A Reappraisal of the H- κ Stacking Technique: Implications for Global Crustal Structure

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¹ Summary

H- κ stacking is used routinely to infer crustal thickness and bulk-crustal V_P/V_S ratio from teleseismic receiver 10 functions. The method assumes that the largest amplitude P-to-S conversions beneath the seismograph station 11 are generated at the Moho. This is reasonable where the crust is simple and the Moho marks a relatively abrupt 12 transition from crust to mantle, but not if the crust-mantle transition is gradational and/or complex intra-crustal 13 structure exists. We demonstrate via synthetic seismogram analysis that H- κ results can be strongly dependent on 14 the choice of stacking parameters (the relative weights assigned to the Moho P-to-S conversion and its subsequent 15 reverberations, the choice of linear or phase-weighted stacking, input crustal P-wave velocity) and associated data 16 parameters (receiver function frequency content and the sample of receiver functions analyzed). To address this 17 parameter sensitivity issue, we develop an H- κ approach in which cluster analysis selects a final solution from 18 1000 individual H- κ results, each calculated using randomly-selected receiver functions, and H- κ input parameters. 19 Ten quality control criteria that variously assess the final numerical result, the receiver function dataset, and the 20 extent to which the results are tightly clustered, are used to assess the reliability of H- κ stacking at a station. 21 Analysis of synthetic datasets indicates H- κ works reliably when the Moho is sharp and intra-crustal structure is 22 lacking but is less successful when the Moho is gradational. Limiting the frequency content of receiver functions can 23 improve the H- κ solutions in such settings, provided intra-crustal structure is simple. In cratonic Canada, India and 24 Australia, H- κ solutions generally cluster tightly, indicative of simple crust and a sharp Moho. In contrast, on the 25 Ethiopian plateau, where Paleogene flood-basalts overlie marine sediments, H- κ results are unstable and erroneous. 26 For stations that lie on thinner flood-basalt outcrops, and/or in regions where Blue Nile river incision has eroded 27 through to the sediments below, limiting the receiver function frequency content to longer periods improves the 28 H- κ solution and reveals a 6–10 km gradational Moho, readily interpreted as a lower-crustal intrusion layer at the 29 base of a mafic $(V_P/V_S=1.77-1.87)$ crust. Moving off the flood-basalt province, H- κ results are reliable and the 30 crust is thinner and more felsic $(V_P/V_S=1.70-1.77)$, indicating the lower crustal intrusion layer is confined to the 31 region covered by flood-basaltic volcanism. Analysis of data from other tectonically-complex settings (e.g., Japan, 32 Cyprus) shows H- κ stacking results should be treated cautiously. Only in regions of relatively simple crust can H- κ 33 stacking analysis be considered truly reliable. 34

35 2 Key Words

³⁶ Crustal imaging, Crustal structure, Cratons, Large igneous provinces, Statistical methods, Body waves, Ethiopia

37 **3** Overview

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The H- κ stacking technique (*Zhu and Kanamori*, 2000) is a widely-used method to obtain bulk-crustal information 38 from teleseismic receiver functions by searching for the combination of Moho depth (H) and V_P/V_S ratio (κ) 39 that maximizes the amplitude sum of P-to-S conversions from beneath a seismograph station. Central to the H- κ 40 method is the assumption that the Moho is the sharpest sub-station velocity contrast, and that it produces the largest 41 amplitude P-to-S conversions and reverberations in the receiver function (Figure 1a). Previous studies have reduced 42 the effect of noisy data in several ways: phase-weighted rather than linear stacking (Crotwell and Owens, 2005) and 43 varying the weighting of the Moho P-to-S conversion relative to subsequent reverberations (e.g., Eaton et al., 2006; 44 Thompson et al., 2010; Vanacore et al., 2013). Other studies have highlighted the importance of anisotropy (e.g., 45 Levin and Park, 2000) and back-azimuthal variations in crustal structure (e.g., Dugda et al., 2005) when interpreting 46 H- κ results. However, as far as we have been able to determine, very few studies have addressed the fundamental 47 question of whether H- κ stacking should be used at all in some complex tectonic settings. For example, in areas 48 where the crust-mantle transition is gradational (e.g., regions of lower-crustal intrusions (Mackenzie et al., 2005), or subduction zones (Bostock et al., 2002)). Moho P-to-S converted energy will have low-amplitude (e.g. Gallacher 50 and Bastow, 2012) (Figure 1b). In such settings, H- κ stacking will only be sensitive to the Moho using longer period 51 receiver functions (e.g. Frassetto et al., 2011). Where complex shallow crustal structure exists, significant P-to-S 52 converted energy may mask signals from the Moho (Figure 1c). In such scenarios, the fundamental single-layer over 53 a half-space assumption that underpins $H-\kappa$ stacking breaks down. 54

Figure 1

here

In this contribution, we first take a forward modelling approach to exploring the sensitivity of H- κ stacking to 56 complex crustal structure. We examine the impact of varying the H- κ stacking input parameters, including the 57 relative weights assigned to the Moho Ps arrival and its subsequent crustal reverberations, the style of stacking 58 employed (linear versus phase-weight), and the *a priori* choice of crustal P-wave velocity. We also test how the 59 frequency content of the receiver functions can be used to ascertain whether a station is underlain by a sharp 60 or gradational Moho. We then develop a cluster analysis approach to H- κ stacking that rigorously explores its 61 parameter space, including the frequency content of the receiver functions. In doing so, we assign a score to each 62 station using ten criteria that variously assess data signal-to-noise ratio, the ability of a single pair of H and κ values 63 to explain the observations for a given station, and the likelihood that the Moho is gradational rather than sharp. 64 We test our new method on multiple synthetic datasets and several tectonic settings worldwide. While the 65 $H-\kappa$ method can often yield accurate bulk-crustal information in regions of simple crustal structure, it can fail 66 completely in regions where these conditions are not met. Our new approach can provide the analyst with a strong 67 indication for why the H- κ method fails in certain tectonic settings. In such circumstances, more sophisticated 68

⁶⁹ seismological inversion techniques are thus required, such as joint-inversion of receiver functions with surface waves

⁷⁰ for 1D structure beneath the station (e.g. Julià et al., 2009; Gilligan et al., 2016) or Markov Chain Monte Carlo

⁷¹ receiver function analyses (e.g., *Piana Agostinetti and Malinverno*, 2010; Wirth et al., 2016).

⁷² 4 Review of Receiver Functions and H- κ Stacking

Receiver functions are time-series calculated from three component seismograms that capture *P*-to-*S* conversions from velocity discontinuities below a seismograph station (e.g., *Langston*, 1979). The H- κ stacking technique (*Zhu and Kanamori*, 2000) utilizes the arrival times of the converted Moho arrivals *Ps*, *PpPs*, and *PsPs*+*PpSs* (Figure 1a) to determine H and κ , using a grid-search of the plausible H and κ values to maximize the amplitudes of the three phases and therefore maximize the stacking function of the linear 'stack', $s(H, \kappa)$:

$$s(H,\kappa) = \sum_{j=1}^{N} w_1 r_j(t_1) + w_2 r_j(t_2) - w_3 r_j(t_3),$$
(1)

⁷⁸ where w_1, w_2, w_3 are stacking weights (satisfying $\sum w_i = 1$) that govern the influence of each converted phase. ⁷⁹ $r_j(t_i)$ are the receiver function amplitudes at the predicted arrival times of the direct *P*-to-*S* conversion (*Ps*) and ⁸⁰ subsequent reverberations (*PpPs* and *PsPs* + *PpSs*) respectively for the *j*th receiver function. *N* is the number of ⁸¹ receiver functions stacked to improve the signal-to-noise ratio. In this study, the $s(H, \kappa)$ grid-search is performed ⁸² using 100 values of both H and κ . The predicted travel times for each phase, t_i are given by Equations 2–4.

$$t_1 = H\left[\sqrt{\frac{1}{V_S^2} - p^2} - \sqrt{\frac{1}{V_P^2} - p^2}\right],$$
(2)

$$t_2 = H\left[\sqrt{\frac{1}{V_S^2} - p^2} + \sqrt{\frac{1}{V_P^2} - p^2}\right],\tag{3}$$

$$t_3 = 2H\sqrt{\frac{1}{V_S^2} - p^2},\tag{4}$$

where p is the ray parameter.

Phase-weighted stacking (PWS) has been used to reduce the affect of incoherent noise (*Schimmel and Paulssen*, 1997). This is particularly important where Moho signals are weak owing to complex Moho and crustal structure (e.g. *Crotwell and Owens*, 2005). PWS modulates the linear stack with the coherency (c) of the instantaneous phases for each receiver function (Equation 5), amplifying coherent signals but damping incoherent noise,

$$c(H,\kappa) = \frac{1}{N} \sum_{j=1}^{N} \frac{\sum_{k=1}^{N} e^{i} \Phi(t_k)}{3},$$
(5)

where Φ is the instantaneous phase at time t. Values of c range from 0–1 with 0 representing incoherent stacking and 1 representing a completely coherent stack (*Schimmel and Paulssen*, 1997). This is applied to the linear stack as follows:

$$s(H,\kappa) = c^{\nu} \sum_{j=1}^{N} w_1 r_j(t_1) + w_2 r_j(t_2) - w_3 r_j(t_3),$$
(6)

where ν controls the sharpness of the PWS filtering. The linear stack is retrieved if $\nu = 0$, $\nu = 2$ represents PWS.

Stacking weights (w_1, w_2, w_3) are often picked on the assumption that Ps is the highest amplitude and clearest 93 arrival and so should have highest weight; PpPs and PsPs + PpSs are lower amplitude so are generally assigned 94 lower weights in the literature (e.g., Eaton et al., 2006). However, consensus on which values should be used is 95 lacking. The stacking weights are often assigned in a 0.6:0.3:0.1 ratio or similar (e.g. Dugda et al., 2005; Thompson 96 et al., 2010; Vanacore et al., 2013) but the precise choice is usually somewhat ad hoc. For H- κ stacking, P-wave 97 velocity (V_P) is held constant for the whole crust and has to be known a priori or assumed. V_P is often unknown 98 outside areas studied by wide-angle seismic reflection/refraction (e.g., Mackenzie et al., 2005) so the resulting qq uncertainties in H and κ must be borne in mind. Specific H- κ stacking input parameters are the input V_P, the 100 stacking weights $(w_1, w_2 \text{ and } w_3)$ and the type of stacking applied (linear or phase-weighted). Additionally, the 101 receiver function frequency content and the subset of receiver functions for a given station used in H- κ analysis are 102 data parameters that can be varied during H- κ stacking analysis. 103

Previous studies have calculated measurement errors using the shape of $s(H,\kappa)$ (e.g. *Zhu and Kanamori*, 2000; *Eaton et al.*, 2006), however, *Crotwell and Owens* (2005) found this sometimes produced implausibly low errors. Instead, they used a bootstrapping algorithm that resampled the receiver functions multiple times for a given station and used the associated standard deviations in H and κ as error estimates. We calculate both dataset derived and $s(H,\kappa)$ derived errors in this study. We require measurement errors in both H (Equation 7) and κ (Equation 8) for each H- κ stacking attempt, which are calculated using the maximum bounds of the 95% contour of $s(H,\kappa)$ (Figure 2). The generally elliptical nature of the contour provides an uncertainty about the exact $s(H,\kappa)$ maxima. A tighter peak, resulting from a more certain stack will therefore have a smaller 95% contour, and smaller errors.

$$H_{error} = \frac{(Upper H 95\% \, contour - Lower H 95\% \, contour)}{2},\tag{7}$$

$$\kappa_{error} = \frac{(Upper \,\kappa\,95\%\,contour - Lower \,\kappa\,95\%\,contour)}{2}.$$
(8)

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To address the issue of noise in receiver functions and to quantify the extent to which a receiver function carries information that cannot be described by a single layer over a half space, we introduce the Amplitude Comparison Estimate (ACE), the signal-to-noise ratio (SNR) and cross-correlation coefficient (CCC) measures. ACE (Equation 9) compares the amplitude at the predicted t_1 arrival time for each receiver function, assuming that H- κ stacking has correctly identified the Moho Ps arrival, with the root mean square (RMS) amplitude of the receiver function between $t_1 + 2s$ and $t_2 - 2s$ (Figure 3).

$$ACE = \frac{1}{N} \sum_{j=1}^{N} r_j(t_1) \left(\frac{\sum_{t=t_{1+2s}}^{t_{2-2s}} r_j(t)}{rate(t_{2-2s} - t_{1+2s}) + 1} \right)^{-\frac{1}{2}},\tag{9}$$

where rate is the sample rate of the receiver function $(r_i(t))$. A simple layer over half-space model with a sharp 119 Moho theoretically has a larger amplitude Ps phase compared to the general signal of the receiver function. A 120 gradational Moho produces a lower amplitude Ps phase than a sharp Moho, and thus a lower ACE. Similarly, a 121 model with complex intra-crustal structure will have additional P-to-S conversions between $t_1 + 2s$ and $t_2 - 2s$, 122 that lower the ACE. Using the predicted t_1 time from the chosen final H- κ solution, ACE becomes a measure of 123 how prominently the Ps arrival stands out from the rest of the receiver function. The SNR (Equation 10) compares 124 the amplitude of the predicted Ps phase (defined by the H- κ solution for that station) with the RMS amplitude 125 of 8s of pre-P arrival noise (Figure 3). A larger Ps amplitude, indicative of a sharper Moho, will produce a larger 126 SNR than for a gradational Moho. 127

$$SNR = \frac{1}{N} \sum_{j=1}^{N} r_j(t_1) \left(\frac{\sum_{t=t_{P-10s}}^{t_{P-2s}} r_j(t)}{rate(t_{P-2s} - t_{P-10s}) + 1} \right)^{-\frac{1}{2}}.$$
 (10)

Finally, the CCC tests the effect of noise and back-azimuthal variations at a station by measuring the mean

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¹²⁹ cross-correlation coefficient of all possible pairs of receiver functions calculated with the same frequency, for each ¹³⁰ different frequency of receiver function. Stations with highly correlated receiver functions will yield more stable H- κ ¹³¹ estimates. These three receiver function analytics (ACE, SNR and CCC) supplement the overall stacking approach ¹³² from Equations 1 or 6 by providing direct information about how the final H- κ solution relates to the receiver ¹³³ functions used in the stack.

Figure 3

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¹³⁵ 5 The Sensitivity of H- κ Solutions to Input Parameter Selection

To determine the effect of varying each H- κ input (V_P, w_1 , w_2 , w_3 and stacking type) and data (receiver function 136 frequency content and the subset of receiver functions chosen) parameter on the final result, we conduct tests 137 using synthetic receiver functions which represent a variety of tectonic scenarios. Synthetic seismograms for flat 138 layered models are generated using the ray tracing program respknt (Randall, 1989) with a one second Gaussian 139 pulse and no noise added to demonstrate the purely seismological challenges that complex structures present during 140 H- κ stacking. To test the effect of crustal anisotropy and a dipping Moho, we calculate seismograms using the 141 raysum method of Frederiksen and Bostock (2000). Horizontal component seismograms are rotated into radial and 142 tangential components and receiver functions are computed using the Extended-Time Multitaper Frequency Domain 143 Cross Correlation Receiver Function Estimation method (ETMTRF, Helffrich, 2006). ETMTRF computes receiver 144 functions using a low-pass \cos^2 taper with the maximum frequency chosen by the user. We automatically set the 145 receiver function window as 10s before the P-arrival, and 100s after the P-arrival. Other receiver function calculation 146 strategies exist (e.g. Langston, 1979; Ligorria and Ammon, 1999; Park and Levin, 2000) and, for moderate-to-high 147 quality seismograms they yield similarly robust results (Rondenay et al., 2016). 148

We present a sharp Moho model with an abrupt V_P change from mantle (8.0 km/s) to continental crust (6.5 km/s) (Figures 4a, 4c and 6a). The second model replaces the sharp Moho with a gradual velocity change over a depthrange of 15 km represented by a series of finite steps (Figures 4b, 4d and 6g). Conceptually, the steps represent

a zone of lower crustal mafic intrusions (e.g., Mackenzie et al., 2005). In each test, H- κ input parameters are 152 varied systematically between plausible limits defined in Table 1, with only one parameter varied for each test 153 while the rest remain constant. We test the effect of stacking weights but retain the limit $w_3 \leq 0.5$ in line with 154 the observation that PsPs + PpSs is usually a low amplitude signal compared to Ps. w_1 and w_2 in most cases 155 will thus have highest weights. However, we do test the effect of w_3 having the largest weight to allow thorough 156 examination of the parameter space. This encompasses tectonic scenarios where, for example, dipping layers may 157 produce larger PsPs + PpSs conversions than PpPs (Frederiksen and Bostock, 2000). Because $\sum w_i = 1$, two of 158 the stacking weights must change synchronously in the weight tests; 21 combinations of the stacking weights satisfy 159 this condition. V_P is varied since it is often unknown a priori. To identify the influence of linear stacking and 160 PWS, we re-run all the tests for both stacking strategies. Finally, previous studies have varied receiver function 161 frequency content to investigate Moho sharpness (e.g. Frassetto et al., 2011), so we test this also. Lower frequencies 162 are required to detect a gradational Moho to which higher frequency H- κ analysis is blind. 163

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For the sharp Moho model (Figures 4a and 4c), the final H- κ solution is independent of frequency and stacking weights, and the grid-search reliably returns the correct H- κ solution for both stacking types. For the gradational model (Figures 4b and 4d), the final result is highly dependent on the choice of both input and data parameters, and the input model is not identified correctly. For both models, as V_P increases, H increases and κ decreases systematically: a 0.1 km/s change in V_P translates to a ~0.71 km variation in H and a ~0.002 change in κ . Table 1 h

Figure 4

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Figure 4 demonstrates that the H- κ input parameters can dictate the H- κ solution obtained; it also indicates 171 that the frequency content of receiver functions influences the H- κ solutions. To ascertain if receiver functions 172 can resolve a crust-mantle boundary that is manifest over an increasingly larger depth range, we produce a suite 173 of synthetic models with Moho thicknesses ranging from 0 km to 15 km. In each model, the crustal V_P and V_S 174 transition towards mantle values over a series of small steps to simulate a gradient; crustal V_P/V_S is 1.765 in 175 all models. If H- κ stacking is reliable for a model, it will identify the centre of the Moho depth range (40 km) 176 successfully. From the sharp Moho synthetic tests (Figures 4a and 4c), a 6.2-6.8 km/s change in V_P produced 177 ranges of 4.2 km and 0.013 in H and κ , respectively. Accounting for the individual measurement errors of those H 178 and κ solutions, all subsequent H- κ solutions are expected to fit within the H range 37.1–42.9 km and the κ range 179 1.723 - 1.807.180

For each Moho model we sample the H- κ stacking input and data parameters randomly and repeat 1000 times (according to parameter ranges defined in Table 1). In each test, 80% of the available synthetic receiver functions are selected randomly with no duplicates. Each of the 21 possible combinations of stacking weight has an equal

chance of selection. We extract the H- κ stacking solutions and their associated measurement errors for each receiver 184 function frequency value separately and determine how many individual solutions for that frequency fit within the 185 aforementioned ranges of H and κ . The percentage of solutions within these limits for each Moho thickness/frequency 186 combination are shown in Figure 5. When the Moho thickness is $\leq 5 \, \mathrm{km}$, all frequencies identify the input model 187 correctly. For Moho thicknesses ≥ 14 km, H- κ stacking fails across all frequencies. At intermediate Moho thicknesses 188 (6–13 km), lower frequency receiver functions identify the Moho most consistently (Figure 5). The general decrease 189 in frequency required to accurately resolve a Moho of increasing thickness provides us with a useful, if imprecise, 190 proxy for diagnosing Moho architecture. 191

¹⁹³ We next examine two models with complex upper crustal structure, with a sharp (Figure 6g) and a gradational ¹⁹⁴ (Figure 6m) Moho, respectively. Both models fail at all frequencies, indicating that complex near-surface structure ¹⁹⁵ can preclude H- κ from working at all. Estimating Moho thickness by varying receiver function frequency content ¹⁹⁶ is thus only feasible when intra-crustal structure is relatively simple.

¹⁹⁷ Having demonstrated that full exploration of H- κ input parameter space, including the frequency content of ¹⁹⁸ the receiver function dataset, is essential for robust crustal study, we now seek a semi-automated means of (*i*) ¹⁹⁹ determining whether or not H- κ analysis works for a given station, and (*ii*) gleaning a preferred H- κ solution, where ²⁰⁰ appropriate.

²⁰¹ 6 Parameter Search Approach to H- κ Stacking

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²⁰² Our new approach to H- κ stacking repeats the standard H- κ method 1000 times per station, randomly selecting ²⁰³ input and data parameters each time. The challenge now is to obtain a preferred solution from this dataset in a ²⁰⁴ quantitative, semi-automated manner. To this end, we pursue a hierarchical cluster analysis (e.g. *Everitt et al.*, ²⁰⁵ 2001) approach. A methodological summary is documented by *Everitt et al.* (2001), and an analogous workflow to ²⁰⁶ ours is presented by *Teanby et al.* (2004). Appendix A provides a more detailed description of the mathematical 207 steps followed here.

Since H and κ have different orders of magnitude (20–55 km for H and 1.65–2.2 for κ), they are re-scaled between 208 0 and 1 using their respective ranges (Equations A1 and A2) to avoid the much larger Euclidean distances in H 209 dominating the clustering algorithm. We begin with N=1000 scaled H- κ solutions, and split the data into M 210 clusters, each containing one solution. The grid-search nature of H- κ stacking produces discrete data, which can 211 cause hierarchical clustering to falter (e.g. Teanby et al., 2004). To counter this, each initial cluster is assigned a 212 scaled numerical error in H and κ corresponding to the interval size of the grid-search with a value of 1/99 used 213 because 100 values of H and κ are used in the grid-search. The inter-cluster Euclidean distances are calculated for 214 all possible pairs of clusters and the closest two combined into one, reducing the number of clusters by one. The 215 number of points per cluster is calculated, alongside the mean centroid position of each cluster centre according to 216 Equations A3 and A4 for H and κ , respectively. Using the position of the newly merged cluster, Euclidean distances 217 are re-calculated between all remaining clusters and the process is repeated until one cluster of 1000 data points 218 remains. This produces the so-called hierarchical structure of clusters where the optimum number of clusters lies 219 between 1 and 1000 (Everitt et al., 2001). 220

²²¹ We desire a method to automatically choose the optimum number of clusters that best represents the 1000 ²²² individual H- κ measurements. There are several methods to achieve this (see *Milligan and Cooper*, 1985, for a ²²³ review) but the criteria of *Caliński and Harabasz* (1974) and *Duda et al.* (1973) are used here. Following *Caliński* ²²⁴ and Harabasz (1974):

$$c(M) = \frac{(N-M)trace(B)}{(M-1)trace(W)},\tag{11}$$

where *B* is the between-cluster covariance (Equation A6) and *W* is the within-cluster covariance (Equation A7), both calculated at each cluster step. When c(M) peaks, the between-cluster variance is maximized compared to the within-cluster variance indicating individual clusters are well spaced but that data points within each cluster are tightly distributed. The optimum number of clusters is therefore found when c(M) is a maximum. The criterion of *Duda et al.* (1973) uses the ratio of within-cluster variances before (σ_2^2 , Equation A10) and after (σ_1^2 , Equation A11) the clusters are combined into a single cluster, assuming the two clusters will always be combined into one. This is rejected when:

$$\left(1 - \frac{\sigma_2^2}{\sigma_1^2} - \frac{2}{\pi p}\right) \left(\frac{N_j p}{2[1 - 8/(\pi^2 p)]}\right)^{1/2} > c_{critical},\tag{12}$$

where p = 2 and is the number of parameters in the analysis, and $c_{critical} = 3.20$ and is the typical value assumed if the data points within a cluster are normally distributed (*Milligan and Cooper*, 1985). The optimum ²³⁴ number of clusters is found when Equation 12 is invalidated as the number of clusters is reduced progressively. ²³⁵ The criteria that produces the larger number of clusters is taken to be the optimum number of clusters, up to a ²³⁶ maximum M = 7; larger numbers are considered indicative of poor clustering (*Teanby et al.*, 2004).

With the optimum number of clusters calculated, the most representative cluster must be identified, from which 237 the final individual H- κ solution will be chosen. The within-cluster variance ($\sigma_{c_i}^2$, Equation A13) and error variance 238 $(\sigma_{d_j}^2)$, Equation A14) are calculated for all clusters with $N_j > 15$ (*Teanby et al.*, 2004). The within-cluster variance 239 measures cluster tightness; the error variance quantifies the measurement errors within each cluster. A diffuse 240 cluster with small individual measurement errors will have large within-cluster variance but small error variance; a 241 tight cluster with large measurement errors will have small within-cluster variance but large error variance (Teanby 242 et al., 2004). Clusters containing <15 data points are rejected because they could have un-representatively small 243 within-cluster variances (indicative of a tight cluster). We desire the cluster that optimizes these two variances. 244 The overall variance ($\sigma_{o_i}^2$, Equation A15) finds the maximum of the within-cluster variance and error variance for 245 each cluster with the best cluster having the minimum $\sigma_{o_i}^2$. From this cluster, we define the final H- κ solution 246 to be the measurement with smallest combined rescaled errors in H and κ . If the 1000 H- κ stacking solutions do 247 not form one cluster, H- κ stacking is not consistently identifying the Moho arrival and respective reverberations. 248 Multiple clusters result from arrivals from intra-crustal velocity discontinuities, particularly when the Moho arrivals 249 are indistinguishable from the trace (e.g. a gradational Moho). 250

The result for the sharp Moho synthetic model (Figures 6a-c) has all 1000 repeat solutions clustering tightly 251 around the true H and κ values. This is clear evidence that a sharp Moho is insensitive to changes in the H- κ input 252 parameters, and is therefore the ideal example of H- κ stacking. When a 3 km-thick surface layer of low velocity 253 sediment is added, H- κ still retrieves the input model, albeit with a larger spread of results (Figures 6d-f). Adding 254 a surface layer of higher velocity basalt above the sediment (Figures 6g-i) disperses the solutions, such that the 255 mean H and κ values no longer match the input model. This implies complex upper crustal structure can cause H- κ 256 stacking to fail. For the gradational model (Figures 6j-l), the results are dispersed into a much larger cluster and 257 $H-\kappa$ stacking fails to identify a single reliable answer. Furthermore, adding the high velocity basalt layer overlying a 258 low velocity sediment layer (Figures 6m-o), the results become further dispersed into a number of clusters indicating 259 a complete failure of H- κ stacking. The effect of 5% crustal anisotropy with fast axis directed northwards (with 0° 260 dip) is to again disperse the results (Figures S1a-c) but the input model is largely returned. A 15° dipping Moho 261 is also successful in identifying the Moho (Figures S2a-c). We thus demonstrate that only by varying the input 262 parameters of H- κ stacking can the reliability of the technique be truly tested. This is not possible to detect when 263 only one set of parameters are chosen and the method performed using these alone. 264

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We characterize and visualize the overall quality of a station using ten pass/fail criteria (where C is the number 266 of passed criteria) (Table 2) and a diagnostic result figure (e.g. Figure 7). Criteria 1 and 2 assess the numerical 267 quality of the final H- κ solution, which are failed respectively if the solution lies on the edge of the H- κ grid space, 268 and if errors exceed $\pm 2.5 \,\mathrm{km}$ in H (defined by the resolvable Moho thickness in Figure 5) and ± 0.042 in κ (limit 269 defined by the sharp Moho synthetic test in Figure 4). Criteria 3, 4, and 6 assess how well clustered the solutions 270 of the 1000 H- κ repetitions are. Criteria 5, 7, and 9 analyze the receiver functions directly and assess whether or 271 not the Ps phase and its reverberations are impulsive in nature. Criteria 8 assesses whether the receiver functions 272 are coherent, or reflective of a noisy dataset and/or strong back-azimuthal variations in crustal structure. Criteria 273 10 compares linear and phase weighted stacking H- κ strategies. 274

A seismograph station that overlies a sharp Moho, with no near surface structure and little back-azimuthal variation, passes ≥ 9 of the criteria, indicating a successful H- κ stacking result from which bulk crustal properties can be reliably inferred. Stations passing <6 criteria have an unreliable H- κ result and their results should not be trusted. Stations with an intermediate number of passed criteria must be analyzed carefully to ascertain result reliability prior to interpreting Moho depth and V_P/V_S ratio.

In the event that criteria are failed solely because the Moho below a given station is gradational, not sharp, 280 we next investigate if the frequency content of the receiver functions can be limited to improve the H- κ solutions 281 at stations that previously failed. We detect the frequency above which the H- κ solutions start to disperse. The 282 maximum frequency is chosen to be the one above which the standard deviation of the solutions exceed 2.5 km in H 283 or 0.042 in κ . The cluster analysis is then repeated using only the longer-period solutions, removing the solutions 284 calculated using higher frequency receiver functions (identified as causing H- κ stacking failure in Figure 5). Limiting 285 the analysis to longer-period data may resolve a gradational Moho, but will not necessarily improve the solution 286 when complex intra-crustal structure exists (e.g. Figures 6g and 6m). In such instances, it is recommended that 287 the analyst pursue more sophisticated analysis techniques such as Markov Chain Monte Carlo receiver function 288 analysis (e.g., Piana Agostinetti and Malinverno, 2010; Wirth et al., 2016) or 1D joint inversions of surface waves 289 and receiver functions (e.g. Julià et al., 2009; Gilligan et al., 2016). We next examine the applicability of our new 290 H- κ strategy to a number of tectonic settings worldwide. 291

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²⁹³ 7 Data Processing

We extract three-component seismograms from the IRIS and ORFEUS data centres for all $mb \ge 5.5$ teleseismic 294 earthquakes listed in the NEIC earthquake catalog in the epicentral distance range 30–90° from each individual 295 station. Seismograms are Butterworth bandpass filtered with 0.04Hz and 3Hz corner frequencies to reduce noise 296 and visually inspected for pre P-wave noise to determine if they are suitable for analysis. Receiver functions are 297 again extracted using ETMTRF (*Helffrich*, 2006). All receiver functions with pre-P-arrival amplitudes $\geq 25\%$ of 298 the P-arrival amplitude at any time in the preceding 10s are automatically removed, those remaining are visually 299 inspected to ensure quality. Stations with fewer than eight acceptable receiver functions are not analyzed because 300 they are deemed unsuitable for stacking in our parameter search approach. A detailed list of stations used in this 301 study and their respective results can be found in Table S1. 302

8 Case Study 1 - Simple Crustal Structure

To test our H- κ approach on regions of simple crustal structure, we analyze receiver functions from station HYB on the East Dharwar craton in India (e.g. *Haggerty and Birkett*, 2004), station KMBL on the Yilgarn craton in Western Australia (e.g. *Swager et al.*, 1997) and on the POLARIS/HUBLE seismic networks (*Eaton et al.*, 2005; *Bastow et al.*, 2015, respectively) from northern Canada. We choose these stations because (*i*) they are installed on crystalline basement rocks, avoiding the effect of sedimentary layers; (*ii*) we have *a priori* constraints on Moho depth at these locations from wide-angle seismic refraction and/or joint inversion of surface waves with receiver functions; (*iii*) they have undergone no major tectonic activity since the Precambrian.

Station HYB, situated on the East Dharwar craton in India, is expected to display reliable results owing to a simple crustal structure imaged by both long period P-waves (*Singh and Rastogi*, 1978) and joint inversions of surface wave group velocities with receiver functions (e.g., *Rai et al.*, 2003; *Julià et al.*, 2009; *Borah et al.*, 2014). HYB exhibits extremely tight clustering of results in H- κ space (Figure 7e) and the crustal thickness of 33.8 km agrees with previous estimates (36 km from *Singh and Rastogi* (1978), 34 km from *Rai et al.* (2003), 35 km from Julià et al. (2009) and 34 km from *Borah et al.* (2014)). Station KMBL, on the Yilgarn craton in Western Australia, also returns well clustered results and a crustal thickness value (37.3 km) is in agreement with the 36 km crustal thickness extracted from the nearby deep-crustal seismic reflection line of *Swager et al.* (1997) and the 36 km value derived by *Collins et al.* (2003).

320

Figure 7

Figure 8

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here

Northern Canada is an ideal study locale to test $H-\kappa$ stacking owing to its lack of surface sediments, removed 321 by billions of years of erosion (e.g. St-Onge et al., 2006). We analyze several stations from the Canadian National 322 Seismograph Network (Geological Survey of Canada, 1989), POLARIS (Eaton et al., 2005) and HUBLE (Bastow 323 et al., 2015) seismic networks using our broad parameter search approach (Figure 8a). In 29 of the 37 stations deemed 324 suitable for analysis, H- κ stacking is reliable at all frequencies, and final estimates for H and κ are recorded for 325 these locations (Figure 8b and c). Station ILON produces a reliable H- κ result, with H=36.6 km in close agreement 326 with Thompson et al. (2010) (they found H=37.7 km for linear, H=38.4 km for PWS), although our lower value of 327 crustal thickness is simply due to a smaller V_P value selected by our analysis. Across northern Hudson Bay, bulk 328 crustal V_P/V_S is low, consistent with the region's felsic tonalite-trondhjemite-granodiorite Precambrian geology 329 (*Thompson et al.*, 2010). 330

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Station SCHQ in Quebec (Figure 8a) allows examination of the suitability of H- κ stacking to constrain 332 crustal properties in a region lacking near-surface complexity (St-Onge et al., 2002) but where the Moho is known 333 to be gradational (Gilligan et al., 2016). Using joint inversion of surface waves and receiver functions, Gilligan 334 et al. (2016) observed an increase in shear-wave velocity from 3.8 km/s to 4.5 km/s over a 20 km depth range (see 335 Figure S3). Our result for SCHQ exhibits a large data spread, very weak and incoherent $P_{s_{Moho}}$ arrivals (Figure 336 9f), and reverberations are completely incoherent despite little pre-P-arrival noise. Surface sediments are lacking, 337 hence scattering in H- κ space must be produced by a gradational crust-mantle transition. SCHQ therefore provides 338 an opportunity to investigate whether limiting the frequency content of the of receiver functions can be used to 339 identify the Moho. At every frequency band, the standard deviations in H and κ exceed the allowed limits, perhaps 340 indicating the Moho is >13 km thick beneath SCHQ (Figure 5). However, reanalysing the H- κ stacking solutions 341 with frequencies $\leq 1.2 \,\mathrm{Hz}$ (Figure S4), we obtain an improved, but sub-optimal solution. The crustal thickness of 342 46.5 km and κ of 1.750 are consistent with other stations in the Canadian shield and corroborate the 40–50 km 343 Moho depth observed by *Gilligan et al.* (2016) (Figure S3). Station SCHQ therefore acts as a cautionary warning 344 that H- κ cannot always be relied upon, even in cratonic areas and our parameter search approach is necessary to 345 decipher this. 346

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ACE, SNR and CCC values for the shields all generally pass the minimum cut-off limits for their respective criteria (Figure 10), with the highest values of ACE (HYB: 5.96), SNR (ILON: 12.31) and CCC (SRLN: 0.80) all associated with Precambrian terranes. This supports the view that shields have generally simple, laterallyhomogeneous crustal structure, with a sharp Moho. There are exceptions however: the high CCC value (0.72) at the Canadian station SCHQ suggests it is a low-noise station with relatively laterally-homogeneous crust, but its low ACE (2.07) and SNR (3.71) values imply low-amplitude Ps Moho arrivals from a gradational Moho, consistent with the conclusions of *Gilligan et al.* (2016).

Overall, of the 55 stations that fail the ACE criteria (criteria 5), 51 pass ≤ 8 criteria overall. Similarly, 42 of 52 stations that pass the ACE criteria, also pass ≥ 9 criteria overall. ACE therefore identifies erroneous H- κ analysis 87% of the time. The equivalent predictive success rates for SNR and CCC are 77% and 78% respectively, demonstrating the collective utility of our three receiver function analytics when carrying out H- κ analysis.

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Figure 10 here

9 Case Study 2 - The Ethiopian Traps: near surface complexity and a gradational Moho

The Ethiopian Traps largely formed at 30 Ma, with 2–3 km flood-basalts erupting atop marine sediments during 362 the development of the Red Sea rift (e.g., Hofmann et al., 1997; Rooney et al., 2012, 2018). Wide-angle seismic 363 (Mackenzie et al., 2005) and gravity surveys (Cornwell et al., 2006) reveal a 8–12 km-thick, lower-crustal intrusion 364 layer below the Ethiopian plateau. Thus, low-amplitude, diffuse Moho P-to-S conversions (Figure 1b), coupled 365 with arrivals/reverberations from the near-surface are expected to render H- κ stacking unreliable. To explore this 366 hypothesis, we analyze stations from several permanent and temporary networks in Ethiopia (e.g. Nyblade, 2000; 367 Bastow et al., 2011; Keranen, 2013; Ebinger et al., 2017). Figure 11a demonstrates that most stations located 368 directly on the flood-basalts produce unreliable results (e.g. CHAE, Figure 12; FURI, Figure S5). Eleven of twelve 369 off-flood-basalt stations yield reliable results, for example stations ABMD (Figure 13) and HYNE exhibit tight 370

clustering similar to those from cratonic Canada. The slight increase in the spread of data as compared to cratonic 371 settings (Figure 7e) is due to the sediments (Figure 6f) on which these stations sit. Our result at HYNE (H=34.8 km, 372 κ =1.761) matches closely the 35 km and κ =1.74 obtained by Hammond et al. (2011). V_P/V_S ratios of 1.71–1.76 at 373 stations where H- κ works well in Ethiopia are lower than the global average of 1.765. This implies that the crust 374 beneath these stations is predominantly Precambrian in age, and lacking in modification by hotspot-related mafic 375 magmatism in the form of dyke intrusions and/or lower crustal intrusions. ACE and SNR values at these off-flood-376 basalt stations (Figure 10) are generally high, consistent with the conclusion that the Ps arrival at these stations 377 is high-amplitude. The mean CCC values are lower than for shields, indicative of a more variable back-azimuthal 378 structure. 379

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Towards the western edge of the flood-basalt province and/or where the flood-basalts have been eroded by Blue 381 Nile river incision, stations pass an intermediate number of criteria (e.g. CHGE; C=6, Figure S6). Frequency 382 limited analysis improves the results (Table S2) significantly (e.g CHGE; C=8, Figure 14) and reduces the spread 383 of the remaining H- κ solutions. The Moho is $\sim 4 \,\mathrm{km}$ deeper for these stations than below the adjacent off-flood-384 basalt stations. Noting that H- κ analysis selects the centre of the Moho velocity gradient, this can be interpreted 385 as a crust that is $\sim 8 \,\mathrm{km}$ thicker. Corroborating this, the 0.6–1.4 Hz frequency limit for these stations implies a 386 gradational Moho of thickness 6–10 km (Figures 5 and 11b), in close agreement with the 8–12 km-thick fast P-387 wavespeed (~7.38 km/s) layer found by *Mackenzie et al.* (2005). κ also increases for these stations (Figure 11c), 388 indicative of a more mafic bulk-crustal composition which, when interpreted in light of the thicker crust suggests 389 lower-crustal intrusions exist below the western extent of the flood-basalt province. Mean ACE and SNR values for 390 these stations (Figure 10) are generally low (e.g. GIDA; ACE = 2.05, SNR = 4.39), suggesting that although the 391 frequency limited analysis has improved the solutions, these stations have genuinely low Ps amplitudes indicative 392 of a gradational Moho. 393

Stations in the centre of the flood-basalts fail across all frequencies, indicating the Moho is >13 km thick and/or 394 that arrivals from the basalt-sediment contact are causing H- κ stacking to fail. The ACE, SNR and CCC values from 395 stations on the flood-basalts (Figure 10) consistently fail their respective criteria, supporting the hypothesis that 396 the Ps arrival is low-amplitude and/or not always discernible from arrivals produced by intra-crustal structure. Our 397 observations may thus imply that the lower-crustal intrusion layer and flood-basalts are thickest in the centre of the 398 Ethiopian traps, near the major Paleogene eruptive centres and thinner ($\leq 5 \,\mathrm{km}$) or non-existent at off flood-basalt 399 stations, consistent with petrological studies of the Ethiopian traps (Rooney et al., 2016; Rooney, 2017; Rooney 400 et al., 2018). 401

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Figure 11 here Figure 12 here Figure 13 here

Figure 14

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⁴⁰³ 10 Case Study 3 - Subduction Zones

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Another tectonic regime on which to test our new H- κ stacking approach is subduction zones, where crustal complexity is expected owing to the presence of two tectonic plates (and therefore two Moho discontinuities). Magmatism and a thick mantle wedge are also expected to add complexity (e.g., *Bostock et al.*, 2002).

Japan is an archetypal example of a subduction zone, where the Pacific plate is subducting below Eurasia. In addition to the expected presence of multiple velocity discontinuities associated with two tectonic plates, a thick mantle wedge and voluminous crustal magmatism (e.g., *Nakajima et al.*, 2005) are expected to render H- κ stacking challenging on the island. To test this hypothesis, we analyze seismograms from a selection of Japan Meteorological Agency Seismic Network (*Tatehata*, 1997) and Global Seismograph Network (*ASL/USGS*, 1988) stations. Predictably, our H- κ approach generally obtains unreliable results (Figure 15b) across the island.

The Cyprus arc in the eastern Mediterranean has developed due to subduction of the African Plate beneath 414 the Anatolian Plate (e.g., Robertson and Mountrakis, 2006). Unlike Japan, the $\sim 8 \text{ mm/yr}$ convergence rate (Gripp 415 and Gordon, 2002) is slower and arc magmatism is lacking, perhaps leading to the expectation of a simpler crustal 416 structure. However, a velocity discontinuity between the high-velocity Troodos Ophiolite and slower wave-speed 417 underlying Anatolian continental crust (Mackenzie et al., 2006; Feld et al., 2017) may introduce receiver function 418 complexity. Terrestrial sediments of thickness $\sim 3 \,\mathrm{km}$ (Harrison et al., 2008) surrounding the ophiolite may also 419 generate additional P-to-S conversions (Figure 1c). To explore these issues, we analyzed data from the Cyprus 420 Broadband Seismological Network (Cyprus Geol. Survey Dept., 2013), the TROODOS temporary broadband de-421 ployment (Bastow et al., 2017), and the Kandilli Observatory Broadband Network (BUKO, 2001). Of 18 stations 422 on the island, only six have eight or more acceptable-quality receiver functions (Figure 15a) and all of these lie on 423 ophiolitic material. Nowhere on Cyprus is $H-\kappa$ stacking deemed reliable. 424

⁴²⁵ Our H- κ stacking analyses in Japan and Cyprus are by no means a complete analysis of the global subduction ⁴²⁶ zone system. However, we contend that the failure of H- κ stacking in both regions suggests all H- κ stacking results ⁴²⁷ in subduction zone settings should be treated with extreme caution.

428 11 Conclusions

We have demonstrated via analysis of synthetic seismograms that key to resolving where the H- κ stacking method succeeds and fails is a rigorous search of the H- κ stacking parameter space (including the relative weights assigned to the Moho *P*-to-*S* conversion and its subsequent reverberations, the choice of linear or phase-weighted stacking, and P-wave velocity). Data parameters including the receiver function frequency content and the subset of receiver functions selected for analysis must also be explored thoroughly.

To address these issues, we have developed an H- κ stacking approach in which cluster analysis selects a final 434 solution from 1000 repeat results, each calculated using randomly-selected input and data parameters. We define 435 ten criteria that variously assess the final numerical result, the receiver function dataset, and the extent to which 436 the results are tightly clustered. If a station passes ≥ 9 criteria, H- κ stacking is reliable and crustal structure 437 can be considered simple. If a station passes ≤ 5 criteria its H- κ results cannot be interpreted reliably and more 438 sophisticated seismological techniques (e.g., Julià et al., 2009; Wirth et al., 2016) are required to characterise crustal 439 architecture. Synthetic testing of our new approach shows that when the Moho is sharp, H- κ solutions cluster tightly 440 at all frequencies and return the input model; in areas of more complex crustal structure, H- κ stacking yields erratic 441 results and cannot be trusted. Limiting the frequency content of the receiver functions can allow an estimation of 442 the thickness of a gradational Moho, provided that complex intra-crustal structure is lacking. 443

Applying our H- κ cluster analysis method to the East Dharwar craton, Yilgarn craton and Canadian shield 444 demonstrates the suitability of the H- κ method in regions where the crust is simple and the Moho sharp. Our three 445 new receiver function analytics (ACE, SNR and CCC), have generally high values in these shields, supportive of 446 a sharp Moho at the base of simple crust, and little back-azimuthal variation in crustal structure. In contrast, on 447 the younger recently-volcanically active Ethiopian plateau where 2 km-thick flood-basalts overlie marine sediments, 448 and the Moho is known a priori to be a gradational feature due to an 8-12 km-thick layer of lower-crustal mafic 449 intrusions, H- κ stacking is particularly unreliable. By limiting the frequency content of receiver functions to longer 450 periods, at stations where the flood-basalts are thinner and/or have been eroded by Blue Nile incision, the quality 451 of H- κ solutions improves. These stations have elevated κ (1.77–1.87) values, with ACE and SNR values lower 452 than on the shields, evidence that these stations overlie a gradational Moho of \sim 6–10 km thickness. Moving just 453 a few kilometers off the western extent of the flood-basalt province, solutions cluster tightly at all frequencies and 454 crustal thicknesses are $\sim 4 \,\mathrm{km}$ thinner than the adjacent flood-basalt stations. Bulk-crustal V_P/V_S ratios are low 455 (~ 1.73) at these stations compared to the global average of 1.765. Unreliable H- κ results at the Cyprus and Japan 456 subduction zones are an inevitable consequence of their complex Moho and crustal architectures. H- κ stacking is 457 therefore a valuable tool to infer crustal thickness and V_P/V_S ratio in locations where the crust is relatively simple. 458 However, the technique should be used with extreme caution where crustal structure is complex. 459

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⁶¹⁸ 13 Appendix A - Cluster Analysis

⁶¹⁹ Before hierarchical clustering can be performed, H and κ must span normalized ranges to avoid the much larger ⁶²⁰ Euclidean distances in H dominating the clustering algorithm. H and κ values are thus re-scaled between 0 and 1 ⁶²¹ using their respective ranges:

$$H_{scaled} = \frac{H - H_{min}}{H_{max} - H_{min}},\tag{A1}$$

$$\kappa_{scaled} = \frac{\kappa - \kappa_{min}}{\kappa_{max} - \kappa_{min}},\tag{A2}$$

where H and κ are the original values and H_{min} , κ_{min} , H_{max} and κ_{max} are the minimum and maximum gridsearch values of H and κ , respectively. Henceforth, H and κ represent the re-scaled measurements and distances are between re-scaled measurements.

Initially there are N = 1000 scaled measurement pairs (H_i, κ_i) with variances $(\sigma_{H_i}^2, \sigma_{\kappa_i}^2)$ where i = 1...N. The data are divided into M clusters with each cluster, C_j , containing N_j data points, where j = 1...M. To reduce the effect of discrete data, each initial cluster is assigned an initial error of 1/99 in H and κ that corresponds to the 99 intervals used in the grid-search.

Starting with M = N clusters, the inter-cluster Euclidean distances are calculated for all possible cluster pairs and the closest two clusters are combined into one, reducing the number of clusters by one. The number of points (N_j) per cluster C_j is calculated, and the mean centroid position of each cluster centre $(\bar{H}_j, \bar{\kappa}_j)$ is calculated as:

$$\bar{H}_j = \frac{\sum_{i=1}^{N_j} H_i^{(j)}}{N_j},\tag{A3}$$

$$\bar{\kappa}_j = \frac{\sum_{i=1}^{N_j} \kappa_i^{(j)}}{N_j},\tag{A4}$$

where $H_i^{(j)}$ and $\kappa_i^{(j)}$ refer to the *i* number of data points within cluster *j*.

Euclidean distances are re-calculated between all remaining clusters, including the newly merged cluster, and the process is repeated until one cluster remains containing all N data points. The optimum number of clusters is between $1 \le M \le N$ (*Everitt et al.*, 2001). The optimum number of clusters is chosen automatically using the criterion of *Caliński and Harabasz* (1974) and *Duda et al.* (1973). The criteria of *Caliński and Harabasz* (1974) is defined by:

$$c(M) = \frac{(N-M)trace(B)}{(M-1)trace(W)},\tag{A5}$$

where B is the between-cluster covariance and W is the within-cluster covariance, both calculated at each cluster step (M = 1...N). The optimum number of clusters is found when c(M) is a maximised. The between-cluster covariance (B) and within-cluster covariance (W) are:

$$B = \begin{bmatrix} \sum_{j=1}^{M} (\bar{H}_{j} - \bar{H})^{2} & \sum_{j=1}^{M} (\bar{H}_{j} - \bar{H})(\bar{\kappa}_{j} - \bar{\kappa}) \\ \sum_{j=1}^{M} (\bar{H}_{j} - \bar{H})(\bar{\kappa}_{j} - \bar{\kappa}) & \sum_{j=1}^{M} (\bar{\kappa}_{j} - \bar{\kappa})^{2} \end{bmatrix},$$
 (A6)

$$W = \begin{bmatrix} \sum_{j=1}^{M} \sum_{i=1}^{N_j} (H_i^{(j)} - \bar{H}_j)^2 & \sum_{j=1}^{M} \sum_{i=1}^{N_j} (H_i^{(j)} - \bar{H}_j) (\kappa_i^{(j)} - \bar{\kappa}_j) \\ \sum_{j=1}^{M} \sum_{i=1}^{N_j} (H_i^{(j)} - \bar{H}_j) (\kappa_i^{(j)} - \bar{\kappa}_j) & \sum_{j=1}^{M} \sum_{i=1}^{N_j} (\kappa_i^{(j)} - \bar{\kappa}_j)^2 \end{bmatrix},$$
(A7)

where $H_i^{(j)}$ and $\kappa_i^{(j)}$ are the H and κ values of each measurement (i) in each cluster (j), and \overline{H} and $\overline{\kappa}$ are the mean H and κ values for the entire dataset:

$$\bar{H} = \frac{\sum_{i=1}^{N} H_i}{N},\tag{A8}$$

$$\bar{\kappa} = \frac{\sum_{i=1}^{N} \kappa_i}{N}.$$
(A9)

The criteria of *Duda et al.* (1973) uses the ratio of within-cluster variances before and after the two clusters are combined into a single cluster. The within-cluster variance of the two clusters prior to being combined is:

$$\sigma_2^2 = \sum_{j=1}^2 \sum_{i=1}^{N_j} [(H_i^{(j)} - \bar{H}_j)^2 + (\kappa_i^{(j)} - \bar{\kappa}_j)^2],$$
(A10)

and the within-cluster variance once the two clusters are combined is:

$$\sigma_1^2 = \sum_{i=1}^{N_1} [(H_i^{(1)} - \bar{H}_1)^2 + (\kappa_i^{(1)} - \bar{\kappa}_1)^2].$$
(A11)

The assumption is that the two clusters will be combined into one cluster which is rejected when:

$$\left(1 - \frac{\sigma_2^2}{\sigma_1^2} - \frac{2}{\pi p}\right) \left(\frac{N_j p}{2[1 - 8/(\pi^2 p)]}\right)^{1/2} > c_{critical},\tag{A12}$$

where p = 2 and is the number of parameters in the analysis and $c_{critical} = 3.20$, the value assumed when the data points within a cluster are normally distributed (*Milligan and Cooper*, 1985). The optimum number of clusters ⁶⁴⁹ is found when Equation A12 is invalidated as the number of clusters is reduced.

The optimum number of clusters is taken to be the criteria that indicates the larger number of clusters up to a maximum of M = 7 clusters. To find the most suitable cluster, we define the within-cluster variance $(\sigma_{c_j}^2)$ and error variance $(\sigma_{d_j}^2)$ according to *Teanby et al.* (2004) for each cluster containing >15 points.

$$\sigma_{c_j}^2 = \frac{\sum_{i=1}^{N_j} (H_i^{(j)} - \bar{H}_j)^2 + (\kappa_i^{(j)} - \bar{\kappa}_j)^2}{N_j},\tag{A13}$$

$$\sigma_{d_j}^2 = \left[\sum_{i=1}^{N_j} \frac{1}{(\sigma_{H_i}^{(j)})^2}\right]^{-1} + \left[\sum_{i=1}^{N_j} \frac{1}{(\sigma_{\kappa_i}^{(j)})^2}\right]^{-1}.$$
(A14)

We define the overall variance $(\sigma_{o_j}^2)$ for each remaining cluster as:

$$\sigma_{o_j}^2 = max(\sigma_{c_j}^2, \sigma_{d_j}^2), \tag{A15}$$

The best overall cluster has the minimum $\sigma_{o_j}^2$ and the final H- κ solution is measurement with smallest combined rescaled errors in H and κ from within this chosen cluster.

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Table 1: H- κ input parameter ranges for analysis, resulting in 4998 possible unique combinations.	There are 21
unique possible combinations of the stacking weights which satisfy $\sum w_i = 1$.	

Parameter	Minimum	Maximum	Interval	Possible Combinations
$\mathcal{V}_P~(km/s)$	6.2	6.8	0.1	7
w_1	0.4	0.9	0.1	-
w_2	0.1	0.6	0.1	21
w_3	0	0.5	0.1	-
Stack type	Linear	PWS	_	2
Fmax (Hz)	0.4	2.0	0.1	17

Number	Criterion	Criteria Assesses
1	Chosen H and κ solutions lie within the boundaries of the	Numerical H- κ solution
	H- κ grid space.	
2	H and κ errors for the chosen result are ${<}\pm2.5\rm km$ in H and	Numerical H- κ solution
	± 0.042 in κ .	
3	Standard deviation in H after all 1000 repetitions is	Cluster analysis
	$<\pm 2.5$ km.	
4	Standard deviation in κ after all 1000 repetitions is	Cluster analysis
	$<\pm 0.042.$	
5	Mean average ACE of the 1000 repetitions is >3 .	RF datatset
6	Mode H and κ lie within the same cluster as the mean H	Cluster analysis
	and κ .	
7	Summed amplitudes of Ps , $PpPs$ and $PsPs + PpSs$ for all	RF datatset
	stacked receiver functions, are positive, positive and nega-	
	tive respectively.	
8	Mean average CCC of all receiver functions at each indi-	RF datatset
	vidual frequency is >0.6 .	
9	Mean average SNR of the 1000 repetitions is >5 .	RF datatset
10	Overall mean H and κ for the linearly stacked repetitions	Cluster analysis
	lie within one standard deviation of H and κ for PWS rep-	
	etitions, and vice versa.	

Table 2: The ten criteria used for determining result quality. RF dataset: refers to the N receiver functions for the station.

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Figure 1: The impact of crustal structure on receiver functions. a) Sharp Moho with high amplitude, impulsive P-to-S conversions. b) A gradational Moho, for which P-to-S conversions occur over a large depth range. Receiver function signals weaker and more diffuse. c) When near-surface layers exist, resulting P-to-S conversions can distort Moho signals.



Figure 2: Errors in H and κ are calculated using the 95% contour of $s(H,\kappa)$ for each repetition. In both H and κ the mean average of the minimum and maximum errors is calculated to obtain the final errors in H and κ .



Figure 3: ACE value (demonstrated for a receiver function recorded at station HYB in Hyderabad, India) is determined by dividing the Ps amplitude by the RMS value of amplitude within the green shaded region. Similarly the SNR value is calculated by dividing the Ps amplitude by the RMS amplitude of the orange shaded region prior to the P arrival.



Figure 4: Distribution of H- κ results from a) sharp Moho with linear stacking, b) gradational Moho with linear stacking, c) sharp Moho with phase-weight stacking, d) gradational Moho with phase-weight stacking, as individual H- κ input parameters are varied. Black cross indicates the input model values of H and κ . The color indicates the parameter being varied while the rest are held constant. n.b. in the case of w_1 , w_2 and w_3 , two are varied synchronously to satisfy $\sum w_i = 1$.



Figure 5: The effect of varying Moho thickness and receiver function frequency content on the accuracy of H- κ solutions. At Moho thickness $\leq 5 \text{ km}$, H- κ stacking is reliable and accurately constrains the input model for all frequency bands. Between 6–9 km, H- κ stacking becomes unreliable at high frequencies and results should be interpreted cautiously. H- κ stacking maintains reliability at very low frequencies until the Moho thickness is $\sim 13 \text{ km}$. However, when the Moho is $\geq 14 \text{ km}$ thick, H- κ stacking becomes unreliable for all frequencies of receiver functions.



Figure 6: H- κ results for various synthetic models. Left column: Blue dashed line indicates V_P with depth, red dashed line indicates V_S with depth. Central column: Final H- κ stack solution for the model. Right column: The distribution of H and κ solutions for the model. Dot color indicates the cluster that a result belongs to in the hierarchical cluster analysis. Black cross is the expected H and κ from the input model, red cross is the mean of H and κ from the 1000 repeats, yellow cross is the mode combination of H and κ , blue cross is the combination of H and κ selected by the cluster analysis. Black box marks one standard deviation in H and κ calculated for the 1000 repeat results. a-c) Sharp Moho synthetic model. d-f) Model with a sharp Moho and 3 km-thick, low velocity, near-surface sediments. g-i) Model with a sharp Moho, and 3 km of high velocity basalts overlying 3 km of low velocity sediments. j-l) Model with a 15 km gradational Moho centred at 40 km depth. m-o) Model with a gradational Moho, and 3 km of high velocity basalts overlying 3 km of low velocity sediments.



Figure 7: Final result diagram for station HYB on the East Dharwar craton. a) H- κ stack of the selected repetition. Red ellipse outlines the 95% amplitude contour, blue cross is the final H and κ solution. b) H result, c) κ result, and d) ACE result for each repetition, with running means marked by the orange lines. e) All 1000 H- κ solutions with color representing the cluster that a result is assigned to. Red cross is the mean of H and κ from the 1000 repeats, yellow cross is the mode combination of H and κ , blue cross is the combination of H and κ selected by the cluster analysis, black box marks one standard deviation in H and κ . f) Accepted receiver functions plotted by horizontal slowness, t_1 , t_2 and t_3 denote the predicted arrival times from the chosen H and κ solution. Peaks/troughs are colored when their amplitude is >10% of P arrival. g) Receiver functions arranged by back-azimuth. h) Distribution of linear stacking results. i) Distribution of phase-weighted stacking results.



Figure 8: Results from stations in northern Canada. a) Number of criteria passed. b) Crustal thickness (H). c) Bulk-crustal V_P/V_S (κ).



Figure 9: Final result diagram for station SCHQ in the Canadian shield (Figure 8) which displays incoherent *P*-to-*S* conversions and an unreliable H- κ result. Figure details are as per Figure 7.



Figure 10: A comparison of the mean ACE, SNR and CCC analytics for stations used in the study. Squares are results from stations analysed at 2 Hz, circles are stations analysed with limited frequencies. Colors indicate the number of criteria passed according to scale in Figure 8a. Red lines indicate the cut-off limit for each respective analytic. CFB: Continental flood-basalt.



1.651.701.751.801.851.90

Figure 11: Results from stations in Ethiopia. a) Number of criteria passed. Black crosses indicate analyzed stations where fewer than eight suitable receiver functions were calculated. Red line delineates the spacial extent of the 30 Ma Ethiopian flood-basalt province (after Rooney, 2017). b) Crustal thickness (H). Squares are results from stations that passed ≥ 8 criteria with all frequencies, circles are solutions for stations from which the frequency dependent analysis produced a reliable result. c) Bulk-crustal V_P/V_S (κ).



Figure 12: Final result diagram for station CHAE on the Ethiopian Plateau (Figure 11). Figure details are as per Figure 7.



Figure 13: Final result diagram for station ABMD, just off the westernmost extent of the flood basalts (Figure 11). Figure details are as per Figure 7.



Figure 14: Final result diagram for station CHGE on the Ethiopian Plateau (Figure 11), where only solutions using receiver functions with frequencies ≤ 0.9 Hz are sampled. Figure details are as per Figure 7.



Figure 15: Results from stations in a) Japan and b) Cyprus with stations plotted by number of criteria passed. Black crosses indicate analyzed stations where fewer than eight suitable receiver functions were calculated. Blue dashed line outlines the surface extent of the Troodos Ophiolite.