

Supplementary information

Antarctic geothermal heat flow and its implications for tectonics and ice sheets

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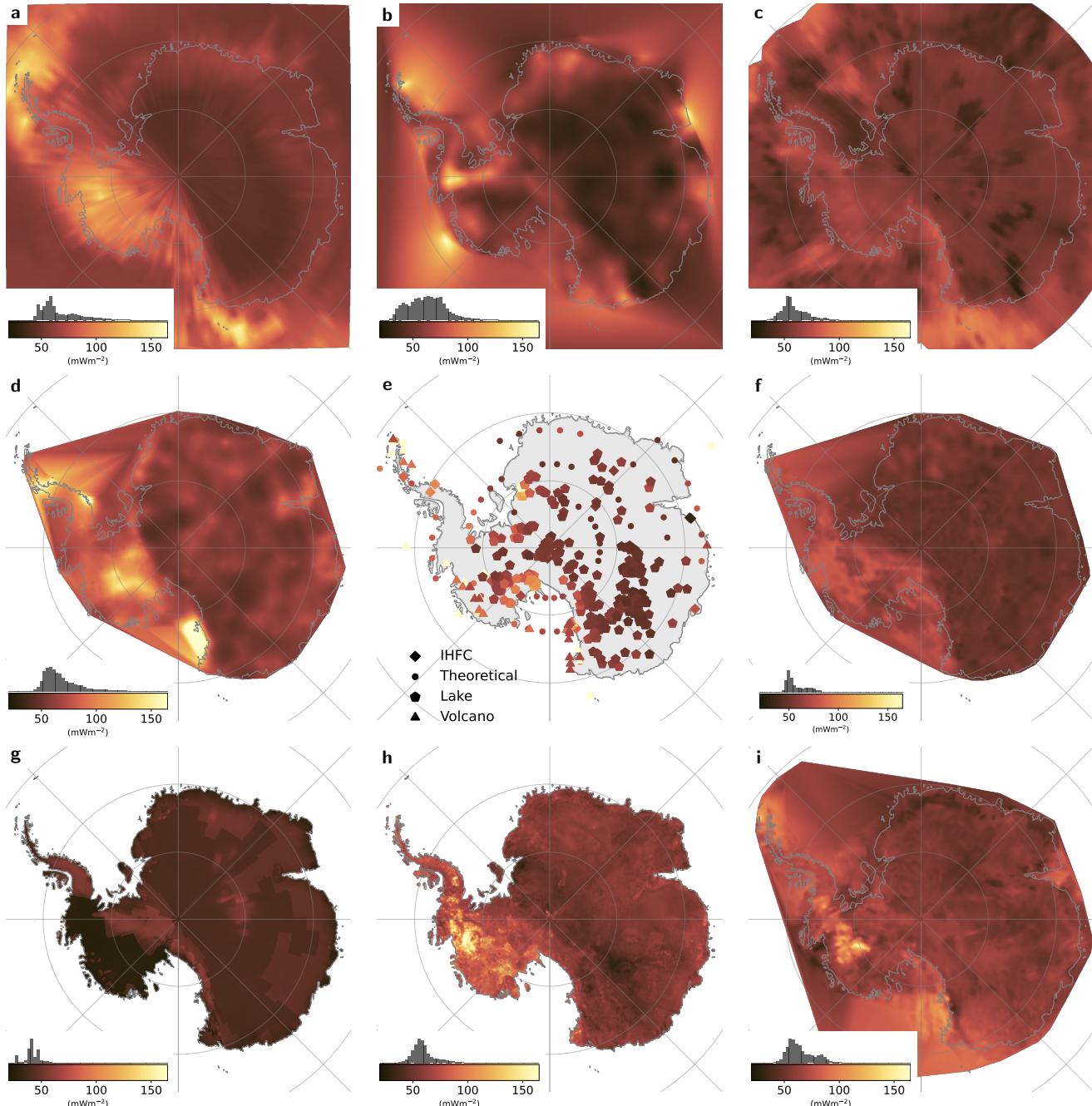
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Supplementary Note 1. Geothermal heat flow models (to date)

A near-comprehensive summary of existing geothermal heat flow models for the continent of Antarctica is provided (Supplementary Figure 1).



Supplementary Figure 1. Existing GHF models for Antarctica with available data shown at their full extent, using consistent colour scales. In order of publication: (a) SR04¹³ (b) FM05⁷⁵ (c) AW15⁷⁶ (d) MC17⁷⁴ (e) GV20¹⁷⁴ (f) SW20¹⁶ (g) AqSS²⁰ (h) Aq1¹⁷ (i) LE21¹⁸.

Supplementary Note 2. GHF methodology descriptions

In this supplement, we outline the methodology behind indirect geophysical methods of determining GHF (q , BOX 1, main text) that have been used to infer such models for Antarctica. While summary descriptions are given for several approaches (Supplementary Figure 2), we note that a previous review of wide scope¹⁵ outlined the forward modelling approaches. We therefore provide a more extended account of the methods behind empirical models not included therein (i.e. a similarity method, and a machine learning approach).

Forward modelling, magnetic data

Modelling GHF using magnetic data is based on constraining the temperature gradient below a given point on the Earth's surface. A point on the temperature gradient may be determined from magnetic data to yield the depth to the bottom of the magnetic source, or Curie Point Depth (CPD), together with the assumption that this depth corresponds to the temperature at which magnetite loses its magnetisation (580°C). The use of spectral analysis (as in MC17)⁷⁴ requires high resolution airborne data with sufficient cover. Also required is an estimate of spatially heterogeneous thermal properties (thermal conductivity k ; heat production A) derived from the geology of the crust, which may be accounted for in very low resolution by assigning different parameters to West and East Antarctica (WA and EA)⁷⁴. Using a different crustal component for WA and EA can result in an artificial contrast between those geographic domains.

An alternative method of inferring the CPD makes use of equivalent magnetic dipoles^{75,175}. The approach produces relatively robust results, and better correlation with observed heat flow⁷⁹. It is again necessary to account for the thermal properties of the crust. As an alternative to assigning average values for these properties, the assigned parameters may be tuned based on a stable continent (as in FM05), which accordingly emphasises those aspects of the tectonic setting in the resulting model.

While the uncertainty in fitting the spectra in the course of the magnetic data analysis can be quantified, methodological assumptions are not captured by that metric. Examples of such assumptions that merit consideration include: a) exactly how GHF relates to CPD, the relationship between these properties is assumed to be consistent, but in fact can vary quite considerably⁷⁸; and b) the impacts of the assumed or inferred crustal component on the model. A further point of discussion is how to handle the CPD when this is calculated as deeper than the Moho: either by limiting the CPD to the Moho depth, or adding the need to assign thermal properties (k, A) to the mantle. The lack of resolution in satellite data and/or the spectral gap to airborne data can also have an impact in sparsely surveyed locations.

Forward modelling, seismic data

Modelling GHF using seismic data is, once again, based on constraining the temperature gradient below a point on the Earth's surface⁷⁶. In the case of seismic wavespeed, a key point of reference is the depth of the lithosphere-asthenosphere boundary (1330°C). It is necessary to account for the thermal properties of the lithosphere above this point. When point locations are examined in forward models^{74–76}, unrealistic thermal gradients at depth can be implied²⁰. Generally; compared with observables derived from magnetic data, those derived from seismic data show a significantly better direct correlation with observed heat flow in global compilations^{11,17}.

Empirical, seismic data

Seismic observables may also be used as an empirical constraint on GHF. Broadly speaking, this is a successful approach because seismic observables allow material properties to be inferred that combine numerous features of the tectonic setting. The first such study, SR04¹³, made use of a global seismic model to assign GHF values to locations in Antarctica using a similarity approach. In a later study, SW20¹⁶, a high quality reference dataset from the US is employed to assign GHF values from the 0.5% structurally most similar grid cells to Antarctica. In the latter case, where similar tectonic settings exist in the US model, the resulting model is likely to be of high quality. Some tectonic settings are missing, however, so the model should be used accordingly.

Empirical, multivariate data

An empirical, similarity approach is used to assign values to the model Aq1¹⁷ in a refinement of the method developed for global studies^{11,27}, with consideration thus given to matching the reference global datasets to lower-resolution or otherwise problematic Antarctic datasets using multiple observables. This approach has the advantage of not relying upon the determination of a thermal gradient, nor upon the direct application of an assumed lithosphere or crustal model. The main shortcomings of empirical, multivariate approaches are that they depend on comparability between reference and target observables, and the representation of tectonic settings contained within the global heat flow catalogue¹².

Some datasets have a distinct correlation with GHF in themselves^{11,17} while others have little direct correlation, but contribute information to the multivariate determination of the tectonic setting. All observables are equally weighted in Aq1 (weighting was tested using Monte Carlo method, and it was found that optimal misfit in LOOCV, 'leave out one cross-validation', was produced with all observables weighted to 1: Fig. S4 in ref.¹⁷). The refined similarity method used to produce

Aq1 does not operate according to 'one dataset, one vote', hence, there is no concern if some observables are not independent (for example seismic wavespeed, and depth to seismic Moho). Additional datasets add stability to the distribution of GHF values and the resulting model.

To constrain the match of the tectonic setting to the GHF value, Aq1¹⁷ includes information such as the magnetic and seismic datasets used in the forward modelling, tectonic regionalisation⁹⁰, geological components through lithology reduced to 14 classes, computed heat production values³¹ with the weight decreased with the distance from the sample analysed, the distance-to-volcano observable from the global catalogue⁸⁹) and suggested subglacial volcanoes¹⁰⁹ with certainty above 2.5/5. Aq1 was tested excluding the volcano observable and some seismic observables, and the difference is within uncertainty for Aq1 (Fig. S14 in ref.¹⁷). The similarity method is not likely to introduce artifacts to the resulting model, however, the stability comes with the price of relatively large uncertainty range. The resolution depends on the weights of all observables in each location, themselves often varying depending on data density. High GHF locations of relatively small spatial extent could be missed in the Antarctic interior. This is almost certainly the case for large areas in East Antarctica.

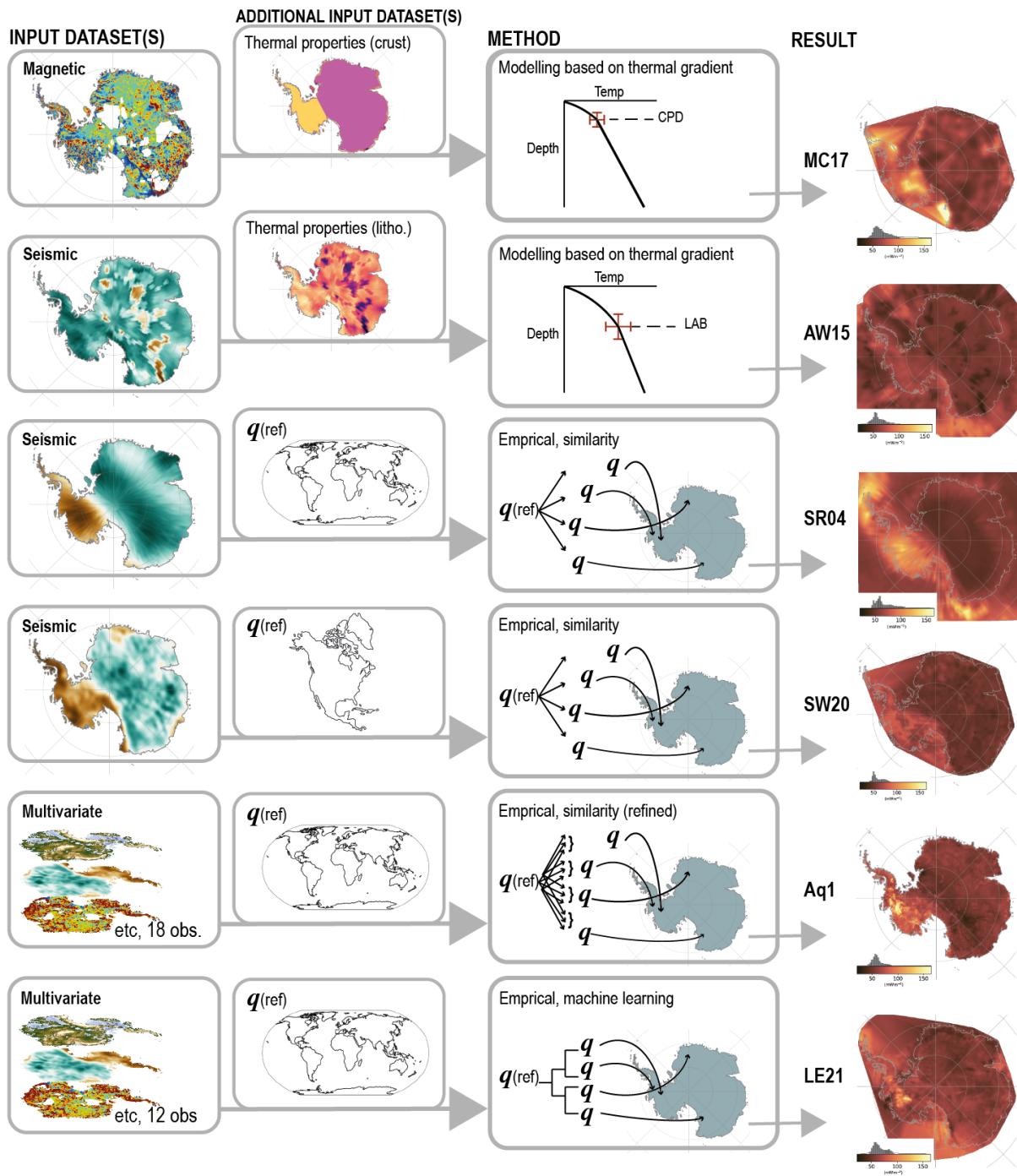
Taking the example of the Thwaites Glacier region, the multiple datasets jointly suggest a match between tectonic settings that have elevated GHF values elsewhere. In this complex region, multiple tectonic settings have an impact on the final model. a) Crustal thinning, by whatever mechanism (including rapid glacial erosion) steepens the thermal gradient, and the cooling of the mid and lower crust is observed as elevated heat flow. b) Topographic troughs focus heat if heat is removed from the through, or, the thermal conductivity of the trough is higher than the ridges. c) In the case of fast-flowing glaciers, heat is efficiently removed by subglacial hydrology and ice. The combination of observables points toward tectonic regions of the world with active tectonism and elevated heat flow. Notably, Aq1 does not predict extreme GHF values associated with glaciers in East Antarctica with deep troughs (e.g. Denman Glacier) in the elevation model used, Bedmachine⁶⁷. It is likely that all three mechanisms contribute to the elevated values observed for the Thwaites Glacier, in general agreement with conclusions drawn from airborne geophysical data in higher resolution studies^{46,72}.

Empirical, machine learning

A comparable, though not identical, smaller collection of datasets is used to define LE21 using a machine learning approach to predict GHF values for matching tectonic location in Antarctica from global datasets¹⁸. Geological contributions are included in the form of maps of volcanoes and recent rifting. In this study, a gradient boosted regression tree algorithm is used, the goal of which is to find a decision tree that best fits the training data and target values, subject to review through the optimisation of an objective function. The importance of an individual dataset for the model is calculated for every tree and subsequently averaged over the whole. The reduction of uncertainty of the target values provided by each attribute split point is calculated, weighted by the number of observations in the respective node. Consequently, a dataset becomes more important when it is essential for reducing the loss function (a term in the objective function) and, therefore, contributes to improving the prediction model. Reducing the number of strongly correlated features is, therefore, essential for a sensible analysis. LE21 has a narrower range in quantified uncertainty, in comparison to the relatively large quantified uncertainty of Aq1, but can be more subject to the choice of included datasets. Tests carried out in course of generating LE21 find that proximity to volcanoes, Moho thickness, distance to trenches and LAB are observables that significantly improves the predictions of heat flow. Magnetic properties and topography have lower impact.

Future directions in geophysical models

While GHF models of Antarctica derived from forward modelling and empirical approaches have all made contributions to progressing the field with the goal of improving our knowledge of the spatial variation of this property in Antarctica, and its implications, they differ in their capacity for further improvement. Forward models that make use of the relationship between GHF and CPD are fundamentally limited on a continental scale because of the potential for variation in this underpinning assumption. Using high-resolution airborne magnetic data to constrain GHF over a limited area^{47,72} has ongoing potential provided further information is known to provide context to that key underpinning assumptions, noting that contributions of the crustal component still need to be incorporated in a well-posed way. Empirical models of GHF have great potential for ongoing improvement. Hybrid models that reduce uncertainty by incorporating constraints from forward models (for example, the upper range of steady state heat transfer) into an empirical model can also be considered.



Supplementary Figure 2. Comparison of methods used to determine GHF for Antarctica. q = geothermal heat flow; CPD = Curie Point Depth; LAB = Lithosphere-Asthenosphere boundary. Graphical representations of datasets and models are indicative.

Supplementary Note 3. Model uncertainty

Best practice in the display of mapped physical properties includes provision of uncertainty bounds on the model result values. Maps displayed in the main text (FIG. 3 and 4) aim to separate some of the contributions to the total geothermal heat flow (GHF) model value (of Aq1¹⁷) through subtracting a reference steady state model value (AqSS²⁰). Both these models have associated uncertainties, and therefore the difference between the models (Aq1 - AqSS) is shown together with the minimum and maximum model differences.

Quantified uncertainty

Quantified uncertainty is an inherently useful concept¹⁰³, in that it highlights which parts of a model are better defined, given the modelling approach together with any parameter choices, and the interplay of these decisions with the input datasets. Further, it points to which parts of a model most merit (for example) further data collection or analyst review. This uncertainty is defined differently according to the inference technique that is employed to produce the model. The uncertainty range associated with Aq1¹⁷ and SW20¹⁶ is the standard deviation of the similar reference heat flow distribution calculated for each grid cell. Alternative metrics to quantify uncertainty have been proposed¹⁰⁴, and include information entropy. This metric may be calculated for the similarity distribution¹⁷ and combined metrics may also be informative. The uncertainty of AqSS is defined from the heat production ranges for each suggested crustal age^{20,105}. Uncertainty in LE21 is defined from the maximum absolute difference between produced prediction models¹⁸.

Unquantified uncertainty

Sources of unquantified uncertainty, in the case of GHF originates from modelling choices, the characteristics of input datasets, and the interplay of factors between or within these categories. The global datasets for GHF, as used for Aq1 and LE21, are improving with time but are likely to retain some old and uncertain measurements, and sampling biases to some regions, geological, and topographic settings. The US dataset used to infer SW20 has a more consistent quality than the global dataset, but less comprehensive in terms of sampled tectonic settings. As GHF is inferred indirectly, and is controlled by multiple different mechanisms, in some cases it remains open to discussion how well the datasets represent such mechanisms (main text FIG. 5b). Understanding such unquantified sources of uncertainty explains the patches of disagreement between the selected models in Supplementary Figure 1.

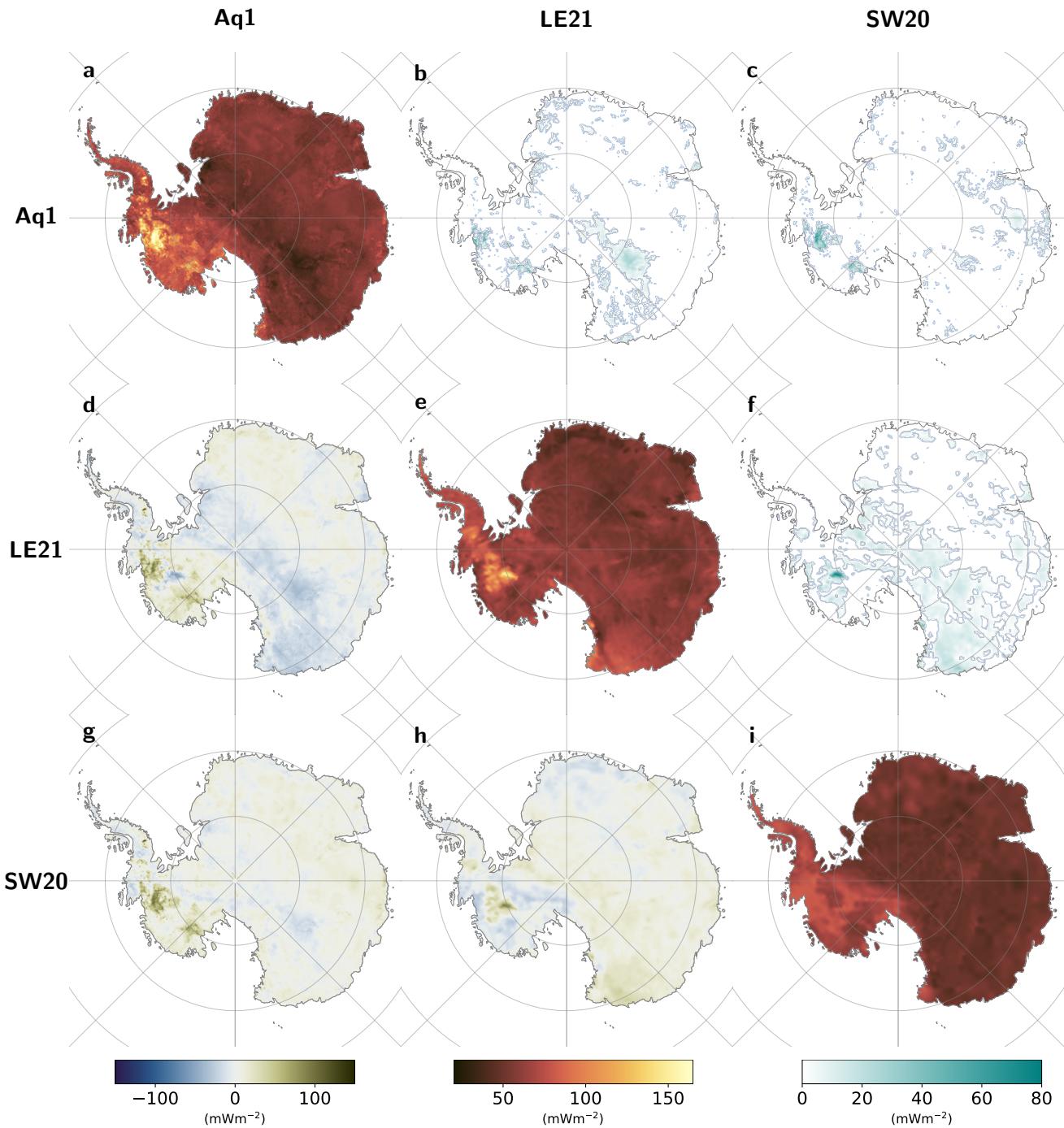
As an illustrative example, both Aq1 and LE21 are likely to capture the crustal contribution reasonably well, since they use extensive global datasets as a reference to assign their given values. SW20 is likely to give better constrained results, including the crustal component, where the tectonic setting is captured in the US dataset, but some tectonic settings are less well represented, or unrepresented. As a second example, Aq1 has (from the modelling choices made, in most areas) a higher quantified uncertainty and less impact on the choice of input datasets whereas LE21 has lower quantified uncertainty but the impact of the choice of input data is greater. In general, most GHF model results are presented together with a transparent appraisal of quantified and unquantified uncertainty, but such information can be difficult to interpret by subsequent users of the model.

GHF model comparisons

A comparison of GHF models of Antarctica, inferred using empirical techniques, is shown by maps of model difference values (Supplementary Figure 3 d,g,h). A remarkable level of agreement between the three models exists, as the difference maps show values close to zero in all but a few locations. The spatial extent of regions where unquantified uncertainty represents a significant component of the difference between the models is illustrated by showing the spatial distribution of the disagreement metric calculated as follows:

$$a = |M_1 - M_2| - \frac{\varepsilon_1 + \varepsilon_2}{2}$$

where M_1 and M_2 are two model values, ε_1 and ε_2 are uncertainties. Negative values indicate that the models agree (the joint uncertainty is larger than the disagreement; Supplementary Figure 3b,c,f shown together with zero values as unshaded regions of the continent) while a positive value indicates that the disagreement is larger than the defined uncertainty (cyan shading, showing level of disagreement). The most notable region of model disagreement between Aq1 and LE21 (Supplementary Figure 3b) is the elevated subglacial topography that separates the Wilkes and Aurora Subglacial Basins. The regions of most notable model disagreement between Aq1 and SW20 (Supplementary Figure 3c) are the Byrd Subglacial Basin, and Ross Province, of the West Antarctic rift. LE21 and SW20 show extensive regions in apparent (slight) disagreement, which largely relate to their respective unquantified uncertainty.



Supplementary Figure 3. Comparison of Antarctic GHF models (selected, based on empirical methods). The panels show GHF models, difference between models, and the relation between difference between models and their uncertainty. (a) Aq1¹⁷, (b) Disagreement Aq1 and LE21, (c) Disagreement Aq1 and SW20, (d) Difference Aq1 - LE21, (e) LE21¹⁸, (f) Disagreement LE21 and SW20, (g) Difference Aq1 - SW20, (h) Difference LE21 - SW20, (i) SW20¹⁶. Subplots b,c and f show disagreement taking into account the model uncertainty; $|M_1 - M_2| - (\varepsilon_1 + \varepsilon_2)/2$. A positive residual value (shaded) indicates model disagreement beyond the provided uncertainty, the contour (blue-grey) shows where model disagreement equals the provided uncertainty, and negative values (unshaded) show where the models agree, that is the disagreement lies within the provided uncertainty metrics.

Supplementary Note 4. Supporting information for main text FIG. 5

The indicative relationship between the scale length of GHF anomalies and the potential contribution (positive or negative) to observed GHF for the given sources can be compared to the frequency power spectra of selected GHF models (main text FIG. 5). This indicative comparison shows which mechanisms can potentially be captured by the spatial resolution of each the approaches used. This analysis contain inherent assumptions and simplifications (Supplementary Note 2, main text TABLE 1).

Calculation of contribution to GHF

The heat flow range associated with the impact of each source is derived from a linear regression of the cross correlation as used in Aq1¹⁷. The topographic factor is derived from numerical analysis of topography and shallow temperatures³⁸ and is in agreement with analytical approaches³⁷. The range of values assigned for neotectonism is indicated by comparative studies¹⁵⁵. The scale length for each contribution is indicative, and derived from a number of studies^{15, 17, 44, 102, 155–157, 180}. The ranges are estimates of how much each contribution can affect the observed heat flow. For example, shallow ground water can disperse heat from deeper sources, land forms can converge or diverge heat depending on how the isotherms relates to the surface.

Calculation of spectral content of GHF models

The spectral content of the GHF models (main text FIG. 5) is calculated as follows. All models are re-sampled with bilinear interpolation to a 5×5 km regular grid, and for consistency between models, clipped at present coastline and grounding line. Every second row (X axis) is reversed, and the 2D array is converted to 1D time series. The power spectra is calculated using Welch's spectral density estimation separately for X, and Y axis, and normalised to the mean value for each model. This approach somewhat distorts models that include the continental shelf.