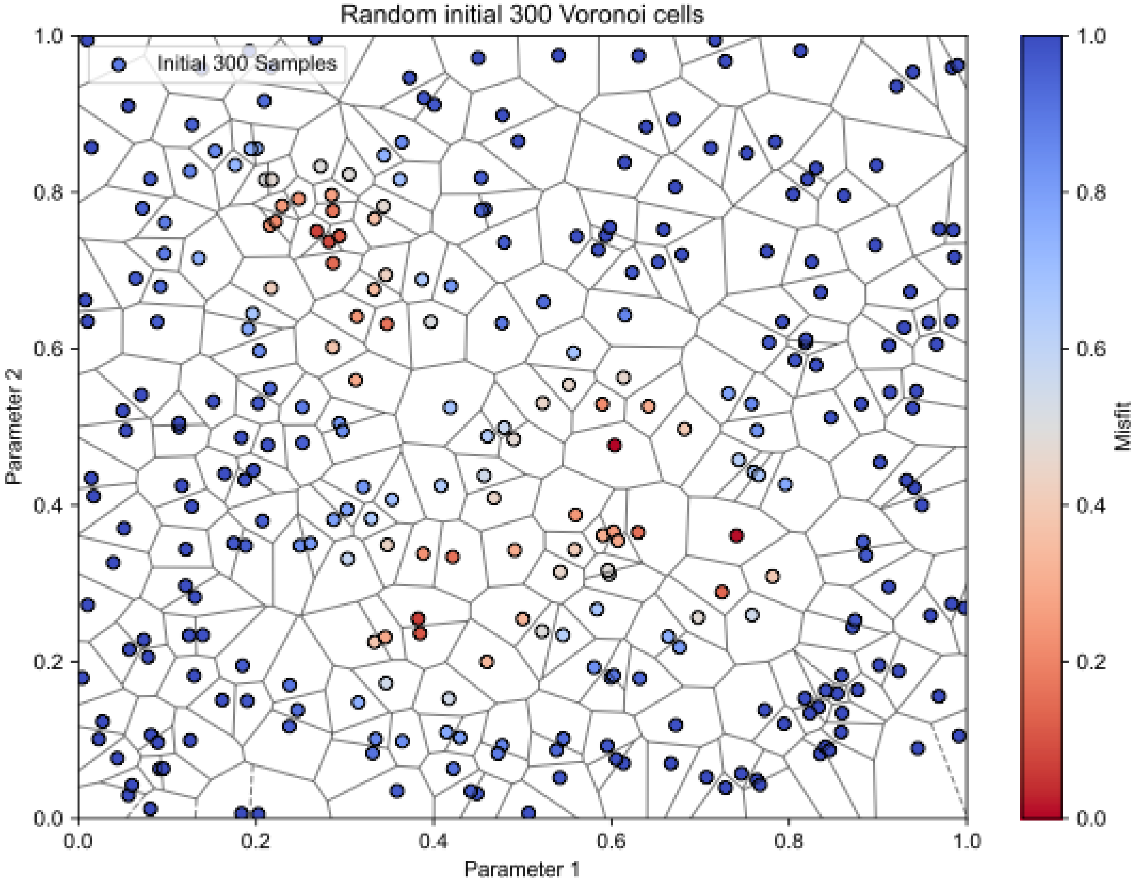
e.g., HeFTy

e.g., QTQt

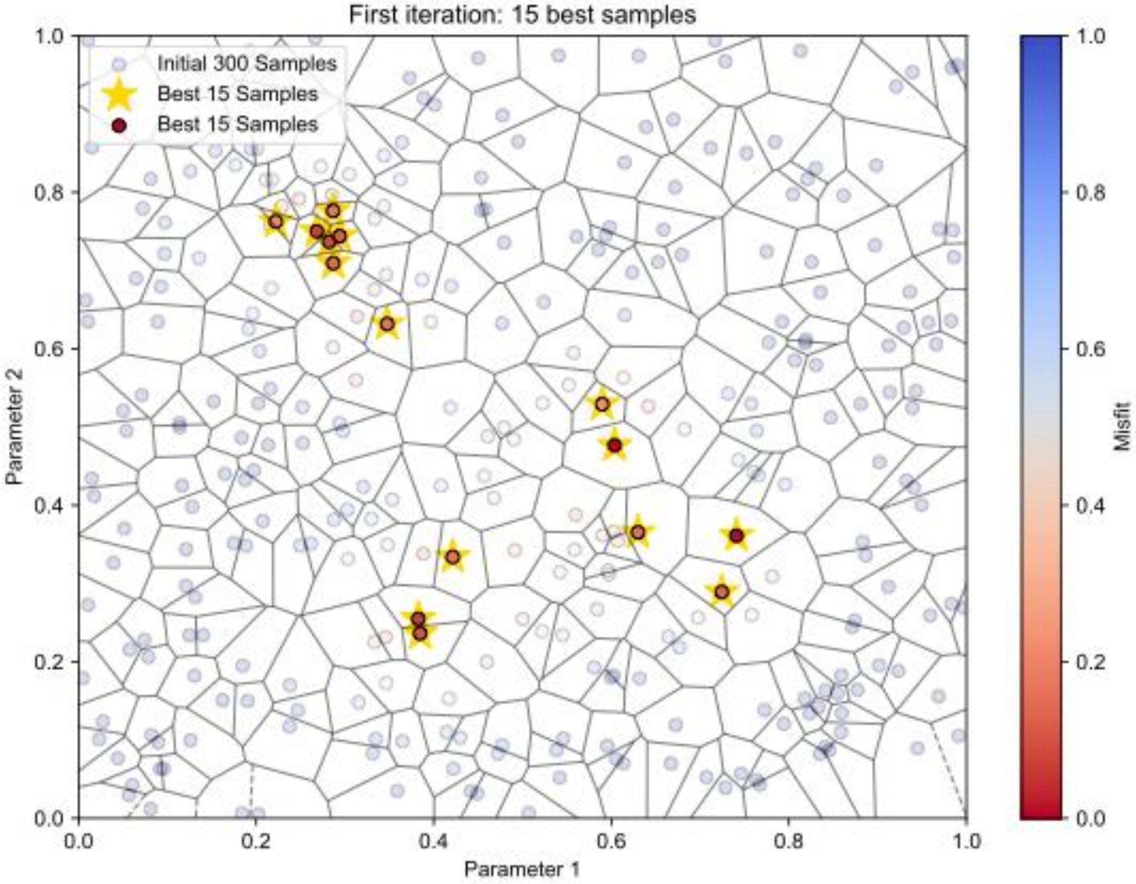
e.g., Pecube

Inversion in Pecube-GUI: Neighbourhood Algorithm (NA)

Define *nearest neighbours* and divide up model space using *Voronoi cells*



Step 1, *n*: search in *j* Voronoi cells that contain *j* best models from previous step



Inversion in Pecube-GUI: Neighbourhood Algorithm (NA)

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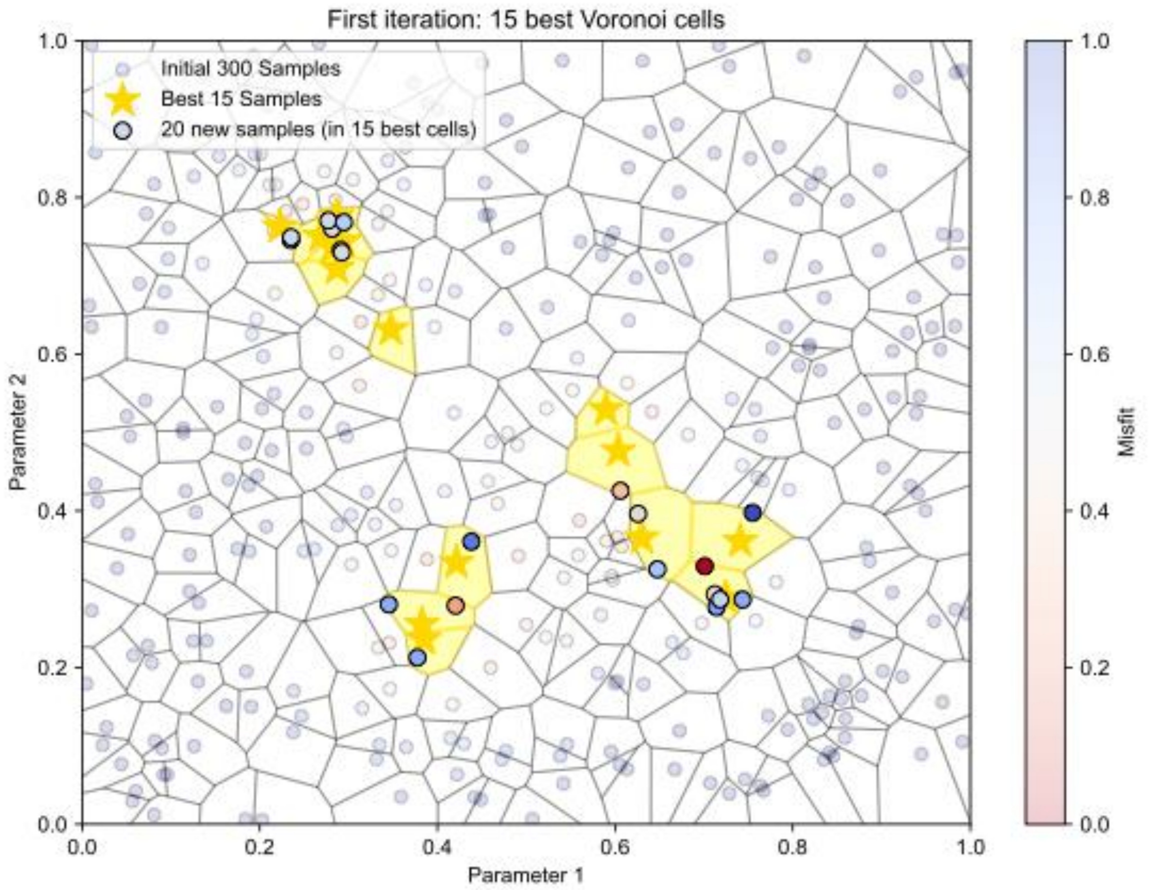
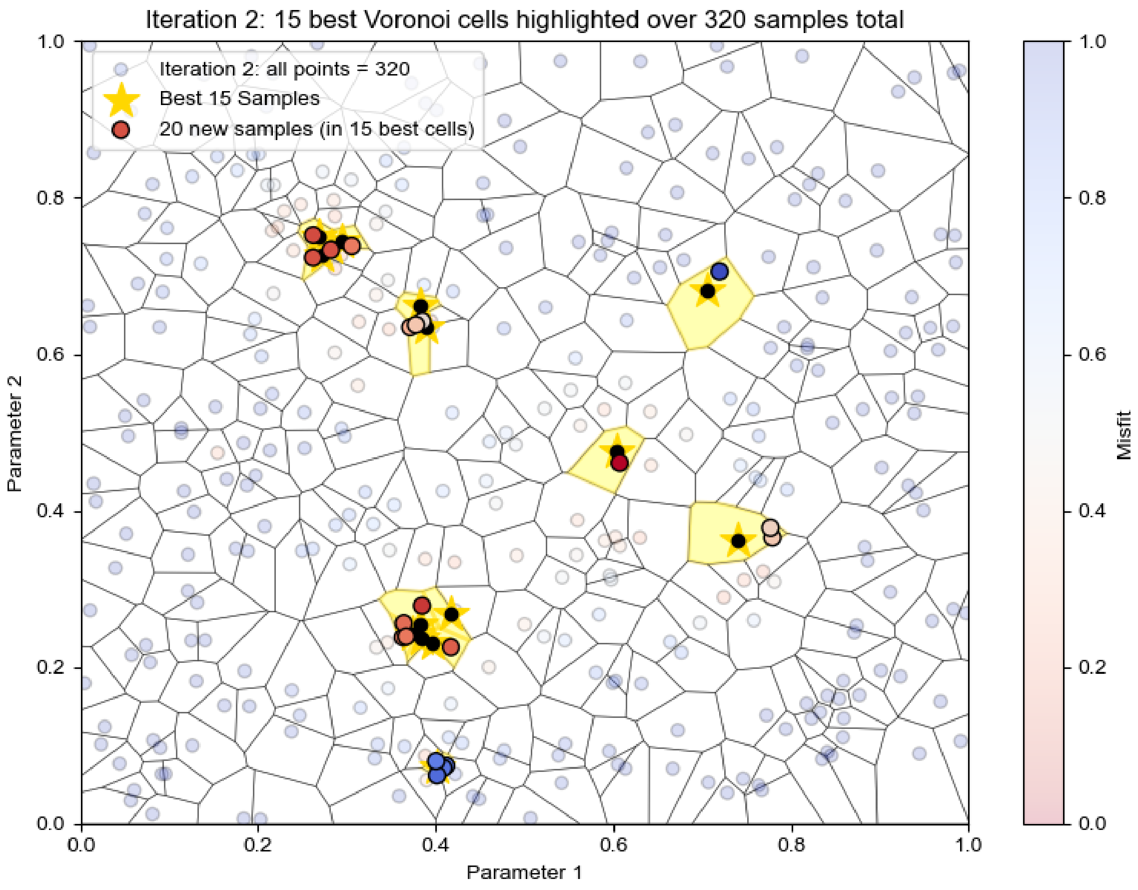
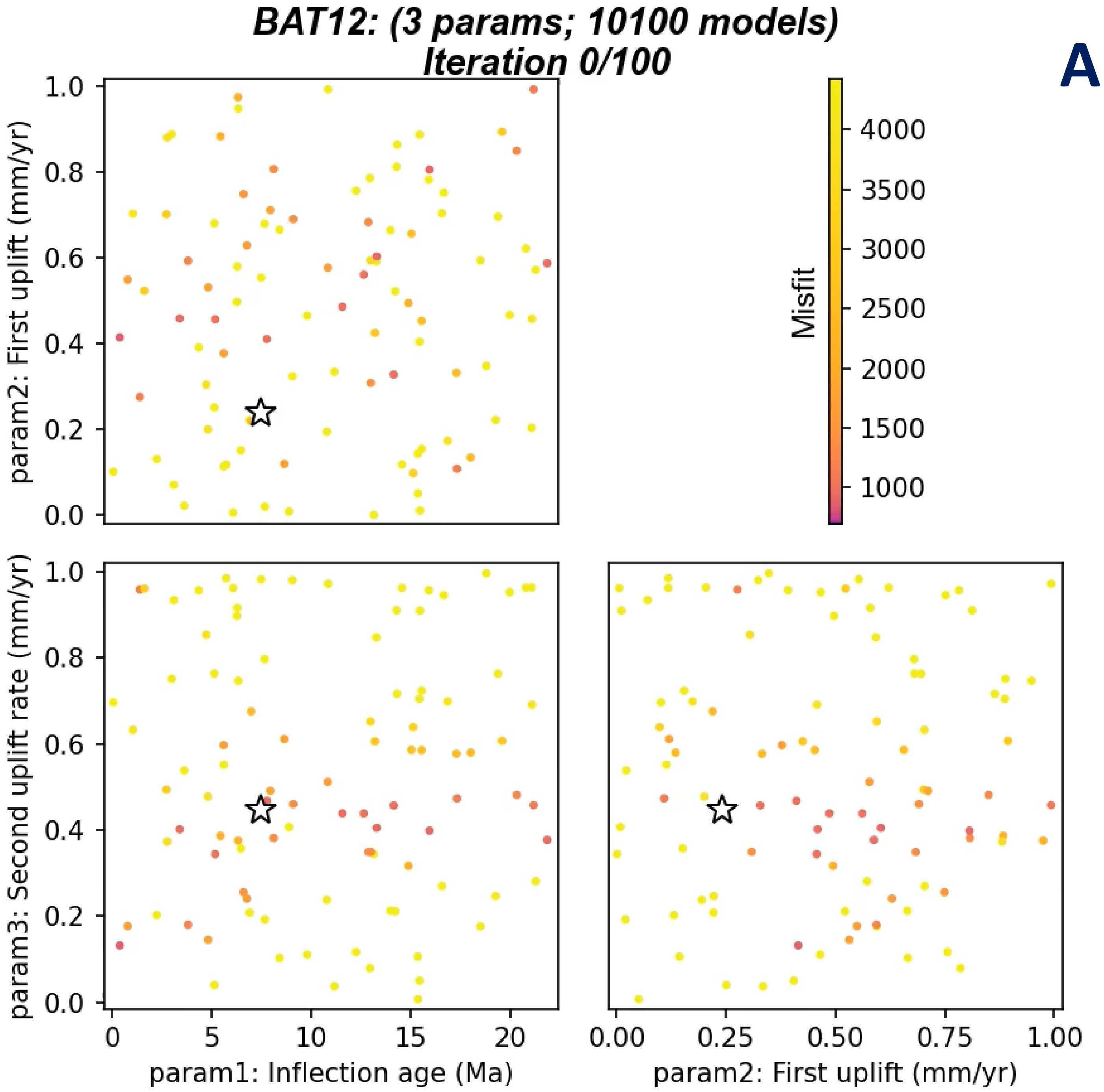


Step 1, *n*: search in *j* Voronoi cells that contain *j* best models from previous step



and so on …

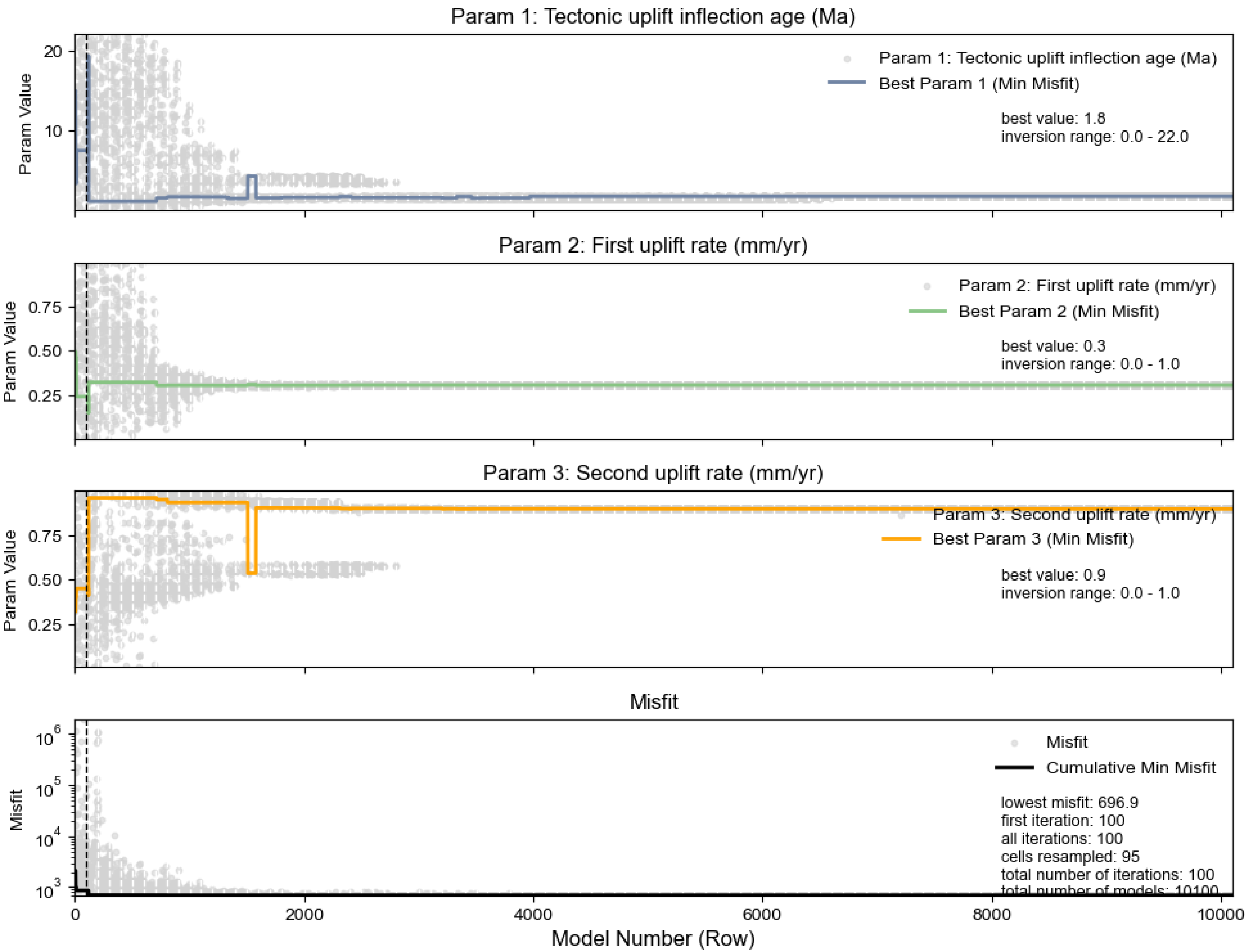


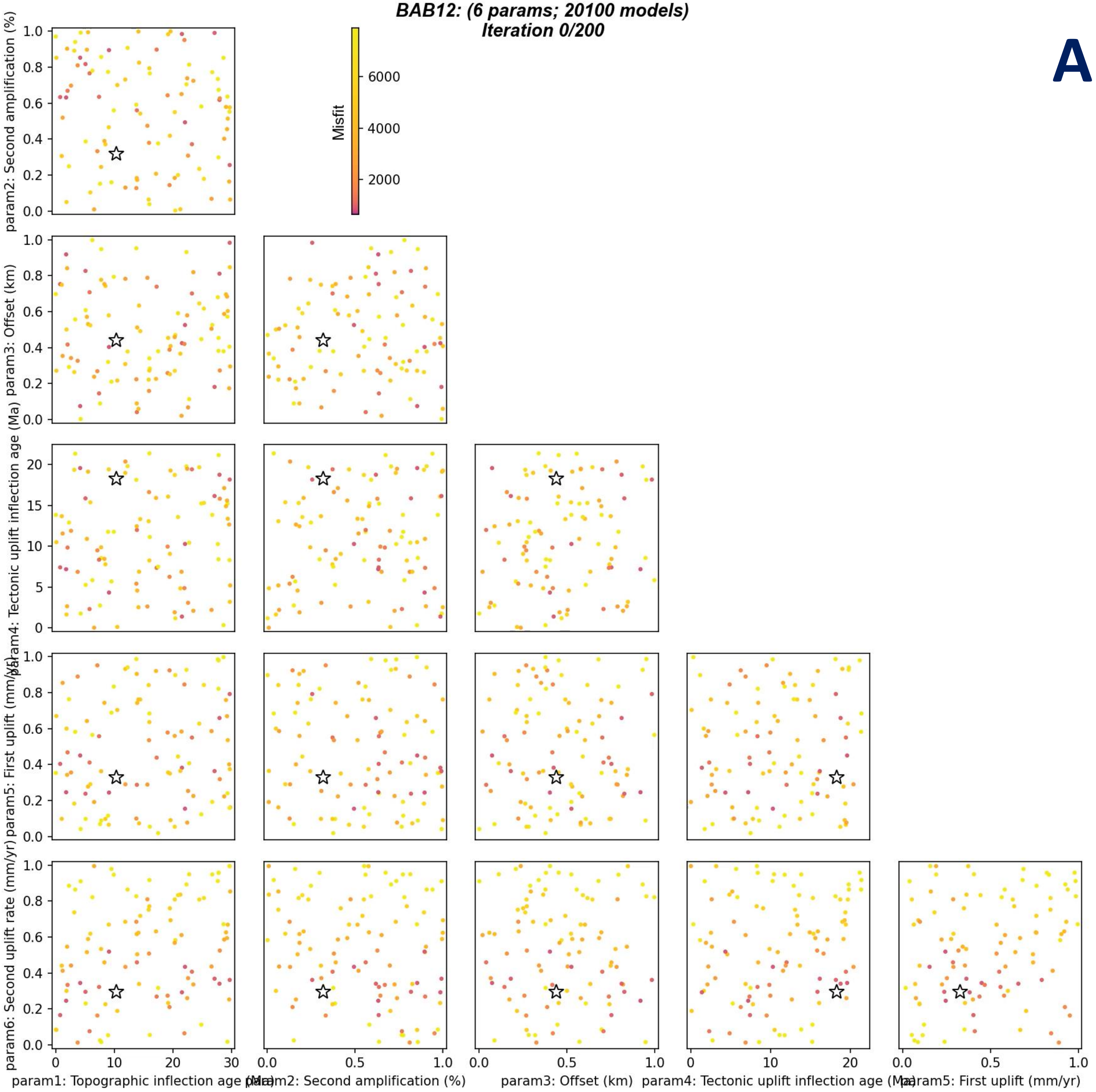
A simple example

3-parameter model – tectonic scenario only

- Initial rock-uplift rate (param 2)
- Final rock-uplift rate (param 3)
- Time of change (param 1)

A simple example

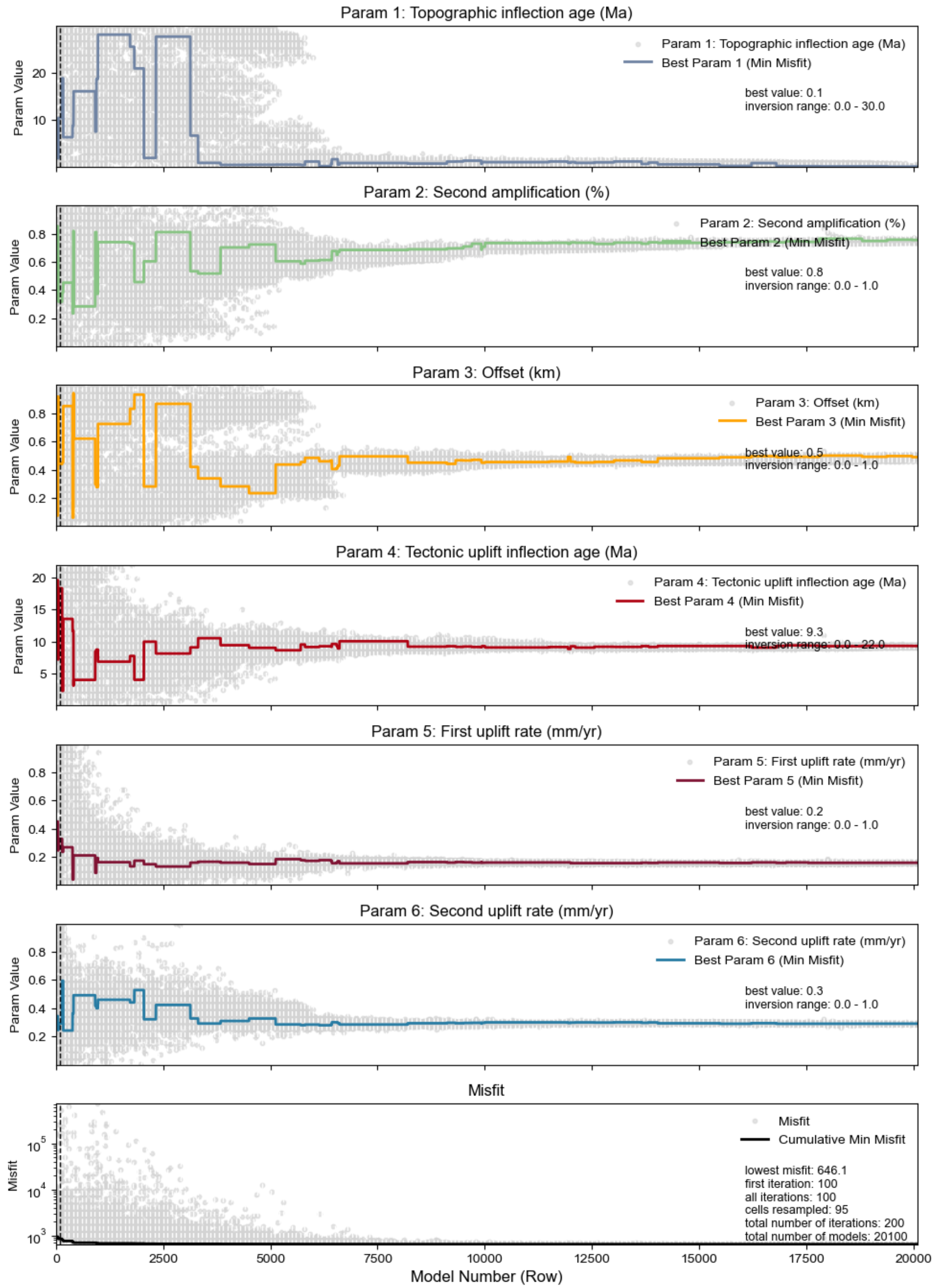




A more complex example

6-parameter model: tectonic and geomorphic scenario

- Initial rock-uplift rate (param 5)
- Final rock-uplift rate (param 6)
- Time of tectonic change (param 4)
- Time of geomorphic change (param 1)
- Initial topographic amplification (param 2)
- Initial topographic offset (param 3)



A more complex example

6-parameter model: tectonic and geomorphic scenario

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- Time of tectonic change (param 4)
- Time of geomorphic change (param 1)
- Initial topographic amplification (param 2)
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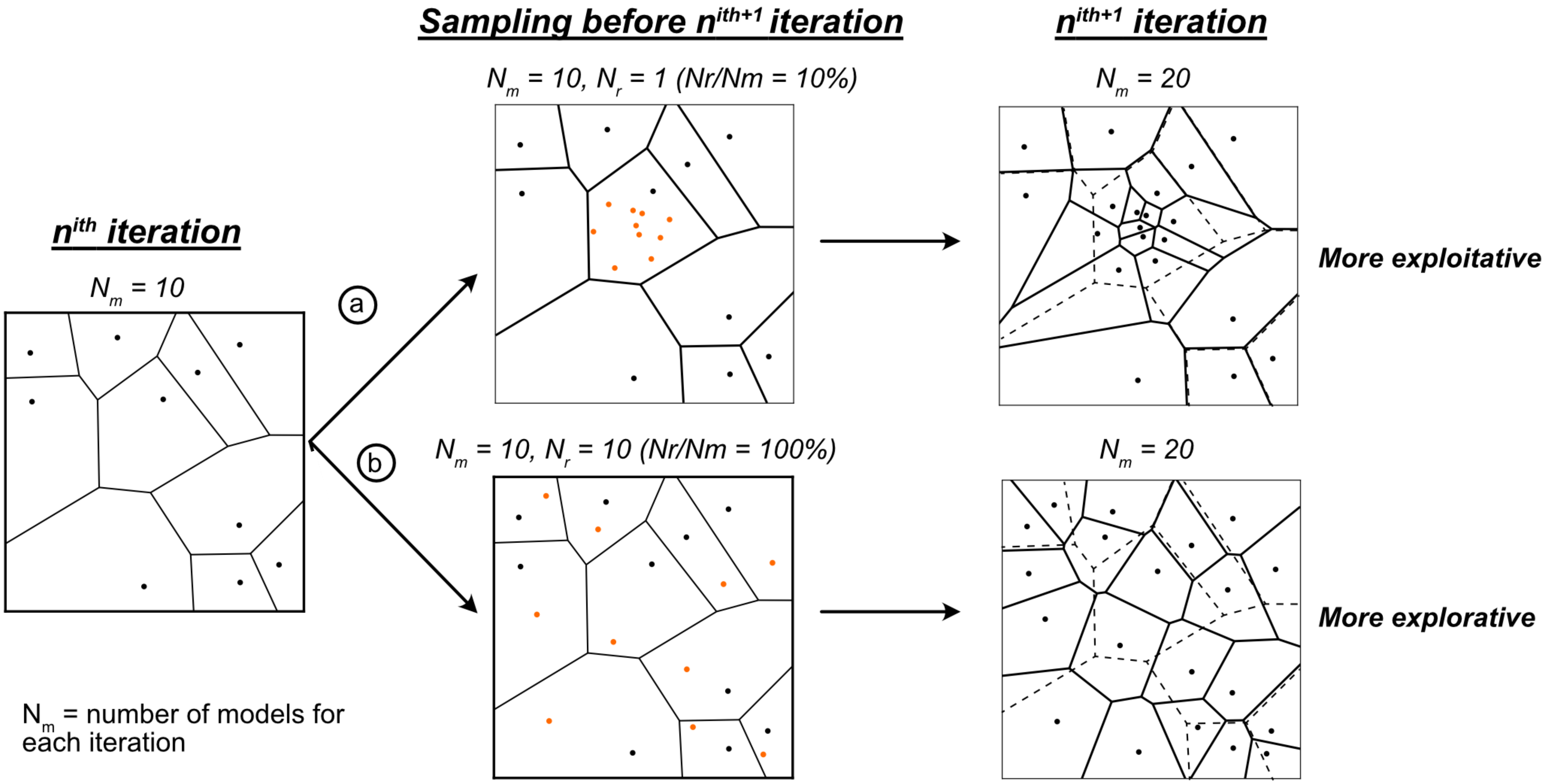
NA inversion strategies

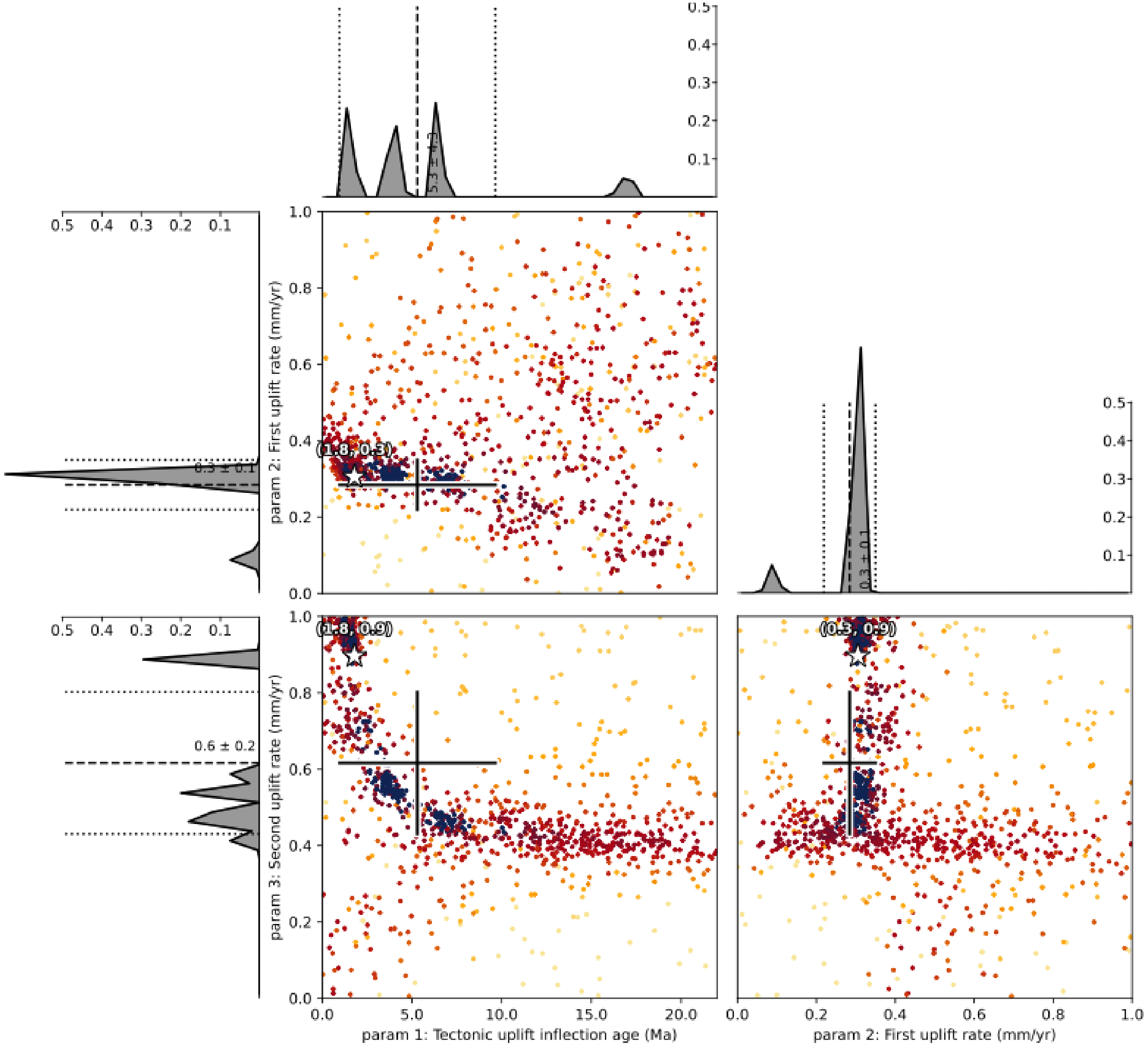


N_m = number of models for each iteration

N_r = number cells to resample (i.e., the N_r best-models)

After *Bernard et al., in prep.*

What does the "best fit" model mean?



After an NA-inversion, you can (it would be better to) run ***NA-Bayes*** to:

- Get an estimate of resolution;
- Assess uniqueness

- Initial rock-uplift rate (param 2): well defined
- Final rock-uplift rate (param 3)
- Time of change (param 1).

} several minima and significant tradeoff

NA-Bayes is (currently still) a stand-alone Fortran code but the tools to visualise the predicted parameter PDF's and estimated uncertainties (as shown here) are now available on Zenodo as *Python* and *Matlab* scripts.

See links on: https://erc-cooler.eu/codes/