# Bayesian inference of mantle viscosity from whole-mantle density models

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#### Abstract

The long-wavelength geoid is sensitive to Earth's mantle density structure as well as radial variations in mantle viscosity. We present a suite of inversions for the radial viscosity profile using whole-mantle models that jointly constrain the variations in density, shear- and compressional-wavespeeds using full-spectrum tomography. We use a Bayesian approach to identify a collection of viscosity profiles compatible with the geoid, while enabling uncertainties to be quantified. Depending on tomographic model parameterization and data weighting, it is possible to obtain models with either positive- or negative-buoyancy in the large low shear velocity provinces (LLSVPs). We demonstrate that whole-mantle density models in which density and  $V_S$  variations are correlated imply an increase in viscosity below the transition zone, often near ~1000~km. Many solutions also contain a low-viscosity channel below 650~km. Alternatively, models in which density is less-correlated with  $V_S$  – which better fit normal mode data – require a reduced viscosity region in the lower mantle. This feature appears in solutions because it reduces the sensitivity of the geoid to buoyancy variations in the lowermost mantle. The variability among the viscosity profiles obtained using different density models is indicative of the strong non-linearities in modeling the geoid and the limited resolving power of the geoid kernels. We demonstrate that linearized analyses of model resolution do not adequately capture the posterior uncertainty on viscosity. Joint and iterative inversions of viscosity variation and scalings between material properties.

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# Key Points:

- We model mantle flow with density variations from full-spectrum tomography.
- We generate Bayesian estimates of the radial viscosity profile with uncertainties.
- There is evidence for a low-viscosity channel below the transition zone and a viscosity increase in the mid mantle.

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#### 1 Abstract

The long-wavelength gooid is sensitive to Earth's mantle density structure as well as ra-2 dial variations in mantle viscosity. We present a suite of inversions for the radial viscos-3 ity profile using whole-mantle models that jointly constrain the variations in density, shear-4 and compressional-wavespeeds using full-spectrum tomography. We use a Bayesian ap-5 proach to identify a collection of viscosity profiles compatible with the geoid, while en-6 abling uncertainties to be quantified. Depending on tomographic model parameterization and data weighting, it is possible to obtain models with either positive- or negative-8 buoyancy in the large low shear velocity provinces (LLSVPs). We demonstrate that whole-9 mantle density models in which density and  $V_S$  variations are correlated imply an increase 10 in viscosity below the transition zone, often near 1000 km. Many solutions also contain 11 a low-viscosity channel below 650 km. Alternatively, models in which density is less-correlated 12 with  $V_S$  – which better fit normal mode data – require a reduced viscosity region in the 13 lower mantle. This feature appears in solutions because it reduces the sensitivity of the 14 geoid to buoyancy variations in the lowermost mantle. The variability among the vis-15 cosity profiles obtained using different density models is indicative of the strong non-linearities 16 in modeling the geoid and the limited resolving power of the geoid kernels. We demon-17 strate that linearized analyses of model resolution do not adequately capture the pos-18 terior uncertainty on viscosity. Joint and iterative inversions of viscosity, wavespeeds, 19 and density using seismic and geodynamic observations are required to reduce bias from 20 prior assumptions on viscosity variation and scalings between material properties. 21

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# Plain Language Summary

The viscosity of Earth's mantle affects nearly every aspect of Earth's evolution, in-23 cluding its convective vigor and rate of cooling, the motion of mantle plumes and sub-24 ducted oceanic lithosphere through the mantle, and the deep volatile cycle. We use the 25 long-wavelength geoid to constrain the variation of mantle viscosity with depth. In so 26 doing, we use newly available whole-mantle models of seismic wavespeeds and density 27 that incorporate constraints on lowermost mantle density from the free oscillations of 28 the Earth. We find evidence for an increase in viscosity within the mid mantle and for 29 a low-viscosity region below the mantle transition zone. We demonstrate that depend-30 ing on choices made in the data weighting and regularization of tomographic models, it 31 is possible to obtain solutions that include a reduced viscosity region in the lower man-32

tle as well. We argue that in joint inversions of seismic and geodynamic observations,

viscosity variations must be solved for together with wavespeed and density variations,

 $_{35}$  and should not be assumed *a priori*.

#### <sup>36</sup> 1 Introduction

Long-wavelength components of the geoid are precise geodetic observations that 37 are sensitive to density and viscosity variations in the Earth's mantle, providing an ob-38 servational constraint on these two dynamically significant parameters. Density varia-39 tions drive convection currents that deflect the topography of the Earth's surface and 40 internal boundaries, determining the observed geoid. Patterns and amplitudes of the geoid 41 variations due to these flows depend on the viscosity structure of the mantle. At the longest 42 spatial scales – those represented by the lowest degrees in spherical harmonic represen-43 tations – radial variation of viscosity becomes much more important than lateral vari-44 ations (e.g. Richards & Hager, 1984; Ghosh et al., 2010). If a radial viscosity profile is 45 assumed a priori, geoid observations may be used to constrain density anomalies within 46 the mantle in conjunction with seismological and other geophysical observations (e.g. Sim-47 mons et al., 2010). Alternatively, geoid observations can constrain the depth-dependence 48 of mantle viscosity when estimates of density anomalies in the mantle are available (e.g. 49 Hager et al., 1985). We adopt and extend the latter approach to provide new constraints 50 on radial viscosity structure while exploring the recent seismological constraints on den-51 sity variations in the mantle (cf. Moulik & Ekström, 2016). 52

Since the 1980s, substantial progress has been made in mapping the viscosity of 53 the mantle by approximating density  $(\rho)$  anomalies by scaling them from shear  $(V_S)$  or 54 compressional  $(V_P)$  velocity anomalies mapped by global seismic tomography. Due to 55 the more uniform data coverage afforded by shear waves, global  $V_S$  tomographic mod-56 els are more consistent among groups and better constrain the longest-wavelength struc-57 ture (e.g. Becker & Boschi, 2002; Cottaar & Lekic, 2016; Ritsema & Lekic, 2020). The 58 scaling factors typically used to relate wavespeed to density variations  $(R_{\rho,S} = \frac{d \ln \rho}{d \ln V_s})$ 59 and  $R_{\rho,P}$ ) are informed by laboratory studies of mineral properties, and usually assume 60 that density variations arise due to temperature, neglecting potential contributions from 61 compositional variations (e.g. Karato, 1993). This assumption introduces uncertainty 62 in inferences of mantle viscosity, compounding the limitations arising from uncertain-63 ties in the  $V_S$  tomographic models themselves. 64

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The assumption of uniform composition may be particularly problematic in the Earth's 65 lowermost mantle, where structure is dominated by the two large low shear-velocity provinces 66 (LLSVPs). Multiple lines of evidence suggest that LLSVPs are compositionally distinct 67 from the ambient lower mantle. First, LLSVPs have slower shear velocities and larger 68 velocity gradients across their margins than is expected for uniform composition (e.g. 69 Ni et al., 2002; Wang & Wen, 2007). Second, variations in  $V_S$  and bulk sound speed are 70 anti-correlated in the lower mantle (e.g. Su & Dziewonski, 1997; Masters et al., 2000). 71 Third, the ratio of  $d \ln V_S / d \ln V_P$  is higher and the distribution of velocities broader in 72 the lower mantle than is expected for purely thermal heterogeneity (e.g. Robertson & 73 Woodhouse, 1996; Masters et al., 2000; Brodholt et al., 2007; Deschamps & Trampert, 74 2003). Finally, constraints from normal modes favor anti-correlation between density and 75 velocity variations in the lowermost mantle (e.g. Ishii & Tromp, 2001; Moulik & Ekström, 76 2016). Depending on the relative importance of thermal and compositional contributions 77 to density, the LLSVPs could either be positively or negatively buoyant structures. If 78 positively buoyant, the LLSVPs would be expected to rise, precluding their stability over 79 geologic time, which has been proposed based on multiple lines of evidence (e.g. Burke 80 & Torsvik, 2004; Burke et al., 2008; Dziewonski et al., 2010; Torsvik et al., 2014). Fur-81 ther complicating matters, the LLSVPs may not be compositionally uniform and could 82 consist of a denser sub-region surrounded by a thermal and/or compositional halo (e.g. 83 Simmons et al., 2010; Moulik & Ekström, 2016; Ballmer et al., 2016; Lau et al., 2017). 84 These distinct scenarios differ in their implications for the nature of LLSVPs, their re-85 lationship to geochemical signatures of primordial material, and to large-scale mantle 86 flow. 87

Seismological constraints, derived primarily from normal mode splitting functions, 88 can be used to directly map large-scale density variations in the lowermost mantle (e.g. 89 Ishii & Tromp, 2001; Moulik & Ekström, 2016), thereby reducing the need for a priori 90  $R_{\rho,S}$  and  $R_{\rho,P}$  scaling factors. However, density tomographic models have not been em-91 ployed yet to constrain mantle viscosity due to a lack of consensus among groups, po-92 tential dependence of the tomographic models on the starting structure (Kuo & Romanow-93 icz, 2002), regularization (Resovsky & Ritzwoller, 1999), and lack of sensitivity to odd-94 degree structure (Resovsky & Ritzwoller, 1995). Improved normal mode splitting mea-95 surements based on recent large earthquakes (e.g. Deuss et al., 2011, 2013) have improved 96 our ability to constrain lower mantle density variations. A recent joint inversion of nor-97

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mal mode splitting, waveforms, and travel-times reported a statistically significant argument for negative buoyancy in the bottom ~500 km of LLSVPs (Moulik & Ekström,
2016). Additionally, new tidal constraints on lowermost mantle density structure suggest that the LLSVPs are about 0.5% denser than average (Lau et al., 2017). Further
refinements on density structure from new geophysical constraints could reveal the depth
extent of regions with denser than ambient mantle within LLSVPs.

In order to better understand the relationship between mantle density structure 104 and the geoid based on currently available data, we perform Bayesian inversions for man-105 tle viscosity structure using a similar framework to Rudolph et al. (2015). The inversions 106 employ a suite of 18 whole-mantle density models that are created based on the approach 107 of Moulik and Ekström (2016) while varying data weights on the seismic observations 108 and the model regularization factor that modulates correlation between density and  $V_S$ 109 structure. We analyze the resulting suite of viscosity structures in terms of fit to the geoid 110 and identify persistent features and ones that depend crucially on modeling choices. Fi-111 nally, we discuss the implications for making robust inferences on density, viscosity and 112 wavespeed based on joint modeling of seismic and geodetic data. 113

# 114 2 Methods

We carry out a suite of inversions for the mantle viscosity profile constrained by 115 the long-wavelength non-hydrostatic geoid. We use geoid spherical harmonic coefficients 116 from the GRACE geoid model GGM05 (Ries et al., 2016) and the hydrostatic correc-117 tion from Chambat et al. (2010). There is a rich history of inversions for the mantle vis-118 cosity structure using the long-wavelength geoid and observations related to glacial iso-119 static adjustment using a variety of inverse methods. In choosing an inversion method-120 ology, it is important to consider at the outset the nature of the inverse problem at hand, 121 and in particular its degree of non-linearity. In Figure 1 we show the variation of the mis-122 fit to the geoid for spherical harmonic degrees 2-7 for a piecewise-linear viscosity struc-123 ture constrained by four control points (describing viscosity and depth). Two of the con-124 trol points are fixed at the surface and the core-mantle boundary while the other two 125 are allowed to vary in depth within the mantle. Even for this coarse parameterization 126 of the viscosity structure using only 6 free parameters, it is evident that there are strong 127 tradeoffs between parameters, multiple local minima or "wells" in the misfit surface (e.g. 128 Figure 10,Q). These basic observations suggest that the variation in the misfit may not 129

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be adequately described by linear estimates. We note that the brute-force search illus-130 trated in Figure 1 is not a viable approach to the viscosity inversion problem because 131 the number of forward model evaluations becomes prohibitive very quickly as the num-132 ber of free parameters (control points) increases. Because of the degree of nonlinearity 133 in the problem, we choose to use a model-space search approach. Various model space 134 search approaches including genetic algorithms (King, 1995; Kido et al., 1998, e.g.) and 135 Monte-Carlo approaches (e.g. Mitrovica & Peltier, 1993; Mitrovica & Forte, 1997; Paul-136 son et al., 2007a, 2007b) have been previously applied to inversions for mantle viscos-137 ity, highlighting the viability of this class of inverse methods. 138

We use a transdimensional, hierarchical, Bayesian (THB) inversion method (Bodin 139 et al., 2012; Sambridge et al., 2013) to estimate the mantle viscosity structure. The trans-140 dimensional approach does not specify a priori the number of free parameters such as 141 viscosity values and interface depths. Rather, the number of free parameters is itself a 142 parameter in the inversion procedure, and we explore models with varying levels of com-143 plexity, with an Ockham factor penalizing model complexity. We employ a reversible-144 jump Markov-Chain Monte Carlo (rjMCMC) approach to explore the model space; "re-145 versible jump" refers to the ability of the Markov chain to jump between model spaces 146 with different numbers of parameters. We use a parallel tempering algorithm (Sambridge, 147 2014), in which multiple Markov chains simultaneously explore model spaces with dif-148 ferent "temperatures" that effectively smooth the misfit surface. Parallel tempering ac-149 celerates convergence and reduces the tendency for the Markov Chains to get stuck in 150 local (rather than global) minima of the objective function. In contrast to our previous 151 inferences of viscosity (Rudolph et al., 2015), we (1) use a different and more varied set 152 of buoyancy structures from seismic tomography, (2) parameterize log-viscosity using piece-153 wise linear functions rather than layers, (3) estimate tomographic uncertainty directly 154 from model covariance matrices, and (4) employ parallel tempering. We describe each 155 aspect of the modeling, starting with the generation of density models used to constrain 156 the inversions for viscosity structure. We then describe the process used to generate the 157 covariance matrices representing data and forward modeling uncertainty. Finally, we de-158 scribe the inversion procedure used to estimate the mantle viscosity profile. 159

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Figure 1. Results of a grid search of piecewise-linear viscosity structures with four control points. Density anomalies were derived from SEMUCB-WM1 using a uniform scaling factor  $d \ln V_s/d \ln \rho = 0.2$ , and the residual is computed for spherical harmonic degrees 2-7. (A) Distribution of residuals for all of the models. (B) Bivariate histogram of relative viscosity for solutions representing the 1000 smallest misfits. The solution with the smallest misfit is shown as a red curve. The dashed line in panel (A) indicates the largest residual among the solutions shown in (B). Panels (C)-(Q) show two dimensional slices through the misfit function passing through the minimum misfit value (star). The viscosity values  $\eta_0$  and  $\eta_3$  correspond to the core-mantle boundary and the surface. The additional control points within the mantle correspond to depth and viscosity  $(z_1,\eta_1)$  and  $(z_2,\eta_2)$ .

# <sup>160</sup> 2.1 Forward Model

We model global mantle flow and calculate the geoid anomalies using a propaga-161 tor matrix technique. The forward mantle flow models are performed with HC (Becker 162 et al., 2014), using free-slip boundary conditions at the surface and the core-mantle bound-163 ary. In the present work, we consider only depth-variation of viscosity and neglect lat-164 eral viscosity variations (LVVs). The degree to which LVVs influence the long wavelength 165 geoid is difficult to quantify because it depends on the amplitude and wavelength of the 166 viscosity variations (Ghosh et al., 2010). Zhong and Davies (1999) demonstrated that 167 high-viscosity slabs in the lower mantle could have a strong effect on the geoid, even at 168 spherical harmonic degree 2. On the other hand, lateral viscosity variations based on  $V_S$ 169 heterogeneity from tomographic models have a less significant effect on the long wave-170 length geoid. Moucha et al. (2007) showed that the inclusion/omission of LVVs had a 171 less significant impact on the  $l \leq 20$  geoid than the variability among geoid predictions 172 using density models derived from the tomographic models S20RTS (Ritsema & Van Hei-173 jst, 1999) and TX2002 (Grand, 2002). Yang and Gurnis (2016) found similar radial vis-174 cosity variations in inversions constrained by long-wavelength gravity and topography 175 with and without LVVs, suggesting a limited sensitivity of the long-wavelength geoid to 176 LVVs. 177

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# 2.2 Joint models from full-spectrum tomography

Full-spectrum tomography (Moulik & Ekström, 2014, 2016) employs seismic wave-179 forms and derived measurements of body waves ( $\sim 1-20s$ ), surface waves ( $\sim 20-300s$ ) and 180 normal modes ( $\sim 250-3300s$ ) to constrain physical properties – seismic velocity, anisotropy, 181 density and the topography of discontinuities – at variable spatial resolution. We follow 182 closely the methodology of Moulik and Ekström (2016) to generate a suite of tomographic 183 models with different levels of structural complexity and fit to seismic data. The start-184 ing model is an anisotropic shear velocity model with topographies of transition-zone dis-185 continuities and three  $(R_P^{UM}, R_P^{LM}, R_{\rho}^{UM} = R_{\rho}^{LM})$  optimal scaling factors that describe 186 the relative variations of compressional velocity  $(V_P)$  and density  $(\rho)$  in the upper (UM)187 and lower mantle (LM). The preferred estimate of upper  $(R_P^{UM}=0.7)$  and lower man-188 the velocity scaling ratio  $(R_P^{LM}=0.4)$  and a whole-mantle density scaling ratio  $(R_{\rho}=0.3)$ 189 gives substantial improvements in data fits and is consistent with petrological constraints 190

(e.g. Montagner & Anderson, 1989; Karato, 1993) and earlier tomographic studies (e.g.
Robertson & Woodhouse, 1996).

The splitting of Earth's lowest-frequency observed normal mode  $(_0S_2)$  is strongly 193 sensitive to long-wavelength density structure and prefers models with negative  $R_{\rho}$  and 194 anti-correlated  $V_S - \rho$  structure in the lowermost mantle i.e. scenarios where the base 195 of LLSVPs are denser and more negatively buoyant than the ambient mantle (Fig.12 in 196 Moulik & Ekström, 2016). Motivated by these observations, we explore a range of den-197 sity models by varying the weight  $(w_{_0S_2})$  assigned to the splitting of  $_0S_2$  and the weight 198 assigned to the prior on  $V_S - \rho$  correlation in the lowermost mantle  $(\gamma_{\rho}^{D''})$ , while keep-199 ing identical values in the other regions of the mantle. Varying  $w_{_{0}S_{2}}$  and  $\gamma_{\rho}^{D^{\prime\prime}}$  affects the 200 model density structure and correlation between density and  $V_S$  below ~ 2000 km depth 201 with the most significant changes occurring below 2500 km depth (Figure 2 and S1). The 202 magnitude of  $\gamma_{\rho}^{D''}$  does not have physical dimensions or significance - it is a data weight-203 ing factor in the inversion and the values reported here are consistent with Moulik and 204 Ekström (2016). The scaling complexity is varied by modulating a modified objective 205 function of the joint inverse problem 206

$$\widetilde{\chi}^{2} = w_{0}S_{2}\chi_{0}^{2}S_{2} + \sum_{i=2}^{N} w_{i}\chi_{i}^{2} + \gamma_{\rho}^{D''}\mathcal{R}_{R_{\rho},D''}^{2} + \gamma_{\rho}^{\text{other}}\mathcal{R}_{R_{\rho},\text{other}}^{2} + \sum_{k=1}^{M} \left[\gamma_{h,k}\mathcal{R}_{h,k}^{2} + \gamma_{v,k}\mathcal{R}_{v,k}^{2}\right] + \gamma_{P}\mathcal{R}_{R_{P}}^{2} + \gamma_{a}\mathcal{R}_{R_{a}}^{2},$$
(1)

where N is the number of data in the inversion, 
$$w_i$$
 are the weights assigned to individ-  
ual data. We minimize vertical  $(\mathcal{R}_{v,k}^2)$  and horizontal gradients  $(\mathcal{R}_{h,k}^2)$  for M parame-  
ters and impose scaling relationships between various pairs of parameters  $(v_S - v_P, v_S - \rho$  and anisotropic  $a_S - a_P$ ) with weights  $\gamma_P$ ,  $\gamma_\rho$  and  $\gamma_a$ , respectively (eq. 8–10 of Moulik  
& Ekström, 2016). We construct 18 models which span the range of scenarios of  $\rho$  vari-  
ations given currently-available seismic data across six values of  $\gamma_\rho^{D''}$  and three of  $w_0 S_2$   
(Table 1). Figure 2 shows the lowermost mantle density structure for a subset of 6 of these  
models. Weights to the remaining  $(N-1)$  data,  $v_S - \rho$  scaling in other regions  $(\gamma_\rho^{\text{other}})$   
and rest of the regularization parameters are kept similar to those employed in the pre-  
ferred model from Moulik and Ekström (2016), which corresponds roughly to the Model 161  
 $(w_0 S_2 = 1X, \gamma_\rho^{D''} = 0)$  in our suite. The posterior model covariance matrix,  $\widetilde{C_M}$ , cor-  
responding to each of the 18 tomographic models is also computed; our procedure for

|             |             | Prior $v_S - \rho$ covariance in the lowermost mantle $(\gamma_{\rho}^{D^{\prime\prime}})$ |           |           |           |           |                  |
|-------------|-------------|--|-----------|-----------|-----------|-----------|------------------|
|             |             | 0  | $10^4$    | $10^{6}$  | $10^7$    | $10^{8}$  | 10 <sup>11</sup> |
|             | 0           | Model 155  | Model 156 | Model 157 | Model 158 | Model 159 | Model 160        |
| Data weight | 1X          | Model 161  | Model 162 | Model 163 | Model 164 | Model 165 | Model 166        |
| $(w_0 S_2)$ | 10 <i>X</i> | Model 167  | Model 168 | Model 169 | Model 170 | Model 171 | Model 172        |

**Table 1.** Summary of scaling assumptions and data weights employed in the 18 whole-mantle density models. The data weight 1X represents the preferred weight for  $_0S_2$  from Moulik and Ekström (2016).

propagating uncertainties in tomographic estimations of density variations into the potentially correlated uncertainties on the individual geoid coefficients is described in Section 2.3.

Depending on the values of  $\gamma_{\rho}^{D''}$  and  $w_{0}S_{2}$ , we can generate models that produce 221 either positive or negative correlation between degree-2 density structure and the good 222 (Figure 2). For large values of  $\gamma_{\rho}^{D''}$ ,  $\rho$  variations largely track those of  $V_S$ . As  $\gamma_{\rho}^{D''}$  de-223 creases,  $\rho$  variations reduce in amplitude and become de-correlated from those of  $V_S$ . In-224 creasing  $w_{_0S_2}$  has the effect of amplifying the strength of  $\rho$  variations and a pattern that 225 is anti-correlated to  $V_S$  variations. It is worth noting that not all 18 scenarios are equally 226 preferred by current seismic data; anti-correlated  $V_S - \rho$  structure in the lowermost man-227 tle and associated dense base of LLSVPs are preferred by most normal modes with sub-228 stantial sensitivity to density at these depths. When we allow additional degrees of free-229 dom with such independent  $\rho$  variations in the lowermost mantle, variance is reduced 230 and the reduction is systematic, large (often exceeding 50 percent) and statistically sig-231 nificant for various subsets of normal-mode, surface- and body-wave data (Moulik & Ek-232 ström, 2016, Section 4.4 and Figure 12). 233

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# 2.2.1 Model Parameterization

In previous work (Rudolph et al., 2015), we specified the viscosity profile using constantviscosity layers. In order to permit an efficient representation of viscosity gradients, we



Figure 2. Here we show density variations at 2875 km depth and for spherical harmonic degrees l = 1 - 7 for six of the density models. Lateral variations of density ( $\delta\rho$ ) in the lowermost mantle depend on the amount of imposed scaling ( $\gamma_{\rho}^{D''}$ ) between density and  $V_S$  variation. On the other hand, the weight assigned to  $_0S_2$  affects the amplitude of  $\delta\rho$  variations more than their pattern. Not all scenarios are equally preferred by current seismic data (Section 2.2).

specify the viscosity profile using k control points:

$$\log_{10}(\eta(r)) = \begin{cases} \frac{\eta_2^* - \eta_1^*}{r_2 - r_1} (r - r_1) + \eta_1^*, & r_1 \le r \le r_2 \\ \frac{\eta_{i+1}^* - \eta_i^*}{r_{i+1} - r_i} (r - r_i) + \eta_i^*, & r_i \le r \le r_{i+1} \\ \dots & \\ \frac{\eta_k^* - \eta_{k-1}^*}{r_k - r_{k-1}} (r - r_{k-1}) + \eta_{k-1}^*, & r_{k-1} \le r \le r_k \end{cases}$$

$$(2)$$

where  $\eta_i^*$  and  $r_i$  specify the base-10 logarithm of the viscosity and the radial coordinate of the *i*-th control point.

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# 2.2.2 Inversion method

We use a reversible-jump Markov chain Monte Carlo algorithm (Green, 1995), with 242 parallel tempering (Sambridge, 2014) to find the collection of viscosity profiles compat-243 ible with the observed geoid. The parallel tempering algorithm runs several Markov chains 244 simultaneously at different "temperatures". At increasing temperatures, the objective 245 function is effectively smoother, and higher-temperature chains may more easily move 246 between local minima. The chains are advanced in parallel, and after each 100 steps, pairs 247 of chains are selected via a random permutation and given the opportunity to swap so-248 lutions at different temperatures. Chains with higher temperature therefore perform a 249

more complete exploration of the model space, while the chains with lower temperature explore the neighborhood of the local or global minimum. Only the solutions with temperature T = 1 are sampled in the posterior ensemble. The benefits of parallel tempering are accelerated convergence and a reduced tendency for the chain at T = 1 to find a local, rather than global, minimum in the objective function.

At each step within each of the Markov Chains, we choose one of five events with equal probability: 1) Creation of a new control point; 2) Deletion of an existing control point; 3) Change of viscosity associated with a control point; 4) Change of depth of the control point; and, 5) Change in hierarchical uncertainty parameter. Given a vector  $\underline{m}$ of model parameters, we calculate a vector containing the model geoid spherical harmonic coefficients  $\underline{N}_{model}(\underline{m})$  for comparison with the observed geoid spherical harmonic coefficients  $\underline{N}_{obs}$ . We calculate a residual using the Mahalanobis distance

$$\Phi(\underline{m}) = (\underline{N}_{\text{model}}(\underline{m}) - \underline{N}_{\text{obs}})^{\mathsf{T}} \underline{\underline{C}}_{D}^{-1} (\underline{N}_{\text{model}}(\underline{m}) - \underline{N}_{\text{obs}}).$$
(3)

We introduce a covariance matrix  $\underline{\underline{C}}_{D}$  that represents the data and forward modeling uncertainties, discussed later. We include an additional *hierarchical parameter*,  $\sigma$  with which we scale the covariance matrix,

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$$\underline{\underline{C}}_{D} = \sigma^{2} \underline{\underline{\widetilde{C}}}_{D}.$$
(4)

In an inversion with a hierarchical parameter, it is assumed that the covariance matrix represents the pattern of covariance but not its amplitude, and  $\sigma^2$  can be viewed as an uncertainty hyperparameter. We calculate the likelihood

$$P(\underline{N}_{obs}|\underline{m}, T_i) = \frac{1}{\sqrt{(2\pi)^{n_{lm}} (\sigma^2)^{n_{lm}} \det(\underline{\underline{C}}_D)}} \exp\left(-\frac{\Phi(\underline{m})}{2T_i}\right).$$
(5)

Here,  $T_i$  is the temperature of the *i*-th chain and  $n_{lm}$  is the length of the data vector. Given the likelihood value, we calculate an acceptance probability in log space for the proposed model (denoted with ' and having k' control points) given the current accepted solution (unprimed quantities)

$$\min\left(1, \frac{P(N_{\rm obs}|m')}{P(N_{\rm obs}|m)}\frac{k}{k'}\right). \tag{6}$$

Parallel tempering is implemented through the addition of an exchange step between chains running at different temperatures, following the approach of Sambridge (2014). At each step of the Markov chain, we propose to swap the currently-accepted solutions for *each* of the N chains having temperatures  $T_i, i \in \{1, 2, ..., N\}$ , with a randomly selected chain having temperature  $T_j$ , where  $j \neq i$ . The proposed swap, implemented by swapping temperatures, is accepted with probability

$$\alpha_{ij} = \min\left(1, \left[\frac{P(\underline{N}_{obs}|m_j)}{P(\underline{N}_{obs}|m_i)}\right]^{1/T_i} \left[\frac{P(\underline{N}_{obs}|m_i)}{P(\underline{N}_{obs}|m_j)}\right]^{1/T_j}\right).$$
(7)

We calculate the acceptance probability  $\alpha_{ij}$  in log-space, where

$$\log(\alpha_{ij}) = \min\left(\log\left(1\right), \left(\frac{1}{T_i} - \frac{1}{T_j}\right) \left[\frac{N}{2}\log\left(\frac{\sigma_i^2}{\sigma_j^2}\right) - \frac{1}{2}\left(\frac{\Phi(m_j)}{\sigma_j^2} - \frac{\Phi(m_i)}{\sigma_i^2}\right) + \log\left(\frac{k_i}{k_j}\right)\right]\right).$$
(8)

For each of the inversions, we run 16 Markov chains at temperatures spaced log-285 uniformly from 1–50. Each chain was run for 10 million steps. During the initial phase 286 of the MCMC procedure, we follow Kolb and Lekic (2014) and limit the dimensional-287 ity of the model space by reducing the maximum number of control points that describe 288 the viscosity solution. During this "burn-in" period, we begin by allowing  $N_{\rm max} = 2$ 289 control points and wait  $10,000 \times N_{\text{max}}$  steps before increasing  $N_{\text{max}}$ . The maximum num-290 ber of control points (25) is accessible after  $2.53 \times 10^6$  steps. We begin sampling the pos-291 terior after 5 million steps and verified that the properties of the ensemble had stabilized 292 before sampling began. We verified that the nature of the solutions did not change as 293 the number of control points was increased further for a test inversion. We assume a uni-294 form prior probability density function (pdf) for  $\eta(r)$  that allows for variations over six 295 orders of magnitude. The prior on the number of control points k is proportional to 1/k. 296 New control points are assigned a log-viscosity sampled randomly from the prior. We 297 propose perturbations to the currently accepted solution using gaussian pdfs with a shape 298 parameter of 0.2 log-units for viscosity and 35 km for control point depths. The proposal 299 distribution for changes to the hierarchical parameter  $\sigma$  is a gaussian pdf with shape pa-300 rameter 0.05. To maintain numerical stability, we limit the distance between adjacent 301 control points to 45 km. We verified that our MCMC procedure achieves uniform sam-302 pling of the model space, reflecting the assumption of a uniform prior on viscosity vari-303 ations and a prior on number of control points that is proportional to 1/k. 304

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#### 2.3 Uncertainty quantification

The THB method enables us to estimate the best-fit values of the model parameters and their uncertainty, accounting simultaneously for the effects of data uncertainty (i.e. uncertainty in the density variations from the tomographic model), and in the observational constraints (the geoid spherical harmonic coefficients). The observational un-

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certainties in the geoid spherical harmonic coefficients for the long wavelengths used to constrain our models are very small, on the order of parts per million to parts per thousand (Ries et al., 2016). Therefore, we ignore them in the inversion, and instead focus on quantifying uncertainties in the density variations.

First, for each of the density models, we sample the multivariate random normal 314 distribution described by the posterior covariance matrix of the tomographic model,  $\underline{\underline{C}}_{M}$ , 315 generating an ensemble of models. Each member within this ensemble is a complete whole-316 mantle model of wavespeeds and density evaluated on an equispaced mesh with 2562 points 317 laterally and at 50 km intervals in depth. At each depth, we perform a spherical har-318 monic expansion using routines from the Slepian software package (Simons et al., 2006) 319 which fit the spherical harmonic basis functions to the equispaced point values using a 320 least-squares inversion. Then, for each density model in the ensemble, we perform a for-321 ward mantle flow calculation using a reference viscosity profile (Model C from Steinberger 322 & Holme, 2008) and obtain a set of model geoid spherical harmonic coefficients. These 323 are used to form a sample covariance matrix that represents the data plus forward mod-324 eling uncertainty, with the caveat that we assumed a single viscosity profile when gen-325 erating the ensemble. The number of samples required for accurate estimation of the co-326 variance matrix was not known a priori, but we estimate the minimum number of sam-327 ples required at 35 per pair of parameters. For the 60 geoid coefficients for spherical har-328 monic degrees 2-7, we find that the number of samples is at least  $35 * \binom{60}{2} = 61,950$ . 329 We verified that the eigenvalues of the covariance matrix converge to nearly constant val-330 ues as the number of samples was increased from  $10^3 - 10^5$  (Figure S2). We also car-331 ried out a suite of inversions with a diagonal covariance matrix (i.e. assuming that the 332 combined data and forward-modeling uncertainties associated with each spherical har-333 monic coefficient are equal and uncorrelated). 334

#### 335 **3 Results**

The model viscosity profiles from our inversions are shown in Figure 3 for the endmember density models with least (panels A,C) and most (panels B, D) preferred correlation between  $\rho$  and  $V_S$ . In each panel of Figure 3 we show viscosity profiles (calculated from the mean value in the ensemble solution at each depth) for models constrained by geoid spherical harmonic degrees l = 2 - 3, l = 2&4 (only even degrees), and l =2-7. The shading in Figure 3 represents probability density. Figure S3 shows the pos-

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terior pdf of viscosity for each ensemble separately along with the number of control points 342 and the distribution of variance reduction. We also show mean viscosity profiles and pseu-343 docolor plots of probability density, model complexity, and variance reduction for inver-344 sions with a diagonal data and forward modeling covariance matrix in Figure S4-S5. All 345 of the ensemble solutions have an increase in viscosity between the upper mantle and the 346 lower mantle. The density models with more imposed correlation between  $\rho$  and  $V_S$  (Fig-347 ure 3B,D) yield viscosity solutions that have a low-viscosity channel (roughly 1/10 the 348 average viscosity at 660 km) below the base of the transition zone (660 km) and a rapid 349 increase in viscosity near 1000 km depth. The overall shape of the viscosity profiles ap-350 pear very consistent regardless of which subset of geoid spherical harmonics is used to 351 constrain the inversion. However, the models constrained by more spherical harmonic 352 coefficients in general show more complex viscosity profiles, as expected for the parsi-353 monious inversions employed here. The models with less imposed correlation between 354  $\rho$  and V<sub>S</sub> (Figure 3A,C) show a similar overall increase in viscosity between upper and 355 lower mantle, but more overall variability among the viscosity profiles in the ensemble, 356 as indicated by the broader shaded confidence intervals. We still find evidence for a vis-357 cosity maximum at or somewhat below 1000 km depth. The viscosity profiles shown in 358 Figure 3A,C correspond to density models with less imposed correlation between  $\rho$  and 359  $V_S$  in the lowermost mantle. These density models contain lowermost mantle density het-360 erogeneity that is uncorrelated with the geoid. The low-viscosity region centered between 361 2000–2500 km in panels A,C is required to minimize the sensitivity to density structure 362 at these depths and is discussed later. The systematic development of this low-viscosity 363 region in the lower mantle can be seen as a natural consequence of relaxing the imposed 364 correlation between  $\rho$  and  $V_S$  (i.e. reducing  $\gamma_{\rho}^{D''}$ ) and increasing the data weight assigned 365 to the density-sensitive normal mode splitting measurements (i.e. increasing  $w_{0S_2}$ ). How-366 ever, it may not be a robust feature, as will be discussed later. We show observed and 367 modeled geoids for the four viscosity models from Figure 3 in Figure 4. For all density 368 models, the pattern and amplitude of the synthetic geoid are in reasonably good agree-369 ment with the observations. The variance reduction for the spherical harmonic degrees 370 included in each inversion is shown in Figure 3. 371



Figure 3. Results from viscosity inversions. The density models used in (A,C) have smaller misfit to the normal mode splitting measurements whereas the models in (B,D) have density variations that are strongly correlated with  $V_S$  variations, at the expense of fitting the normal mode constraints. The blue, green, and red curves in each panel correspond to models constrained by spherical harmonic degrees l = 2 - 3, l = 2, 4, and l = 2 - 7 respectively. In each panel, the red, green, and blue colors show the probability distributions for each combination of spherical harmonic degrees. We also show the histogram of geoid variance reduction associated with each model.



Figure 4. Model geoids for l = 2 - 7 for the four end-member density models for inversions with a hierarchical parameter. The model geoids are shown for the "median model" from each ensemble.

#### 372

# 3.1 Interplay of radial viscosity variations and density heterogeneity

We used whole-mantle density models to invert for the mantle viscosity profile as 373 constrained by the long-wavelength geoid. The density models are inverted with full-spectrum 374 tomography using various data-types whose relative contributions in the inversion are 375 set by a priori weights. The scenarios in the model suite differ in their choices for the 376 weight assigned to  $\rho$ -sensitive normal-mode splitting measurements  $(w_0 S_2)$  and the de-377 gree of correlation between  $\rho$  and  $V_S$  variations in the lowermost mantle  $(\gamma_{\rho}^{D''})$ . In gen-378 eral, models with reduced  $\gamma_{\rho}^{D^{\prime\prime}}$  and increased  $w_{_{0}S_{2}}$  provide statistically significant im-379 provements in data fits along with anti-correlated  $V_S - \rho$  structure where the base of 380 LLSVPs are denser than the ambient mantle. In an end-member case, illustrated in Fig-381 ure 2D, the lowermost mantle density structure contains an approximately 1% density 382 excess beneath Africa and the western Pacific, overlapping with the locations of the low-383  $v_S$  LLSVPs but with somewhat discrepant patterns. The preferred density model from 384 (Moulik & Ekström, 2016) adopted a moderate weight ( $w_{0S_2} = 1X$ ) to obtain a den-385 sity excess of around 0.5% in the bottom 500 km of LLSVPs. 386

When lateral viscosity variations are ignored, lateral heterogeneity at a given spherical harmonic degree and order can only cause geoid anomalies at the same degree and order with no coupling across harmonics. It is therefore possible to represent the sen-

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sitivity of the geoid to perturbations in density structure at different depths through the 390 geoid kernel (e.g. Hager, 1984; Richards & Hager, 1984). The misfit between modeled 391 and observed geoid anomalies is minimized when the geoid kernel takes on positive val-392 ues at depths where the pattern of mantle buoyancy variations is strongly correlated with 393 the geoid and negative values at depths where the buoyancy structure is anti-correlated 394 with the geoid. At depths where the mantle buoyancy structure is uncorrelated with the 395 geoid, the residual can only be minimized by ensuring that the geoid kernel, itself a func-396 tion of the radial viscosity structure, takes on a value close to zero. Approximately 70%397 of the power in the dynamic geoid is concentrated in the lowest spherical harmonic de-398 grees 2-3, and power falls off rapidly with increasing degree (e.g. Kaula, 1966). There-399 fore, we conclude that it is possible to obtain reasonable fits to the observed geoid for 400 all density models explored because at the long wavelengths considered here, lateral het-401 erogeneity is either strongly correlated or anti-correlated with the geoid throughout much 402 of the mantle. 403

The correlation between the long-wavelength geoid and density variations in our 404 model suite varies across density models and with depth. In Figure 5(C,F,I,L), we show 405 the correlation between the geoid and the density structure in four end-member density 406 models for spherical harmonic degrees 2, 3, and 4. Models 160 and 172 both exhibit den-407 sity variations that are highly correlated with  $V_S$  variations, and we can see clearly that 408 the degree 2–4 density structure is highly correlated with the geoid in the upper man-409 tle, and that the degree 2–3 density structure is highly anti-correlated with the geoid in 410 the lower mantle. This pattern of correlation is a common feature of almost all published 411 shear-wave tomographic models. On the other hand, models 155 and 167 (Figure 5C,I) 412 that relax the imposed  $V_S$ - $\rho$  correlation and assign more weight to the density-sensitive 413 normal-mode data have degree-2 density structure that is anti-correlated with the geoid 414 through the mid mantle (660–2000 km depth) but positively correlated with the geoid 415 in the bottom  $\sim 500$  km of the mantle. Since our normal-mode data do not constrain 416 the odd-degree density variations (e.g. Resovsky & Ritzwoller, 1995; Deuss et al., 2011), 417 degree-3 density variations do not depart from scaling to the  $V_S$  models, and the degree-418 3 density structure in all density model scenarios shows a transition from anti-correlation 419 to correlation with the good, tracking the behavior seen with  $V_S$  models. Because the 420 degree-2 and degree-3 geoid kernels are generally very similar in their overall shape for 421 a given viscosity structure, it is more challenging to obtain a viscosity profile that matches 422

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the observed geoid. For density models 155 and 167, we recovered viscosity profiles shown 423 in Figure 5(A,G). The geoid kernels corresponding to the "median model" from each en-424 semble are shown in Figure 5(B,H). Here we differentiate between the "ensemble aver-425 age"- the mean viscosity value present in the posterior ensemble at each depth and the 426 "median model" - the individual solution from the ensemble whose likelihood is closest 427 to the peak of the likelihood distribution in the ensemble. Model 155 has degree-2 low-428 ermost mantle structure that is overall less well-correlated with the good than Model 429 167. The viscosity profiles for inversions constrained by l = 2 + 4 and l = 2 - 7 for 430 Model 155, shown in Figure 5B generally remove sensitivity in the lowermost mantle, 431 where much of the power in the buoyancy field is poorly correlated with the geoid. The 432 sensitivity is suppressed by the introduction of a viscosity reduction around 2000 km depth. 433 Model 167 contains degree-2 structure that is more positively correlated with the observed 434 geoid than Model 155, but other spherical harmonic degrees remain negatively correlated 435 (e.g. degree 3) or very weakly negatively correlated (degree 4). Consequently, the vis-436 cosity profiles obtained using Model 167 contain an even more pronounced reduction in 437 viscosity above D'', effectively suppressing geoid sensitivity in the lowermost mantle. Our 438 results demonstrate that the relative patterns and amplitudes of long-wavelength den-439 sity variations influence inferences on radial viscosity structure in a non-linear fashion. 440 Evaluating the consistency between even- and odd-degree density variations with new 441 seismic constraints will be critical to improved constraints on viscosity structure. 442

In Figure 5(A,D,G,J), we show selected models from the posterior ensemble solu-443 tions (dotted lines) as well as the ensemble mean and shaded confidence interval. It is 444 important to note that the individual solutions in many cases possess far more overall 445 variation in viscosity than the ensemble average. Furthermore, because the geoid ker-446 nels depend strongly on the viscosity profile, the ensemble average itself may not pro-447 duce a small misfit to the geoid. Instead, the ensemble average and confidence interval 448 should be viewed as an indicator of the common properties of accepted solutions, and 449 the range of uncertainty in the model parameters. 450

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# 3.2 Uncertainty quantification

The transdimensional, hierarchical Bayesian approach used here yields samples from the posterior that can be used to directly quantify uncertainty in the viscosity profile, regardless of the shape of the posterior distribution. This is in contrast with uncertainty

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quantification in linearized inversions in which the posterior in approximated by a multivariate normal distribution. When the posterior probability density is "close" to a normal distribution, the posterior covariance operator can be approximated through a linearization around the maximum likelihood solution ( $\underline{m}_{ml}$ ) using Equation 3.56 of (Tarantola, 2005)

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$$\underline{\underline{\widetilde{C}}}_{M}^{lin} \simeq \left(\underline{\underline{G}}^{T} \underline{\underline{C}}_{D}^{-1} \underline{\underline{G}} + \underline{\underline{C}}_{M}\right)^{-1} \tag{9}$$

where  $\underline{\underline{C}}_{D}$  is the covariance matrix representing data and forward modeling uncertainty,  $\underline{\underline{C}}_{M}$  is the prior covariance matrix, and  $\underline{\underline{G}}$  contains partial derivatives of the forward model operator (geoid kernels  $g_i$ ) with respect to the model parameters  $\underline{\underline{m}}$ ,

464 
$$G_{ij} = \frac{\partial g_i}{\partial m_j}\Big|_{m=m_{ml}}.$$
 (10)

For the uniform, very broad prior on viscosity assumed here, the prior covariance matrix in Equation 9 effectively vanishes.

To better understand the uncertainty estimates recovered by our method and to 467 compare these estimates with those that could be obtained using other, more established, 468 methods in geophysics, we compute a few illustrative results. First, we compute the es-469 timate of the posterior covariance matrix around the maximum likelihood point. We iden-470 tify the "median model" from the posterior ensemble, interpolate it onto 20 regularly-471 spaced points in depth, and calculate the partial derivatives of the geoid coefficients with 472 respect to viscosity using numerical differentiation. We compute  $\underline{\underline{\widetilde{C}}}_{M}^{lin}$  using the Moore-473 Penrose pseudoinverse because in some cases (especially without a prior on viscosity) the 474 covariance matrices are nearly singular. The posterior covariance matrix  $\underline{\widetilde{C}}_{M}^{lin}$  is shown 475 in Figure 6A and selected rows of the covariance matrix are shown Figure 6B-C. We also 476 computed an estimate of the posterior covariance matrix including prior uncertainties 477 on  $\log_{10} \eta(r)$  of 0.5 (log-units), shown in Figure 6D-F. Regardless of whether the prior 478 on  $\eta$  is included, the covariance matrices shown here represent very strong tradeoffs be-479 tween parameters and depths at which the model has little sensitivity. 480

Figure 7 illustrates the uncertainty on the viscosity profiles implied by the actual posterior ensemble, a re-sampling of the same ensemble, and by the covariance around the maximum likelihood point (Equation 9). The results shown correspond to density Model 155, constrained by spherical harmonic degrees l = 2-7. In Figure 7B, we generated a sample covariance matrix from the posterior ensemble, and then sampled viscosity profiles from this covariance matrix. In Figure 7, we show the pdf corresponding to the linear estimate of  $\tilde{C}_{M}^{lin}$  from Equation 9 with a flat, broad prior on  $\eta$  ( $\underline{C}_{M}^{-1} = \underline{0}$ ). Three key observations emerge from this analysis. First, the posterior pdf in our ensemble solutions is not well-described by a multivariate normal distribution. Second, the posterior is multimodal at some depths. Third, the linearized covariance operator grossly underestimates the true variability among solutions accepted in the posterior ensemble. All three are a direct consequence of the non-linearity inherent in the inversion of geoid data for viscosity, as illustrated in Figure 1.

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# 3.3 Mechanisms for radial viscosity variations

In a mantle with pyrolitic composition, phase transitions of olivine to its high-pressure 495 polymorphs have important implications for the inferences of viscosity in the transition 496 zone. We recover no large variations in viscosity at 410 km and within the mantle tran-497 sition zone (410-650 km), consistent with recent global inversions of shear attenuation 498 (Moulik, 2016). Large changes in viscosity or the potentially related shear attenuation 499 in the transition zone can be disfavored based on mineralogical considerations; phase tran-500 sition from olivine to wadsleyite ( $\sim$ 410 km) and ringwoodite ( $\sim$ 550 km) do not involve 501 a wholesale reordering of the unit cell structure as in the ringwoodite to perovskite tran-502 sition ( $\sim 650$  km). Other complicating effects such as grain size reduction could influence 503 the nature of viscosity variations across the 650-km discontinuity (e.g. Panasyuk & Hager, 504 1998; Solomatov & Reese, 2008; Dannberg et al., 2017). 505

An increase in viscosity below the base of the transition zone is a persistent fea-506 ture among the viscosity profiles from our inversions (Figure 3). The origin of this fea-507 ture cannot be easily attributed to a single physical mechanism since its depth is not co-508 incident with known mantle phase transitions; nevertheless, several plausible explana-509 tions exist, many of which are not mutually exclusive. The inversions using models 160 510 and 172, both of which have density structures that closely resemble scaled  $V_S$  tomog-511 raphy, generally favor the presence of a reduction in viscosity at 660 km depth and a sub-512 sequent increase in viscosity close to 1000 km depth. Similar low-viscosity channels were 513 recovered in viscosity inversions constrained by the global long-wavelength geoid (Forte 514 et al., 1993) and by shorter-wavelength (l = 12 - 25) variations in the oceanic geoid 515 (Kido et al., 1998). 516

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Figure 5. Viscosity profiles, geoid kernels, and the correlation between  $\rho$  and geoid anomaly for Models 155 (A-C), 160 (D-F), 167 (G-I), and 172 (J-L). In panels (A,D,G,J), we show the ensemble mean (solid) and the median model (dotted) for the inversions with hierarchical parameter. The shaded region indicates a 90% confidence interval. (B,E,H,K) show geoid kernels for the median model for each inversion. Blue, grey, and red curves correspond to inversions constrained by spherical harmonic degrees l=2-3, l=2,4, and l=2-7, respectively and the kernels for degrees 2-4 are shown using solid, dashed, and dash-dotted lines. The kernels are normalized to unit amplitude and shifted for clarity. (C,F,I,L) Here we show the correlation between  $\rho$  and the geoid for spherical harmonic degrees 2, 3, and 4 for each of the density models.



Figure 6. Linearized estimates of the posterior covariance matrix  $\underline{\tilde{C}}_{M}^{lin}$  for viscosity for the inversion using density Model 155. Panels (A) and (D) illustrate the pattern of covariance without and with a prior on viscosity. In (D), the prior assumes an uncorrelated uncertainty in viscosity of 0.5 log-units. In panels (B-C) we show rows of the covariance operator for depths closest to 600 km and 1000 km corresponding to (A). Panels E-F show the same information as (B-C) for the covariance operator in panel D.



Figure 7. Posterior probability distribution (pdf) for viscosity. (A) shows the true sampling of the posterior ensemble. (B) shows a multivariate normal distribution approximating the pdf in (A). (C) shows a pdf centered around the maximum likelihood solution (black curve) described by the linearization in Equation 9. We note that the pdf in (B) significantly overestimates the uncertainty of model at most depths while the pdf in (C) underestimates the uncertainty represented by the true posterior.

A reduction in viscosity below 650 km depth might be associated with grain size 517 reduction as downwelling material crosses the perovskite-forming phase transition. The 518 radial extent of the low-viscosity region below the 660 km phase transition could be much 519 smaller than the feature recovered in our inversions, with a thickness of about 1 km es-520 timated on theoretical grounds (Panasyuk & Hager, 1998). Alternatively, upwelling plumes 521 could be blocked partially by an endothermic phase transition, resulting in ponding of 522 warm, low-viscosity material below the transition zone. The presence of a reduced-viscosity 523 channel below the 650 km phase transition may have important dynamical implications. 524 Sinking slabs could move laterally with relative ease through a low viscosity region, pro-525 moting stagnation in the transition zone beneath the northwest Pacific and eastern China 526 as observed in tomographic models (e.g. Fukao et al., 2009; Moulik & Ekström, 2014; 527 French & Romanowicz, 2014) and confirmed using geodynamic models that include a 528 low-viscosity channel and an endothermic phase transition (Mao & Zhong, 2018; Lourence 529 & Rudolph, 2020). 530

An increase in viscosity around 1000 km depth has been supported by multiple stud-531 ies of the mantle viscosity profile constrained by glacial isostatic adjustment and geoid 532 (King & Masters, 1992; Mitrovica & Forte, 1997). For highly simplified two-layer vis-533 cosity structures in which the depth and magnitude of a viscosity contrast are the only 534 parameters, preferred depth of the viscosity increase between the shallow and deep man-535 tle depends on the definition of misfit (e.g. correlation, L2-norm) and on the assump-536 tions used to generate buoyancy structures from mantle tomography, but the results uni-537 formly favor a viscosity increase below 660 km, with preferred depths c. 800-1200 km 538 (Forte, 1989; Rudolph et al., 2015). The reason that geoid inversions favor a deeper vis-539 cosity increase can be understood from an inspection of the geoid kernels and the cor-540 relation between the geoid and tomography models. The degree-2 geoid is positively cor-541 related with buoyancy structure throughout the upper mantle, and while there is a de-542 crease in the correlation coefficient between geoid and buoyancy at 650 km depth, the 543 correlation remains positive for several models down to almost 1000 km. In the presence 544 of an increase in viscosity, the geoid kernels for layered viscosity structure change sign 545 from positive in the upper layer to negative in the lower layer, and the depth of the change 546 547 in sign increases with the depth of the viscosity increase.

<sup>548</sup> Our previous work found that the positive  $V_S$ -geoid correlation persists to ~1000 km <sup>549</sup> depth in models that employ continuous and smooth parameterization thereby recov-

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ering smooth changes in the heterogeneity spectrum across the 650-km phase transition 550 (French & Romanowicz, 2014). Such a paramaterization can lead to smearing of hetero-551 geneity from the transition zone to the uppermost lower mantle (Gu et al., 2001), espe-552 cially when employing data sensitive to these depths such as normal modes (Moulik & 553 Ekström, 2014). Nevertheless, all of the density models used here contain an abrupt re-554 duction in correlation between density variations and the degree 2-3 geoid at 650-km depth 555 (Figure 5(C,F,I,L)), as well as a decrease in the RMS amplitude of both overall power 556 and power at low degrees (Moulik & Ekström, 2014). However, at degrees 2-4, the cor-557 relation between density heterogeneity and the geoid remains positive below 650 km, per-558 sisting to 800-1200 km (e.g. Figure 5F). The dramatic reduction in density-geoid cor-559 relation at 650 km depth coincides with an allowed discontinuity between the 16 cubic 560 splines in the radial direction (Moulik & Ekström, 2016). This choice, common across 561 a subset of recent tomographic models (Kustowski et al., 2008; Moulik & Ekström, 2014), 562 represents the *a priori* information that deviations in large-scale pattern of mantle het-563 erogeneity could coincide with the 650-km phase transition and is substantiated by the 564 improved fits to precursors of the body-wave phase SS that reflect off this discontinu-565 ity (Gu et al., 2003). Boschi and Becker (2011) reported improved fit to body wave travel 566 times with a greater depth of decorrelation ( $\sim 800$  km) but did not include additional 567 data such as SS precursors that directly constrain transition zone topography, which trades 568 off with volumetric wavespeed variations at shallow lower mantle depths (Moulik & Ek-569 ström, 2014). In our previous inferences of viscosity based on SEMUCB-WM1 (French 570 & Romanowicz, 2014), which has a continuous, smooth, parameterization in the radial 571 direction, we recovered solutions favoring an increase in viscosity near 1000 km depth 572 (Rudolph et al., 2015). It is noteworthy that in spite of the allowed decorrelation at 650 km 573 depth in the density models used here, we still recover viscosity structures that prefer 574 a viscosity increase somewhat deeper than the base of the transition zone, which we at-575 tribute to the fact that for spherical harmonic degrees 2 and 4, the correlation between 576 density structure and geoid remains positive below the base of the transition zone, and 577 only becomes negative deeper within the lower mantle. The deeper viscosity increase is 578 driven by the dominant degree-2 variation that has a positive correlation with the geoid 579 which persists to the uppermost lower mantle. 580

Several potential mechanisms exist that could explain an increase in viscosity below the 650-km discontinuity. First, Marquardt and Miyagi (2015) measured the strength

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of ferropericlase and found a threefold increase in strength over the pressure range 20-583 65 GPa. Though ferropericlase constitutes the minority of the lower mantle, Marquardt 584 and Miyagi (2015) argue that it could form interconnected layers/sheets especially in high 585 strain-rate regions, controlling the lower mantle rheology, an idea that is supported by 586 two-phase deformation experiments on analogue materials (Kaercher et al., 2016) and 587 on mixtures of Bridgmanite and Magnesiowüstite (Girard et al., 2016). Second, changes 588 in the proportionation of iron between bridgmanite and ferropericlase in the depth range 589 of 1200-1600 km could produce a mid-mantle viscosity hill (Shim et al., 2017). If a greater 590 proportion of iron is incorporated in ferropericlase, the melting temperature of bridg-591 manite increases, and viscosity is expected to increase based on homologous tempera-592 ture scaling. Shim et al. (2017) predict a viscosity hill with a maximum viscosity at  $\sim$ 593 1200 km depth and a value approximately two orders of magnitude larger than the vis-594 cosity at 660-km depth. The magnitude of the predicted viscosity variation and the depth 595 of the viscosity maximum are in reasonably good agreement with the viscosity profiles 596 shown here. Third, Deng and Lee (2017) measured the solidus and liquidus temperatures 597 of ferropericlase and found a maximum at pressures corresponding to 1000 km depth, 598 again implying an increase in viscosity on the basis of homologous temperature scaling. 599 These various mechanisms do not appear to be mutually incompatible. 600

601

#### 3.4 Implications for joint modeling of seismic and geodynamic data

Some of the earliest tomographic models (e.g. Woodhouse & Dziewoński, 1984) ex-602 hibited large-scale structures that were fairly well correlated with the major surface man-603 ifestations of mantle convection, such as the long-wavelength non-hydrostatic geoid (Hager 604 et al., 1985) and the large-scale tectonic plate motions (Forte & Peltier, 1987). Recent 605 tomographic models, such as the ones used here based on Moulik and Ekström (2016), 606 have afforded refined images and better fits to diverse measurements from broadband 607 seismograms. The analysis presented above has focused on how seismically-inferred man-608 the density structure may be used to model mantle flow in order to predict surface ob-609 servables. However, our results also have major implications for the converse approach, 610 i.e. inferring mantle structure from either geodynamic observations in isolation (e.g. Hager, 611 1984; Ricard et al., 1989; Forte, 1989) or jointly with seismic data (e.g. Simmons et al., 612 2010).613

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The earliest inferences of radial viscosity variation (e.g. Hager et al., 1985) assumed 614 constant scaling throughout the mantle to convert velocity variations to those of den-615 sity that drive mantle flow. This is only appropriate for a purely thermal contribution 616 to seismic velocity heterogeneity throughout the mantle, and is contrary to multiple lines 617 of seismic evidence (e.g. Ritsema & Lekic, 2020) including normal mode (Moulik & Ek-618 ström, 2016) and tidal constraints (Lau et al., 2017). Such scaling assumptions are also 619 employed in the construction of recent tomographic models (e.g. Ritsema et al., 2011; 620 French & Romanowicz, 2014), which assume fixed scalings between  $d \ln V_S$ ,  $d \ln V_P$ , and 621  $d \ln \rho$ , in order to account for data sensitivity to parameters that are not directly inverted 622 for. When attempts are made to jointly model seismic and geodynamic data (e.g. Sim-623 mons et al., 2009), observations such as normal modes that can uniquely disentangle the 624 density contributions from those of other elastic parameters are often excluded. Our re-625 sults demonstrate that inferences of viscosity variations and thereby mantle flow depend 626 strongly on the density models. Inferred jumps and gradients in viscosity from a corre-627 lated  $V_S$ - $\rho$  model can differ from an independent  $\rho$  inversion by up to 2 orders of mag-628 nitude and contain features such as low-viscosity channels. Therefore, dynamical infer-629 ences based on constant  $V_S$ - $\rho$  scaling assumptions or tomographic models constructed 630 therewith may be biased in the dynamically important boundary regions of the Earth 631 e.g. transition zone and lowermost mantle. 632

Several recent studies have attempted to relate dynamical observations (e.g. geoid) 633 to structural heterogeneity (e.g. temperature, velocity, density) to jointly constrain man-634 tle flow dynamics. For example, Simmons et al. (2009) inverted some geodynamic and 635 a small subset of available seismic constraints, primarily body wave arrival times, for lat-636 eral heterogeneity assuming a fixed viscosity profile (Mitrovica & Forte, 2004). We demon-637 strate that sensitivity kernels that relate plate motions and geoid to density variations 638 (Figure 5) depend strongly on viscosity variations. Radial viscosity changes can amplify 639 sensitivity in depth ranges where density variations are consistent with the good anoma-640 lies, and even nullify sensitivity in regions where the two are dissimilar. The use of a con-641 stant radial viscosity profile in earlier studies implicitly introduces a strong a priori as-642 sumption about the relative contribution of heterogeneity at various depths to surface 643 geodynamic observations. An iterative procedure of recalculating sensitivity kernels may 644 help converge towards a self-consistent solution of radial viscosity variations and struc-645 tural heterogeneity. 646

Our results on radial viscosity variations could potentially inform the parameter-647 ization and regularization choices in seismic tomography. Moulik and Ekström (2016) 648 employed a parameterization that allowed various spherical harmonic degrees in density 649 structure to deviate from a scaled  $V_S$  structure as dictated by seismic observations. Since 650 the self-coupled normal-mode splitting observations constrain only even-degree density 651 variations, all inversions strongly disfavored even-degree  $V_S$ - $\rho$  correlation ( $R_2 \sim -0.46$ 652 to -0.25) in the lowermost mantle while retaining the starting assumptions on positive 653  $V_S - \rho$  correlation in the remaining regions and for odd degree variations. The opposing 654 sign of the correlation of the longest wavelength even- vs. odd-degree structure with the 655 geoid maps into a region of reduced viscosity in the lower mantle in our viscosity inver-656 sions. Since this viscosity feature is a product of current limitations in data, it needs fur-657 ther evaluation with odd-degree sensitive observations (e.g. Resovsky & Ritzwoller, 1995). 658

An alternative approach to suppress this even-odd degree dichotomy in  $V_S$ - $\rho$  cor-659 relation is to parameterize structural heterogeneity in terms of a radial  $V_S$ - $\rho$  scaling ra-660 tio and three-dimensional velocity heterogeneity, as used in previous inversion (e.g. Robert-661 son & Woodhouse, 1996; Simmons et al., 2009) and forward modeling schemes (e.g. Lau 662 et al., 2017; Koelemeijer et al., 2017). In contrast to the methods employed in our mod-663 eling, this approach enforces perfect  $V_{S}$ - $\rho$  (anti)correlation with a radially varying scal-664 ing factor that is consistent across spherical harmonic degrees, and would likely disfa-665 vor a low viscosity channel in the lower mantle. However, it is not immediately clear if 666 such a strong prior assumption on  $V_S$ - $\rho$  scaling is either compatible with data or is phys-667 ically reasonable in a strongly heterogeneous boundary region. Various mechanisms (e.g. 668 partial melt, iron enrichment, primordial material, grain size variations) may manifest 669 more strongly at different spatial scales in the lowermost mantle and get expressed as 670 spatially varying correlations and amplitudes of  $V_{S}$ - $\rho$  scaling. For instance, small-scale 671 structures such as Ultra Low Velocity Zones (e.g. Thorne & Garnero, 2004; Rost et al., 672 2005; Cottaar & Romanowicz, 2012) may have a different physical origin (and associ-673 ated  $V_S - \rho$  scaling) than the larger-scale LLSVPs. Joint and iterative inversions of struc-674 tural heterogeneity and radial viscosity variations with new and improved measurements 675 may help disentangle such effects in the Earth's deep interior. 676

# 677 4 Conclusions

We used recently-developed whole-mantle  $V_P$ ,  $V_S$  and density models from full-spectrum 678 tomography (Moulik & Ekström, 2016), together with their associated covariance ma-679 trices, to infer the mantle viscosity profile as constrained by the long-wavelength gooid. 680 The resulting inferences of depth-variation in viscosity contain several persistent features, 681 including an increase in viscosity below the base of the mantle transition zone (often near 682 1000 km depth) and a maximum in mantle viscosity at mid-mantle depths. Our ensem-683 ble solutions permit the quantification of uncertainties in the inferences of viscosity. We 684 found that uncertainty estimates based on linearized inversions are likely to woefully un-685 derstate true uncertainty, and therefore the robustness of specific complexities in viscos-686 ity profiles that were justified using an uncertainty analysis based on covariance around 687 the maximum likelihood point. This might explain why so many different viscosity pro-688 files have been proposed based on inversions constrained by similar gravity data and us-689 ing similar forward modeling assumptions. 690

It is noteworthy that the mid-mantle viscosity increase persists in the suite of in-691 versions presented here despite the use of a radial parameterization in the tomographic 692 model suite that includes a discontinuity at 650 km depth as opposed to the smooth ra-693 dial parameterization used in SEMUCB-WM1, the basis for our previous inferences that 694 favored a viscosity increase at  $\sim 1000$  km depth (Rudolph et al., 2015). The detailed 695 features of our inversions are refined in the upper mantle, within and below the transi-696 tion zone. The robustness of our inferences is evaluated across a suite of density mod-697 els. Density variations that most-closely resemble the  $V_S$  structure predict viscosity struc-698 tures that contain a low-viscosity channel below the 660 km discontinuity. While mod-699 els with anti-correlated  $V_S - \rho$  structure in the lowermost mantle with the base of LLSVPs 700 denser than the ambient mantle fit the seismological constraints significantly better, they 701 currently provide discrepant even and odd-degree correlations with the good and poorer 702 overall correlation. The best-fitting viscosity profiles for these seismically-preferred mod-703 els tend to contain a low-viscosity channel between  $\sim 2000-2500$  km depth that acts to 704 reduce the geoid sensitivity to buoyancy variations in the lowermost mantle. For all of 705 the density models considered, it is possible to find a viscosity profile that accurately pre-706 dicts the geoid. Iteratively solving for radial viscosity variations and density heterogene-707 ity is likely to account for their strong nonlinear relationship in joint inversions of seis-708 mological and geophysical observations. New seismological constraints on density struc-709

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ture and joint modeling with the geoid may provide improved insights on the thermo-

<sup>711</sup> chemical nature of the lowermost mantle.

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