Tomographic filtering of shear and compressional wave models reveals uncorrelated variations in the lowermost mantle

Jun Su[1,2], Christine Houser[1], John W. Hernlund[1,2], Frédéric Deschamps[3]

[1] *Earth-Life Science Institute, Tokyo Institute of Technology, Tokyo* 152-8551*, Japan. E-mail: junsu@elsi.jp*

[2] *Department of Earth and Planetary Science, Tokyo Institute of Technology, Tokyo* 152-8551*, Japan*

[3] *Institute of Earth Sciences, Academia Sinica, Taipei* 11529*, Taiwan*

S.1 SVD inversion results

One utility of using SVD for a tomographic inversion is that it is only necessary to perform the calculation of $\mathbf{G}^\dagger$ once. The final inversion model is then a truncated $\mathbf{G}^\dagger$ at a level which balances fitting the data without over-fitting the inversion. We remind the reader that creating new inversion models is not the goal of this study. Our goal is to establish a quantitative assessment tool utilizing the resolution operator. However, we include a brief discussion here to demonstrate that the SVD is recovering the general patterns of slow and fast velocity anomalies found in lower mantle tomography models.

We can calculate an approximate inverse model in order to check the influence of singular value truncation.

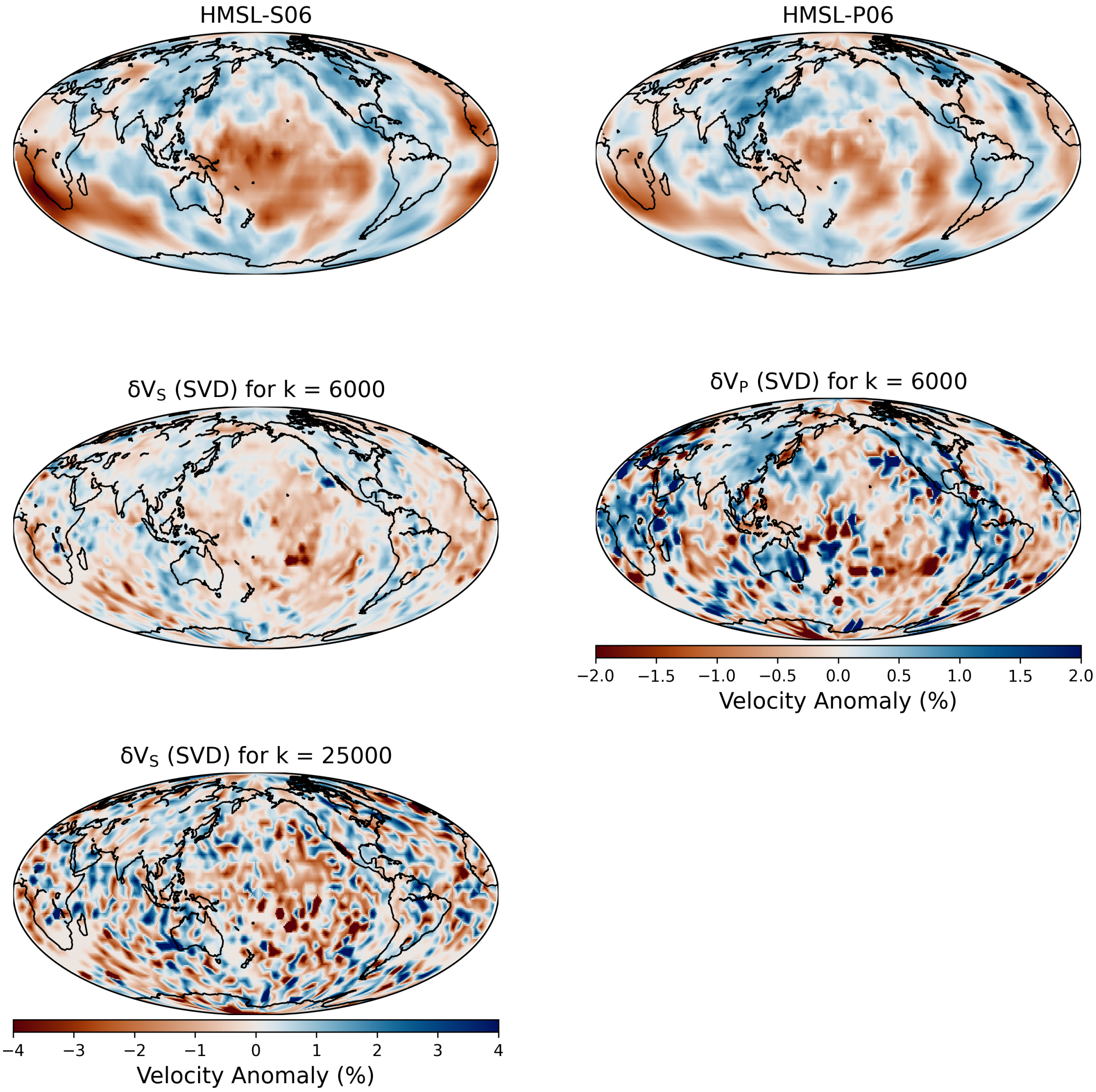
$$\mathbf{m}^\dagger = \mathcal{T}(\mathbf{G}^\dagger)\mathbf{d} = \mathbf{VLZU}^T\mathbf{d}, \quad (1)$$

where we can control the number of singular values by selecting a corresponding $\mathbf{L}$.

When using no regularization (i.e., $\mathbf{L} = \mathbf{I}$) we over-fit and the solution becomes unstable. The solution fluctuates in neighboring blocks similar to Gibb's phenomenon on the edge of a indifferentiable function, with increasing amplitude as more singular values are included until reaching unstable solution.

Supplementary Figure 1 shows the numerical instability that potentially happens when choosing an inappropriate value of truncation factor k that controls the number of singular values being used. For the V_S model, when k equals 6000, we get a rough model that to first-order corresponds to the LSQR approach. However, it starts over-fitting at some point before $k = 25000$, where patchy and large amplitude fluctuations show up globally, and a numerical instability happens in the lowermost mantle when using a full matrix ($k = 36092$) to reconstruct the unevenly sampled lower mantle. A similar pattern appears in the V_P model arguably starting from $k = 6000$, while some regions are still relatively smooth.

We infer this instability to be the result of a lack of constraints on the uncertainty in $\mathbf{d}$, because obtaining $\mathbf{m}^\dagger$ by applying $\mathbf{R}$ to $\mathbf{m}^t$ does not depend on $\mathbf{d}$ as an input such that $\mathbf{G}^\dagger$ implicitly considers the given data must be perfectly consistent with no measurement error.



Supplementary Figure 1: The HMSL model in comparison to inversion δV_S (left column) and δV_P (right column) models obtained by SVD method for the bottom layer at 2800 km. The top row shows the HMSL-S06 model produced using the LSQR method. We construct the inversion models with the truncation factor k, which equals the number of vectors used at $\mathbf{Z}$, in 6000 and 25000.

Truncation gives a larger margin of tolerance to avoid the unstable solution, but it inevitably loses more details.

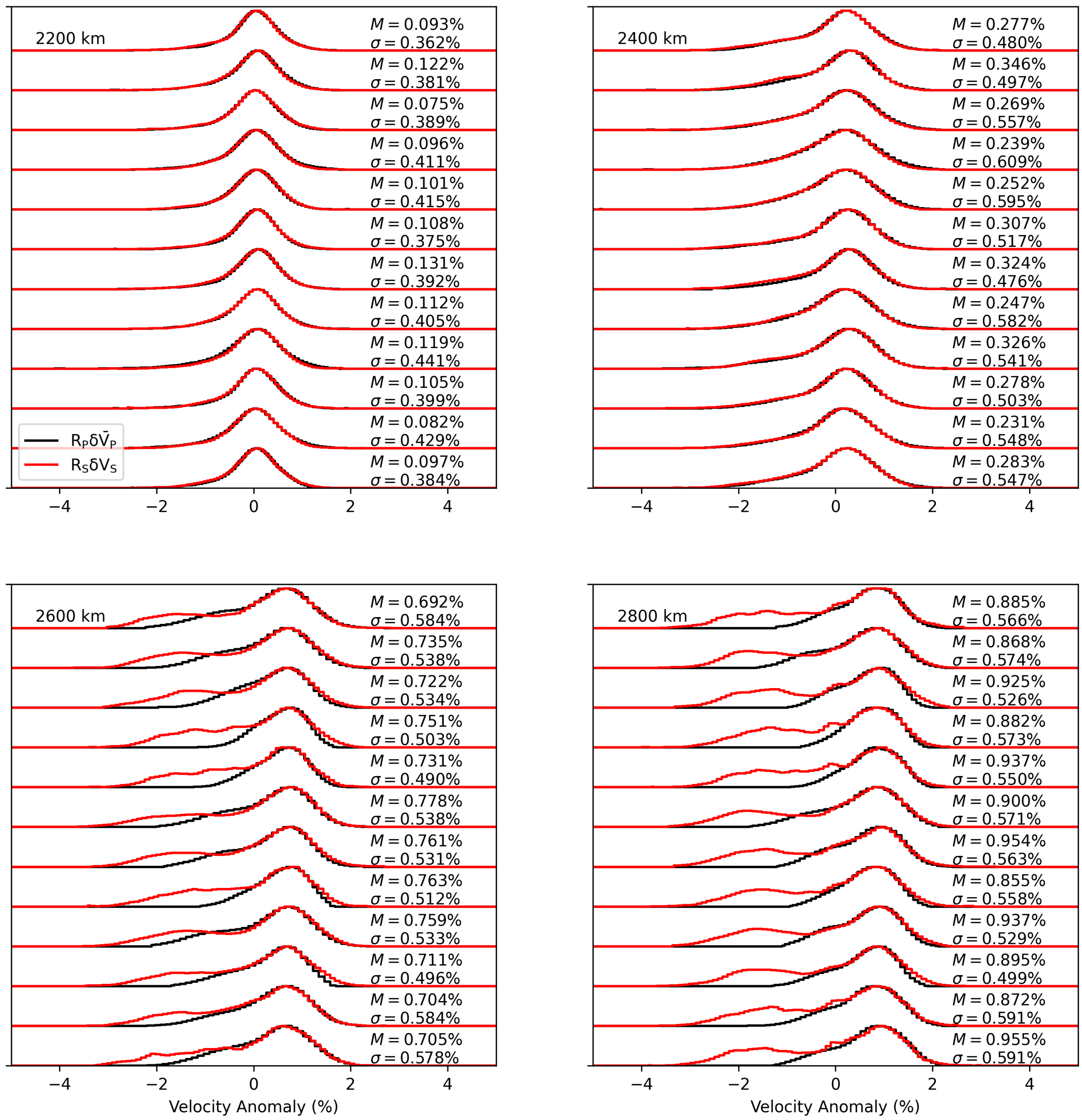
An inversion model using ≈6000 provides a demonstration of our SVD approach applied to the HMSL data. The inversion with 6000 singular values is not as smooth as the original HMSL model, the latter of which used roughness damping that results in a much smoother solution. The pseudo inverse obtained from the SVD is nevertheless suitable for application as a tomographic filter to determine how the ray path coverage represented by the kernel is capable of resolving hypothesized structures in the mantle.

S.2 Influence of geographical difference on the resolution of synthetic models

Geological distribution of the primordial material, post-perovskite, and their derived velocity structure in the geodynamic models is arbitrary and may not seem to represent the Africa-Pacific pattern observed for LLSVPs owing to poorly constrained initial conditions. If most low-resolution areas happen to coincide with the same kind of structure, the measurement of a "slow-tail" in distribution curves would possibly be biased. To test the impact of the relatively lower data coverage in the southern hemisphere where LLSVP reside, we perform the statistical analysis on a set of rotated results and obtain the average value for volume fraction (X_{het}) in Table 2. We utilize Rodrigues' rotation formula to obtain the position vector $\mathbf{v_{rot}}$ of a point in a rotated coordinate:

$$\mathbf{v_{rot}} = cos\theta\mathbf{v} + sin\theta(\mathbf{u} \times \mathbf{v}) + (1 - cos\theta)(\mathbf{u} \cdot \mathbf{v})\mathbf{u}, \tag{2}$$

where $\mathbf{v}$ is the position vector of the point in the original geodynamical model, $\mathbf{u}$ is the axis of rotation, and θ is the rotation angle. We rotate the geodynamic models by moving a reference point $(0°, 90°\mathrm{N})$ on the spherical surface of the polar coordinate to twelve vertices of icosahedron evenly distributed on the same surface, before downsampling the velocity models to the parameterization of HMSL models and applying tomographic filters. Distribution curves derived from the rotated results (Supplementary Figure 2) are consistent at first order, which suggests that the degree-2 velocity structure related to primordial material in TC4-pPv is robust in our measurement and implies that the absence of slow tails in distributions for δV_P is unlikely to be explained by the geographical difference in resolution.

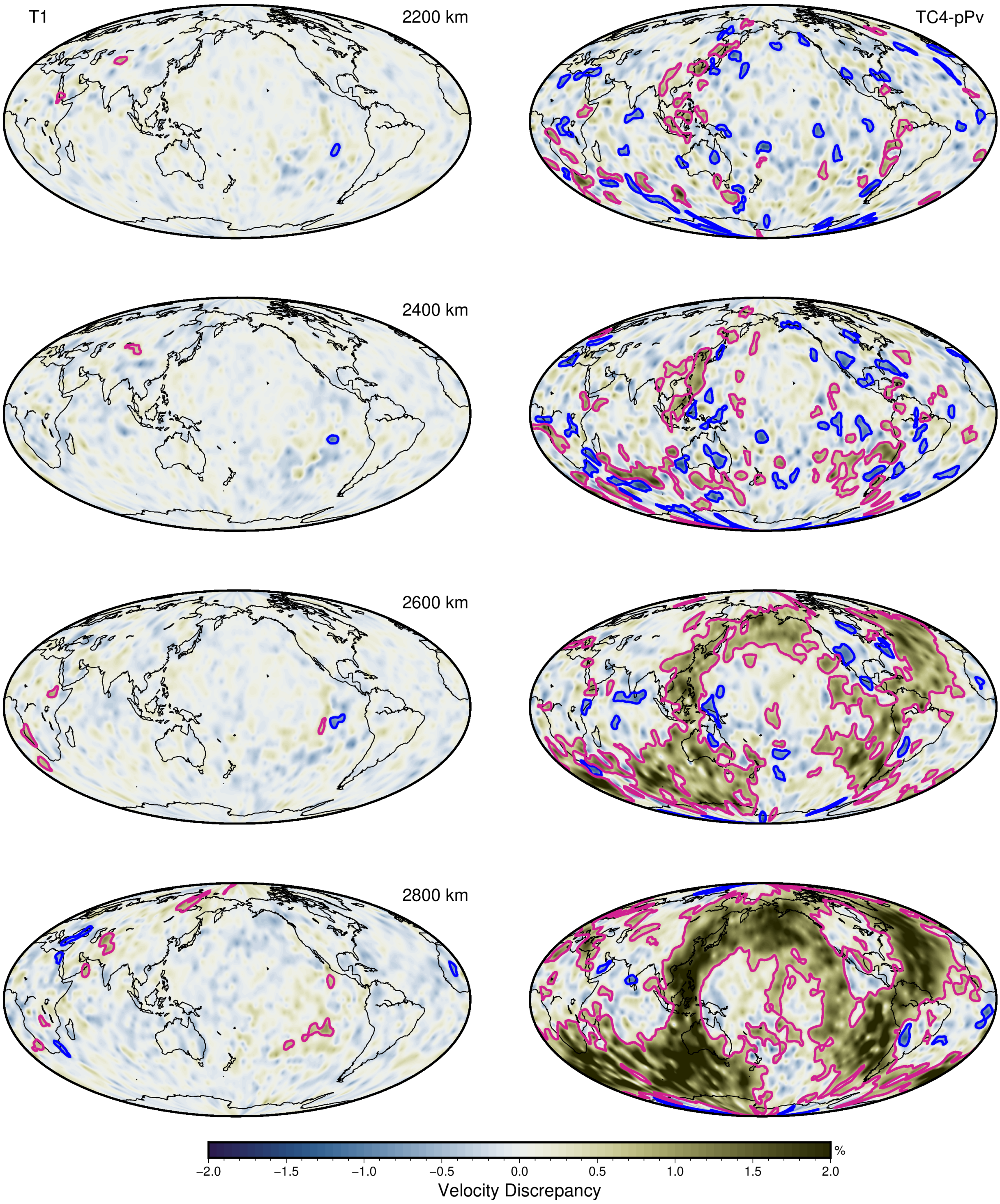


Supplementary Figure 2: Distribution curves for lowermost model layers of TC4-pPv rotated by twelve different angles before applying tomographic filters.

S.3 Assessing the definition of LUMP

In this study, uncorrelated velocity is defined as the departure from $\delta V_P \propto \delta V_S$, measured using the Eq. (7): $\Delta\bar{V} = R_S\delta\bar{V}_P - R_P\delta V_S$. The equation allows us to quantify and visualize potential heterogeneity related to variations in composition and/or phase, which we refer to as large uncorrelated moduli province (LUMP) using the criteria $\Delta\bar{V} > 0.5\%$ and $\Delta\bar{V} < -0.5\%$ for positive and negative LUMP, respectively. Here we evaluate LUMP criteria and the possible influence of artifacts, for example treating velocity discrepancy induced by anelasticity effect in purely thermal structure as LUMP. Therefore, we examine LUMP definition and criteria with geodynamic models, for which we know whether the velocity anomaly is influenced by temperature, composition, or both.

We measure $\Delta\bar{V}$ for tomographic filtering results of T1 and TC4-pPv model from Section 3.2 using a generalized definition $\Delta\bar{V} = R_P\delta\bar{V}_P - R_S\delta V_S$ and draw contours at $\Delta\bar{V} = \pm 0.5\%$ (Supplementary Figure 3). The small area of (both positive and negative) LUMPs in the T1 model suggests that few artifacts are generated, such that a purely thermal model is not consistent with abundance of LUMP material identified in the cross-filtered result shown in Fig. 6. In addition, the large area of positive LUMP in TC4-pPv shows that our method is capable of detecting primordial material. Although this model contains post-perovskite distributed ubiquitously outside the primordial material at the lowermost 200 km, the post-perovskite signal is only loosely recovered as negative LUMP. One possible explanation for this inconsistency is the mineral physical parameters used in geodynamic models are not sensitive to the definition used here. Therefore, the interpretation of negative LUMP with post-perovskite is not as straightforward and requires further work.



Supplementary Figure 3: Similar to Fig. 6 but using the definition $\Delta\bar{V} = R_P\delta\bar{V}_P - R_S\delta V_S$ to measure LUMP material in T1 (left column) and TC4-pPv model (right column).