New normal mode constraints on bulk inner core velocities and density

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ABSTRACT

Inner core elastic parameters $V_p$, $V_s$, and density ($\rho$) inform both experimental and theoretical studies of inner core composition and potential light element candidates. Meanwhile, constraints on the density jump at the inner core boundary offer much-needed observational insight into the processes powering the geodynamo. Thus, obtaining accurate observational constraints on the elastic structure of the inner core is key to gaining better understanding of its composition and dynamics.

While body wave phases provide information on inner core $P$ velocity and anisotropy structure, constraining shear velocity and density currently relies predominately on core-sensitive normal mode observations. Since the construction of the Preliminary Reference Earth Model (Dziewonski and Anderson, 1981), which was largely based on such data, the database of observed normal modes has become both larger and more accurate, and new model exploration methodologies have become computationally feasible.

Here we use recent normal mode center-frequency catalogues to simultaneously explore average shear ($V_s$) and compressional ($V_p$) velocities, as well as density ($\rho$), in the inner core via a Monte Carlo parameter-space search.

We find best-fitting $V_p$ values (11,160–11,180 m/s) in good agreement with PREM, while $V_s$ values (3560–3590 m/s) favor a minor reduction (< 1% relative to PREM). We show that a recently proposed reduction of 2.5% in $V_s$ in the inner core, while keeping the other two parameters constant, is incompatible with normal mode data, and demonstrate the importance of simultaneously exploring the parameters to address trade-off effects. Meanwhile, we show that $\rho$ is the most poorly-constrained parameter, though mode data without any additional constraints favor a density reduction of ~0.7–1.9% with respect to PREM. We also show that the need for this reduction is largely independent of various assumed parameters, including: the choice of reference mantle and outer core model, observational catalog, and the depth of the ICB.

The presented results may be of interest for laboratory and ab-initio studies aiming at constraining IC composition and for studies that consider the energy available to power the geodynamo via compositional convection.

1. Introduction

Seismological observations are central to our understanding of the Earth’s core composition dynamics, and evolution. The fluid core was first discovered using seismic observations in 1906 (Oldham, 1906), by 1936 the existence of an inner-core (IC) was established (Lehmann, 1936), and its solidity finally confirmed in 1970 (Dziewonski and Gilbert, 1971). Meanwhile, Birch established the core’s primary composition: an Iron-Nickel alloy (Birch, 1952) with about ~10 wt% light-elements (LE) (Birch, 1964; Jephcoat and Olson, 1987; Poirier, 1994), leaving the solid IC depleted (~3-5 wt%). The resulting compositional heterogeneity is generally believed to be the driving force for the compositional convection that powers the geodynamo at present (Gubbins et al., 1979; Loper, 1978).

In the years since Birch first proposed the presence of light elements in the earth's core, numerous candidates have been suggested, including Si, O, S and H (Antonangeli et al., 2010; Bazhanova et al., 2012; Belonoshko et al., 2007; Caracas, 2015; Hirose et al., 2017; Martorell et al., 2013; Sakamaki et al., 2016; Tagawa et al., 2016; Vočadlo, 2007). However, both ab-initio and laboratory studies have struggled to reconcile these proposed compositions with seismic observations,
consistently recovering incompatibly high velocities, even when matching density (ρ) (Li et al., 2018). This has led to various proposed mechanisms to lower Vc, such as anelasticity, premelting conditions (Martorell et al., 2013) and multiple LFs (Li et al., 2018).

Body wave travel time measurements provide strong constraints on IC Vp, since PKIKP, the inner-core compressional phase, is routinely observed. However, its Vc equivalent, PKJKP, remains elusive. Of five published observations (Cao et al., 2005; Deuss et al., 2000; Julian et al., 1972; Okal and Cansi, 1998; Wookey and Helffrich, 2008), two are thought to be in the wrong frequency band (Deuss et al., 2000), while a recent paper demonstrated the phase may be too low amplitude to observe (Shearer et al., 2011). Body waves provide even less constraint on IC density, though amplitude ratios can provide information on the relative density jump across the ICB. As a result, constraining bulk Vc and ρ in the IC relies primarily on core-sensitive normal mode observations.

The spherically symmetric Preliminary Reference Earth Model (PREM, Dziewonski and Anderson, 1981) was constructed with constraints from normal mode center-frequency measurements, as well as body wave travel times, Earth's mass/moment of inertia, and from the Adams-Williamson equation. PREM is still widely used as a reference for the average Vc, ρ, and quality factors (Qu and Qc) in the inner core.

Since PREM was developed, 38 years ago, the database of observed normal mode center-frequencies has grown significantly larger and more accurate, with the addition of data from recent large earthquakes, and theoretical improvements in the measurements, such as including mode splitting and coupling due to 3D structure. Additionally, increases in computation power have made more computationally intensive methodologies accessible.

In the last 20 years, several studies have revisited normal mode constraints on IC density and velocity structure. Masters and Gubbins (2003) used a Backus-Gilbert inversion method to isolate the inner-core density signal, examining bulk IC density, and the density jump (Δρ) across the inner core boundary (ICB). The latter is an important parameter, indicative of the degree of LE partitioning between the IC and the outer core, and thus the energy available to power the geodynamo by such a mechanism.

On the other hand, Deuss (2008) fixed inner core density to that of PREM and searched for the average shear and compressional velocities in the inner core using a grid-search forward modeling scheme, finding average velocities remarkably close to that of PREM when assuming PREM's average density. Another study utilized artificial neural networks (de Wit et al., 2014) to explore normal mode constraints on Earth's 1D structure, though its broad focus and large modal dataset predominantly emphasized sensitivity to mantle structure.

As normal mode studies were consistently finding bulk IC parameters (Vp, Vs, and ρ) within 0.5% of PREM (de Wit et al., 2014; Deuss, 2008), an ab-initio study suggested for the first time that these observations could be matched simultaneously, utilizing multiple LE components (Li et al., 2018). However, within months, two papers called bulk core parameters into doubt. A recent Reversible-jump Markov chain Monte Carlo study in the outer core favored a model with increased OC density, drawing into question the robustness of PREM's density structure in the outer core (Irving et al., 2018). Soon after, Tkalič and Pham (2018) attempted to enhance PKJKP signals using a novel coda-wave correlation technique, proposing that Vc in the IC may be lower than that of PREM by ~2.5%. Yet, their best fitting model appears non-unique, and, as we will show, it does not predict the normal mode center-frequency data better than PREM, in general, and provides very poor fits to several specific modes. Additionally, as with other IC studies (Deuss, 2008), density is kept fixed to that of PREM, in spite of known tradeoffs.

Here, we utilize multiple recent normal mode catalogues, a variety of weighting and error schemes, and computational advances, to better constrain the elastic structure of the IC. We simultaneously explore Vp, Vs, and ρ via a Monte Carlo parameter-space search for models composed of a homogeneous IC (i.e. with no depth dependence), overlain by structure in the OC and mantle, which is fixed to a published 1D background model. We explore multiple background mantle models and discuss the possible influence of mantle and outer core structure on our results.

2. Data

2.1. Catalogues

For this study we consider two sets of observed modal center-frequencies:

- REM (2001) a collection of observations from numerous authors and methodologies (“Reference Earth Model,” n.d.)
- DR (2013) observations from Deuss et al. (2013), with the addition of radial mode observations from Roult et al. (2010). Unlike REM, Deuss et al. (2013) accounts for coupling between certain modes and was generated with the addition of data from some recent large events.

2.2. Mode selection

From each of these datasets a subset of IC-sensitive modes were selected. Initially, a list of IC-sensitive modes was compiled from the existing literature (Andrews et al., 2006; Beghein and Trampert, 2003; Deuss, 2008; Deuss et al., 2013; Durek and Romanowicz, 1999; He and Tromp, 1996; Irving and Deuss, 2011; Laske and Masters, 1999; Mäkinen et al., 2014), and 23 modes not present in both REM and DR were discarded (1S7, 2S2, 2S5, 3S5, 4S0, 4S8, 5S6, 6S7, 7S6, 8S5, 9S2, 10S2, 11S1, 12S8, 13S7, 14S5, 15S6, 16S7, 17S8, 18S2, 18S4, 18S6, 20S2, 21S8, 22S2, 25S1). Remaining modes were assessed on their theoretical proportion of total sensitivity within the IC. This resulted in the following 41 modes, used in the present study:

1S0, 1S6, 2S0, 2S1, 3S0, 3S1, 3S2, 4S0, 5S3, 6S3, 7S5, 8S1, 8S5, 9S2, 9S3, 9S4, 11S4, 11S5, 11S6, 13S1, 13S2, 13S3, 14S6, 15S3, 15S6, 16S5, 16S6, 16S7, 17S1, 18S3, 18S4, 20S1, 20S5, 21S7, 22S1, 23S4, 23S5, 25S1, 25S2, 25S5.

2.3. Mode classification

Each normal mode presents different frequency sensitivity kernels for each of the three elastic parameters (Vp, Vp, ρ) as a function of depth (Fig. 1).

Here, we group modes into 3 groups: “radial”, “PKIKP-equivalent” or “PKJKP-equivalent” (Fig. 2). The latter two were separated according to the relative proportion of IC sensitivity to Vp and Vs.

2.4. Observational uncertainty

Accounting for observational uncertainty is important for assessing the physical interpretability of our results. However, published uncertainty values vary by orders of magnitude between different center-frequency catalogues. Therefore, we make a conservative approach by using the measurement variability, i.e. the differences (Δω) between observed center-frequencies in our chosen catalogues, REM and DR (Fig. 3), as an estimation of uncertainty. The corresponding uncertainty estimates are on average an order of magnitude larger than the published estimates in DR, though still significantly smaller than those of REM (Supplementary Fig. S1). Each mode is then assigned a grouping based on the magnitude of the corresponding difference. The estimated observation uncertainty, σω, is calculated as the median difference, Δω, scaled by a factor assigned to each group, G

\[ σω = G Δω \] (1)

Here we assign low (Group 1), intermediate (Group 2) and high Δω (Group 3) modes scaling factors of 1, 2 and 3 respectively. However, we
note that the choice of these factors has little effect on results within reasonable limits (results are stable until the denominator of the cost function varies by a factor of $\sim 750$ between group 1 and 3).

2.5. Background models

To explore the effects of assumed mantle and OC structure on recovered IC structure, we utilize two background models, PREM (Dziewonski and Anderson, 1981) and NREM (Moulik, personal correspondence, 2019 based on Moulik and Ekström, 2016). Both models were independently constructed to fit normal mode observations, using different datasets and assumptions. These models were used here to provide all elastic and anelastic structure outside of the IC, and for IC quality factors.

3. Methodology

We consider average, homogeneous inner core models, ignoring any depth-dependence in $V_p$, $V_s$, and $\rho$. Since these parameters vary slowly within the IC, this is a good first-order approximation of IC structure and helps mitigate computational limitations. We explore this 3-dimensional parameter-space via a grid-search, following the procedure outlined in Fig. 4.

Within some a-priori bounds, containing all proposed seismological and experimental estimates, we generated a suite of 1D models, each composed of a homogeneous IC in $V_p$, $V_s$, and $\rho$, overlain by a published background model (e.g. PREM or NREM). IC quality factors were also fixed to those of the background model, as preliminary testing showed multiple orders of magnitude higher sensitivity to changes in $V_p$, $V_s$ and $\rho$.

Fig. 1. Normalized sensitivity kernels of IC-sensitive modes: $\delta S_0$, $\alpha S_1$, $\beta S_5$ (calculated in PREM), showing the relative predicted center-frequency shift expected for a perturbation in the model in $V_p$, $V_s$, and $\rho$, respectively.

Fig. 2. The relative proportion of IC-sensitivity to $V_p$, $V_s$, and $\rho$ for each mode considered. Values represent the percentage of the sum of the integrals over depth in the IC of each parameter's sensitivity kernel (Fig. 1). Dashed vertical lines separate modes characterized as radial, PKIKP and PKJKP.
ρ, than in Qκ or Qμ. This also limited the dimensions of the problem, further reducing computations. Parameter spacing within the grid search was kept constant across runs, with velocities and ρ varying in increments of 10 m/s and 10 kg/m³, respectively.

For each model, normal mode center-frequencies were predicted for our selection of IC-sensitive normal modes using MINOS (Woodhouse, 1998). A sum of squared differences was computed against a catalog of observed center-frequencies and a cost assigned to each model (Eq. (2)).

\[
\phi = \sum_{i=1}^{N} \left( \frac{\omega_{obs} - \omega_{calc}}{\sigma_i} \right)^2 \frac{1}{C_i} 
\]

(2)

Here \( N \) is the total number of modes, and \( \omega \) denotes mode frequency. Each mode's contribution to the cost function is weighted by two factors, observational error, \( \sigma_i \), and mode character, \( C_i \) (e.g. Fig. 1, PKIKP, PKJKP or radial mode).

We consider two different \( C \)-weighting schemes: (a) where all modes have equal weights – “all-equal” \( (C_i = N \) for all \( i \)'s) and the other and (b) “PPR”, which accounts for the different number of modes in each mode group (PKIKP, PKJKP, radial). In scheme (b) \( C_i = 3M_i \), where \( M_i \) is the number of modes within \( i \)-th mode's mode group. Normalizing by sensitivity groupings can help improve the strength of constraints provided by IC-sensitive normal modes on bulk IC parameters (Deuss, 2008).

The methodology outlined (Fig. 4) was repeated 16 times, for each permutation of 1) our two \( C \)-weighting schemes: PPR and all-equal 2) different observational catalogues: REM and DR 3) different background models: PREM and NREM and 4) different \( \sigma \) values: with our estimation of observation uncertainty \( \sigma = \sigma_{est} \) as described earlier, and using normalization by observed frequency, \( \sigma = \omega_{obs} \). The latter ensures that differences are not unintentionally upweighted for high frequency modes i.e. a 1% difference will be weighted the same at all frequencies.

4. Results

The bulk IC velocities are found to be consistent across all 16 runs (Table 1). \( V_p \) values vary between 11,160–11,180 m/s, with a standard deviation of just 8 m/s, and are in good agreement with Deuss’s proposed 2008 value (11,150 m/s) as well as PREM’s IC average (11,183 m/s). \( V_s \) values are similarly well-constrained (3560–3590 m/s) with a standard deviation of 10 m/s and exhibit a minor reduction of ~1% with respect to PREM (35 m/s) and are in better agreement with Deuss (3550 m/s). N.B. Unless otherwise stated, reference averages computed in the reference PREM model are linear averages, as volumetric averages overly emphasize the outermost inner core's effect on modal frequencies. While we also acknowledge linear averages underemphasize this contribution, we believe the context of our results are largely independent of this decision. Though for clarity, volumetric averages are marked alongside the linear averages in Fig. 5.

Our results provide looser constraints on IC density, with values ranging from 12,720–12,880 kg/m³ (+/- 54 kg/m³) (Fig. 5). Still, the results show a reduction in average IC density with respect to PREM on
Table 1
The homogeneous IC parameters associated with the lowest cost models for each of the 8 runs using NREM in the mantle and OC (top) and those using PREM (bottom). Mean and standard deviation values are also shown for each subset, as are PREM’s linear averages, maximum and minimum values for comparison. A reduction in Vs and ρ with respect to PREM can be seen across all runs and is particularly pronounced in the runs with NREM in the outer core and mantle. The distribution of these models can be visualized in Fig. 5.

<table>
<thead>
<tr>
<th>Background model</th>
<th>NREM</th>
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<tbody>
<tr>
<td>Observations</td>
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<tr>
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<td>All-equal PKIKP:PKJKP:radial</td>
</tr>
<tr>
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<table>
<thead>
<tr>
<th>Background model</th>
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<td>ω obs</td>
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<tr>
<td>Vs</td>
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<tr>
<td>ρ</td>
<td>12,810</td>
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<td>Model name</td>
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Optimal Inner Core Models

Fig. 5. Histogram showing the distribution of parameters in the 16 best-fitting models. Letters correspond to the final letter of the model names shown in Table 1. The grey box represents a 1% variation in PREM’s linear average for each parameter. Models using NREM’s mantle and outer core (solid outlines) are distributed towards lower values in Vs and ρ than PREM’s (dotted outlines), while there is no clear difference between the two background models in Vp.
the order of 1.3%, with a mean density of 12,801 kg/m³.

The level of constraints on each of these variables can be seen in a different way by visualizing the cost function across the parameter-space (Fig. 6). The cost function exhibits a steeper gradient and thus greater sensitivity in $V_s$ while showing less stringent constraints on $V_p$ and relatively weak constraints on $\rho$. Still, the $V_p$ remains the closest to PREM.

5. Discussion

We have shown that the recent normal mode center-frequency catalogues considered provide constraints on bulk IC $V_p$, $V_s$ and $\rho$ that are largely independent of the dataset, data uncertainty, and to some extent on the choice of reference OC and mantle model.

Additionally, to explore the effects of a deviation from PREM’s IC
radius, proposed by a recent normal mode study (de Wit et al., 2014), we performed tests (not shown), finding results were insensitive to changes in IC radius within reasonable bounds (± 20 km). We did not explicitly explore the effect of inner core anisotropy (Woodhouse et al., 1986) on the center frequencies, ignoring the effects of cross-coupling due to IC anisotropy and 3D mantle structure in our simulations. However, in contrast to the construction of PREM, developed before the discovery of anomalous mode splitting, recent normal mode measurements are based on extracting the constant, “00” term in a spherical harmonics expansion of mode splitting functions, while the anisotropy signature is in the higher order terms. Also, since we compare the results based on two different catalogues, constructed from measurements by different authors, using different techniques, we may assume that any hidden effect of anisotropy may be reflected in the conservative errors we have assigned to the data.

We note that a recently proposed reduction in $V_s$ of 2.5% in the IC, keeping $V_p$ and $\rho$ fixed at the PREM values (Tkalčić and Pham, 2018), is incompatible with normal mode observations, ignoring orders of magnitude higher cost than best-fitting models (Fig. 6). Additionally, while most mode center-frequencies in our catalog are arguably fit no worse than by other existing models (Fig. 7), several modes stand out: predictions for modes $s_5$, $s_6$, $18S_6$, $22S_1$, and $2S_2$. Note, $1S_0$ (far right) was not used to generate our models as it was not present in REM. However, it is a PKJKP-like mode with high IC-sensitivity to $V_s$. Please note, all models are depth dependent in the IC other than RR19A (Model A – Table 1) which has a homogeneous IC.

Fig. 7. Comparison of center-frequency predictions to DR observations. For each IC-sensitive mode the difference between its predicted Eigenfrequencies and observed (DR) Eigenfrequencies is shown. Models include: PREM, NREM, PREMQL6 (Durek and Ekström, 1996; Dziewonski and Anderson, 1981), STW105 (Kustowski et al., 2008), and the best-fitting model from Fig. 6 – Model A. Notably, a reduction of 2.5% in IC shear velocity (stars) is associated with increased misfits for many IC-sensitive modes, particularly $s_5$, $s_6$, $18S_6$, $22S_1$, and $2S_2$. Note, $1S_0$ (far right) was not used to generate our models as it was not present in REM. However, it is a PKJKP-like mode with high IC-sensitivity to $V_s$. Please note, all models are depth dependent in the IC other than RR19A (Model A – Table 1) which has a homogeneous IC.

mode observations alone offer poorer constraints for IC density than for other parameters (Fig. 6), and while mass and moment of inertia are well known, these parameters do not help to constrain IC density, given uncertainty in shallower density structure (Irving et al., 2018). We note that slightly lower $V_s$ and $\rho$ values are obtained when fixing structure in the mantle and outer core to that in NREM (Fig. 5), which presumably is an improved 1D model over PREM. Considering the values obtained with NREM, the data require a reduction of 1.1% in $V_s$ and 1.3% in $\rho$ with respect to PREM.

Finally, we acknowledge that mode sensitivity to $V_p$, $V_s$ and $\rho$ reduces to zero at the Earth’s center (Fig. 1). As a result, on average, normal modes have greater sensitivity at shallower depths, so that best-fitting bulk IC parameters may be more representative of the top part of the IC.

It is clear that normal modes favor a reduction in IC density with respect to PREM, though the magnitude of such a reduction is weakly constrained (Fig. 5/6). This reduction may have important implications for our understanding of the driving mechanism of the geodynamo. When considered with PREM's outer core, best-fitting models reduce the magnitude of the density jump ({$\Delta \rho$}) at the ICB in PREM (603 kg/m$^3$) by between 89 and 242 kg/m$^3$. This is significant given the magnitude of the density jump due to solidification alone can be estimated to be about 210 kg/m$^3$ (Allè et al., 2000). As such, our density reduction may reduce the jump associated with light element partitioning by over half, having significant implications for the ability of that mechanism to power the geodynamo. This issue is potentially compounded when considering the results of another recent mode study in the outer core (Irving et al., 2018), which favored an increase in average OC density. This would bring the mode-derived value close to the lower end of the values obtained from recent PKiKP/PcP amplitude ratio measurements, which span a range of 300 to 1200 kg/m$^3$ for $\Delta \rho$ (e.g. Cao and Romanowicz, 2004; Koper and Dombrovskaya, 2005; Shen et al., 2016; Tkalčić et al., 2009; Waszek and Deuss, 2015), although the higher values obtained in some of these studies may be due to amplification due to focusing by topography on the inner-core boundary.

While we present results for the simplest possible parameterization of IC parameters, attempts were made to explore depth dependence via
both linear and quadratic forms. However, when using center-frequency alone, the higher order terms – and so the gradients – were unstable and highly dependent on the choice of grid-search points for the zeroth order term. Introduction of additional independent constraints from mineral physics, such as a Birch type V_p ρ relation (Birch, 1961; Sakamaki et al., 2016), or assuming hydrostatic equilibrium is necessary to stabilize results and reduce the dimensions of the problem.

Overall, our results reaffirm PREM’s average IC V_p, suggest a slight reduction in V_s (~1%) and a larger reduction in density (~0.7–1.9%), while acknowledging limitations in constraining IC ρ based on normal mode center-frequency data alone.

6. Conclusions

Using a catalog of well-characterized IC-sensitive normal mode center-frequencies based on recent measurements, and exploring variations in average V_p, V_s, and ρ in the IC simultaneously, we have shown that IC velocities are well-constrained by these data, independent of choice: dataset, mantle model, data uncertainty and IC radius. We find V_p is in good agreement with PREM and a minor reduction in V_s with respect to PREM is favored (~1%). We show that a more significant reduction of 2.5% in V_s, while fixing ρ to PREM as proposed by Tkalić and Pham (2018), is incompatible with normal mode center-frequency observations. Meanwhile, normal mode center-frequency data favor a reduction in average ρ in the IC of between 0.7 and 1.7%, although data-sensitivity to ρ is significantly lower than to V_p and V_s.

While normal modes alone struggle to constrain the elastic parameters’ depth-dependence within the IC, these best-fitting average values and their associated standard deviations may be useful for laboratory and ab-initio studies aiming at constraining IC composition. If confirmed, the slight density reduction favored by our models may have important implications for the energy available to power the geodynamo, potentially reducing the magnitude of the ICB density jump as-


