

1 **Probabilistic linear inversion of satellite gravity**
2 **gradient data applied to the northeast Atlantic**

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5 **Key Points:**

- 6 • We present a methodology for 3-D linear inversion of satellite gravity gradient data
7 using statistical prior information
8 • We apply the inversion method to estimate the density variation in the upper man-
9 tle beneath the northeast Atlantic Ocean
10 • The predicted density variations are compared to independent results of seismic
11 tomography and linked to distribution of Cenozoic underwater volcanoes and seamount-
12 like features of the seafloor

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Abstract

We explore the mantle density structure of the northeast Atlantic region using constrained linear inversion of the satellite gravity gradient data based on statistical prior information and assuming a Gaussian model. The uncertainty of residual gravity gradient signal is characterized by covariance matrix obtained using geostatistical analysis of controlled-source seismic data. The forward modeling of the gravity gradients in the 3D reference crustal model is performed using a global spherical harmonics analysis. We estimate the model covariance function in the radial and angular directions using a variogram method. We compute volumetric gravity gradient kernels for a spherical shell covering the northeast Atlantic region down to the mantle transition zone (410 km depth). The solution of the linear inverse problem in the form the mean density model follows a least-squares approach. The results indicate a direct relation between the seismic velocity and density anomalies in the Iceland-Jan Mayen region, Greenland and the Norwegian passive margin. The predicted low-density anomalies at the depth of 100-150 km underneath the northeast Atlantic Ocean are correlated with the distribution of Cenozoic underwater volcanoes and seamount-like features of the seafloor.

Plain Language Summary

We image density heterogeneities within the upper 400-km layer of the Earth beneath Greenland and the northeast Atlantic region using satellite gravity gradient data. The observed density anomalies within continental and oceanic lithosphere are linked to the activity of Iceland plume throughout the Cenozoic time (0-60 Ma).

1 Introduction

The GOCE satellite mission was active during 2009-2013 and provided global coverage with gravity tensor data (Fig. 1) (European Space Agency, <https://earth.esa.int/>). Unlike other gravity missions, the GOCE gravity measurements were made directly at the orbit (220-250 km height). The spatial derivatives of gravitational potential help to enhance the signal from lithospheric sources. The GOCE observation level acts as a natural upward continuation filter suppressing a high-frequency "noise" due to superficial structures and enhancing the spectral band of the gravity field linked to the density variation in the upper mantle (Sebera et al., 2017).

The present-day configuration of the lithosphere in the northeast Atlantic is the result of continental rifting, break-up and subsequent seafloor spreading that formed the oceanic basin from about 56 Ma (Gaina, Nasuti, et al., 2017) (Fig. 2). It is postulated that seafloor spreading was initiated after the North Atlantic Igneous Province (NAIP) (e.g. R. White & McKenzie, 1989) was emplaced affecting a substantial part of the Greenland and Eurasia lithosphere. The geodynamic evolution of the northeast Atlantic over the subsequent 50 myr may have developed in a pulsating fashion with periods of high and low magmatic and tectonic activity as documented in Iceland, mid-ocean ridges (Ito, 2001; Jones et al., 2002; Parnell-Turner et al., 2014), by pervasive seamount volcanism (Gaina, Blischke, et al., 2017) and episodic uplift and basin inversion at the passive continental margins (N. White & Lovell, 1997; Rudge et al., 2008).

The early evolution of the northeast Atlantic was inferred from a number of seismic reflection and refraction profiles, mostly at the continent-ocean transition. Both intrusives and extrusive magmatic rocks associated with NAIP has been mapped in detail (Eldholm & Grue, 1994). Variable physical properties of the igneous crust in the deep ocean basin were linked to the Miocene activity of the Iceland hotspot (Parkin & White, 2008; A. J. Breivik et al., 2008). Iceland is presently in the vicinity of the active Mid-Atlantic Ridge, and has been a ridge-centered mantle melt anomaly during late Cenozoic (Ito, 2001). Several studies have recently proposed that basaltic upper crust can be

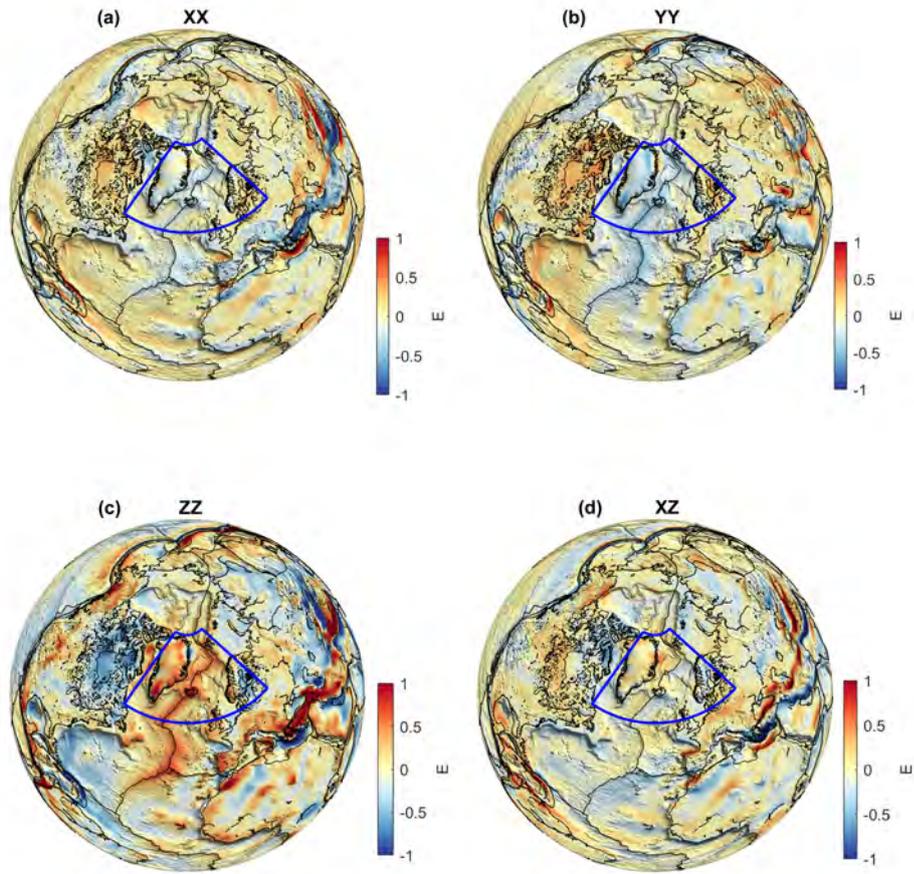


Figure 1. GOCE gravity gradients (a) XX -, (b) YY -, (c) ZZ -, and (d) XZ -components.

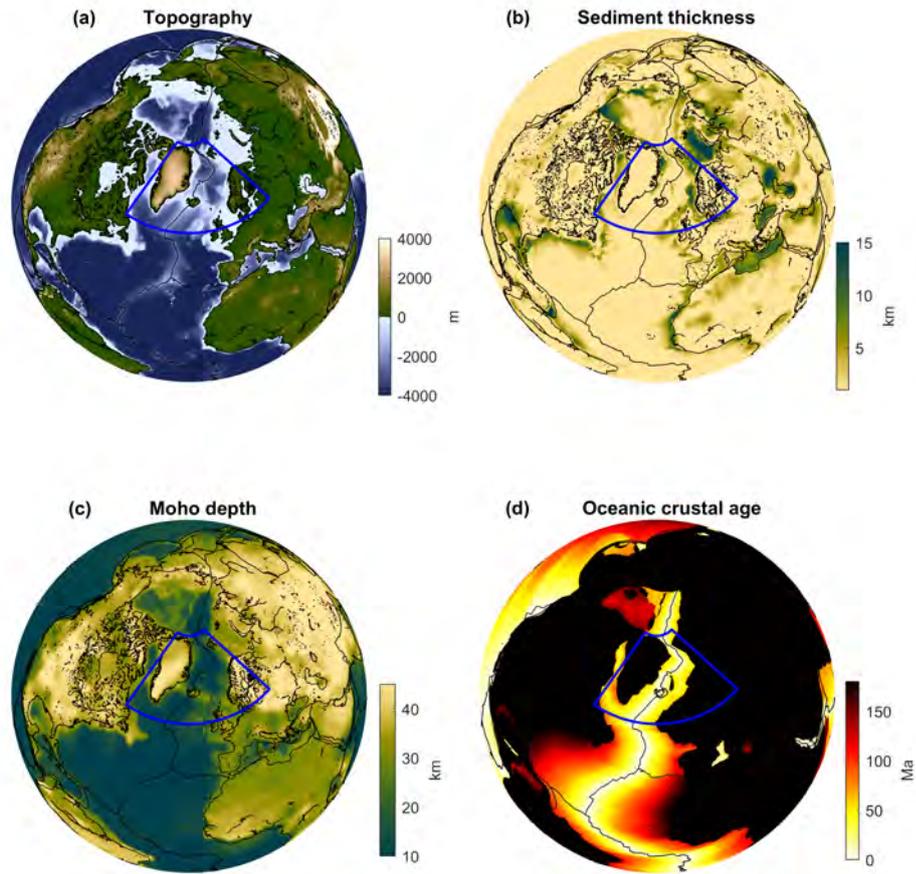


Figure 2. Data-set compilations used in this work: (a) Topography (GEBCO, 2019), (b) Sediment thickness (Straume et al., 2019), (c) Moho depth (Szwilius et al., 2019; Funck et al., 2017), and (d) Crustal age (Gaina, Nasuti, et al., 2017) . The blue sector indicates the northeast Atlantic study region.

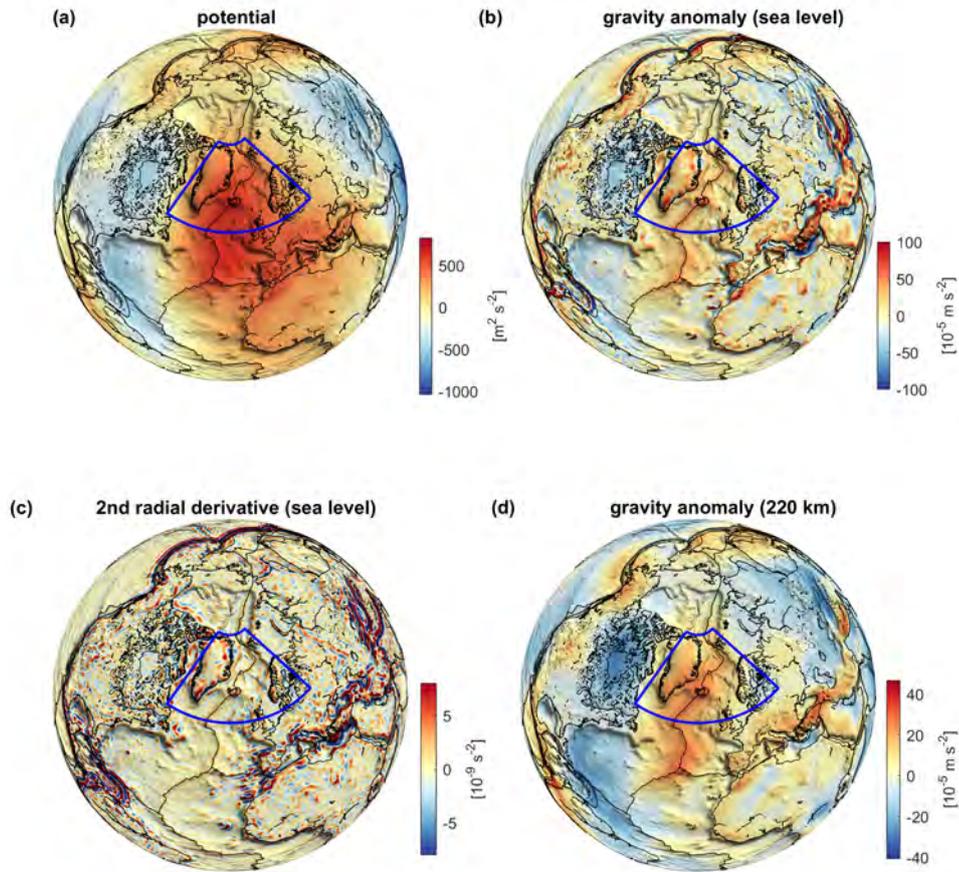


Figure 3. GOCE-derived datasets (a) Gravitational potential anomaly, (b) free-air gravity anomaly (at sea level), (c) radial gravity gradient at sea level, and (d) gravity anomaly (at 220-km height). The blue sector indicates the northeast Atlantic study region. GEBCO topography/bathymetry grid (GEBCO, 2019) is used as shaded relief surface.

62 underlain by extended continental crustal reworked by intrusive magmatism (Torsvik et
 63 al., 2015; Foulger et al., 2019). Petrological models suggest that the mantle source of Ice-
 64 land lavas is a peridotite (80-90%) mixed with basalt (10-20%), and would imply a den-
 65 sity perturbation of $10\text{-}20 \text{ kg m}^{-3}$ (Brown & Leshner, 2014). However, the density distri-
 66 bution within the primary melt source region in the upper mantle remains unknown.

67 The long-term magmatic and tectonic evolution of the northeast Atlantic region
 68 are controlled by processes in the mantle. The present-day mantle density variation
 69 provide important constraints for evolutionary dynamic models and useful for quantitative
 70 understanding of the stress regime in the shallow upper crust. The northeast Atlantic
 71 region is associated with a broad and intense high of the gravitational potential attributed
 72 by a superposition of shallow and deep mantle heterogeneities (Fig. 3 ; Cochran and Tal-
 73 wani (1978)), and disentangling these anomalous density sources is not fully possible due
 74 to non-uniqueness of the inverse gravimetric problem. Moreover, the surface topogra-

75 phy and crustal thickness variation is known to constitute of up to 80 % of the observed
 76 gravity signal (Sebera et al., 2017). To better utilize the physical constraints provided
 77 by gravity data, it is important to assess the contribution of individual density sources
 78 (with a presumably known probability) and provide a statistical measure for the uncer-
 79 tainty of the final density model.

80 The density variation beneath hotspot regions is a key physical parameter for un-
 81 derstanding thermo-chemical convection and distribution of volcanism. At the same time,
 82 a parametric relation between the seismic velocity and density in non-adiabatic and par-
 83 tially molten upper mantle is not available. There have been few attempts to directly
 84 invert the gravity gradient data directly due to non-uniqueness of the solution. Here, we
 85 suggest a method to utilize the prior information in the 3-D sphere in the form of: i) data
 86 covariance matrix; ii) prior model covariance matrix including a model for spatial vari-
 87 ability of mantle heterogeneity; and iii) a stabilizing functional in the form of spatial weight-
 88 ing function. We construct a seismically-constrained 3D crustal reference model includ-
 89 ing ice, water, sediments, and crystalline crustal layers based on spherical kriging inter-
 90 polation (Fig. 2) including a model for the average density of the crystalline crust. Then,
 91 we use the GOCE grids to infer density variation (and associated Gaussian probability
 92 distribution) in the upper mantle in a spherical shell within the northeast Atlantic re-
 93 gion based on constrained linear inversion of gravity gradient data using statistical prior
 94 information.

95 2 Data and Methodology

96 The density structure of the lithosphere and asthenosphere in the northeast At-
 97 lantic region based on the gravity data has been previously addressed in a number of stud-
 98 ies (Haase et al., 2016; Tan et al., 2018; Shulgin & Artemieva, 2019). Tan et al. (2018)
 99 focuses on the lithospheric density structure of the oceanic region around Jan Mayen is-
 100 land and discuss possible impact of the Iceland hotspot on the temperature and density
 101 structure in this region. Shulgin and Artemieva (2019) performed density modeling us-
 102 ing a tesseroïd approach to discuss thermochemical structure of the upper mantle. As
 103 constraints, they used the UNASEis crustal model of Artemieva and Thybo (2013). A
 104 spectral method based on global spherical harmonics analysis, combined with local isostasy
 105 constraints, has been applied by B. Root (2020) to investigate the relation between seis-
 106 mic velocity and density structure of the lithosphere.

107 A population of acceptable solutions of the potential fields inverse problem requires
 108 a priori constraints and regularization. Zhdanov (2015) discussed various stabilizing func-
 109 tionals applied to model parameters which can be instrumental to obtain a solution sat-
 110 isfying certain a priori geological or geophysical knowledge, such as the minimum-norm,
 111 maximum smoothness, total variation, minimum entropy and minimum-gradient sup-
 112 port functionals (Last & Kubik, 1983; Portniaguine & Zhdanov, 1999; Boulanger & Chouteau,
 113 2001). Li and Oldenburg (1996) suggested a stabilizing function for the potential field
 114 inversion in the form of the inverse distance ($1/r^\beta$) to counteract the rapid decay with
 115 distance of the integral kernels. Zhdanov et al. (2011) and Wan and Zhdanov (2013) pro-
 116 posed a method for rapid imaging using gravity gradient data incorporating the depth
 117 weighting of Li and Oldenburg (1996) and a known background density model. Chasseriau
 118 and Chouteau (2003); Barnoud et al. (2016) considered the inverse gravity problem in
 119 a Bayesian formulation implying that the density variation and the observed data can
 120 be considered as Gaussian random fields characterized by their mean and the covariance
 121 matrix.

122 The 3D gravity gradient inversion method has been traditionally used in mineral
 123 and petroleum exploration focusing on the reconstruction of localized density anoma-
 124 lies e.g. (Pilkington, 2014; Wan & Zhdanov, 2013). For a particular case of point mass
 125 sources or weakly interfering localized sources, the eigenvectors of the gravity gradient

126 tensor indicate the direction to the location of point mass (or baricenters of localized bod-
 127 dies) (Pedersen & Rasmussen, 1990; Mikhailov et al., 2007). In general, the vertical (ra-
 128 dial) component of the gravitational tensor is shown to be most informative and often
 129 utilized (Pilkington, 2014).

130 In these previous studies the analysis has been performed for models in Cartesian
 131 coordinates. The applications at a lithospheric or planetary scale are less common and
 132 specifically require a consistency between model parameterization and observation ref-
 133 erence frames. Liang et al. (2014) used a tesseroïd approach and performed linear inver-
 134 sion using a combination of angular and radial weighting functions as constraints. Afonso
 135 et al. (2019) performed constrained non-linear inversion of GOCE gradients (together
 136 with other geophysical constraints) for several lithospheric layers. An efficient method
 137 for forward and inverse gravity modeling of crustal density structure based on spheri-
 138 cal harmonic analysis was introduced by Wieczorek and Phillips (1998). Novák and Gra-
 139 farend (2006) and B. C. Root et al. (2015) have further extended this method for var-
 140 ious geophysical applications. Martinec and Fullea (2015) used the GOCE gravity gra-
 141 dient data to model density structure of the Congo basin based on a spherical harmonic
 142 approach.

143 The modeling method presented in this study combines the computationally effi-
 144 cient spherical harmonics method and the local parameterization to perform a proba-
 145 bilistic linear inversion of satellite gravity gradient data in spherical coordinates. The
 146 input GOCE data have the form of grids in the local (north-oriented) reference frame
 147 (LNOF) (Bouman et al., 2015). The gravity field solutions (grids) contain a detailed sig-
 148 nal at a height of ≈ 220 km with a spatial resolution of ≈ 80 km (Fig. 1).

149 2.1 Preliminaries

The gravity vector can be expressed using a scalar potential as

$$\mathbf{g}(\mathbf{r}) = \nabla U(\mathbf{r}). \quad (1)$$

The gravitation tensor is defined as double gradient of the gravitational potential

$$\mathbf{T}(\mathbf{r}) = \nabla \nabla U(\mathbf{r}). \quad (2)$$

The gravitational potential due to density distribution $\rho(\mathbf{r}')$ at point \mathbf{r} can be computed
 using the volume integral

$$U(\mathbf{r}) = \gamma \int_V \rho(\mathbf{r}') G(\mathbf{r}, \mathbf{r}') dV \quad (3)$$

where γ is the gravitational constant. The scalar Green function G is in the form of in-
 verse distance function:

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|}. \quad (4)$$

The integral forms for the gravity vector and gravity gradient tensor can be ob-
 tained by substituting eq. 3 in eqs 1 and 2

$$\mathbf{g}(\mathbf{r}) = \gamma \int_V \rho(\mathbf{r}') \nabla G(\mathbf{r}, \mathbf{r}') dV \quad (5)$$

$$\mathbf{T}(\mathbf{r}) = \gamma \int_V \rho(\mathbf{r}') \nabla \nabla G(\mathbf{r}, \mathbf{r}') dV \quad (6)$$

150 The ways of solving the integrals 3, 5 and 6 depend on application.

151

In Cartesian coordinates

$$|\mathbf{r} - \mathbf{r}'| = \sqrt{(\mathbf{x} - \mathbf{x}')^2 + (\mathbf{y} - \mathbf{y}')^2 + (\mathbf{z} - \mathbf{z}')^2} \quad (7)$$

$$\rho(\mathbf{r}') = \rho(\mathbf{x}', \mathbf{y}', \mathbf{z}') \quad (8)$$

$$dV = dx dy dz \quad (9)$$

152

The geocentric latitude, longitude and radial distance are related to Cartesian coordinates as

153

$$x = r \cos \phi \cos \lambda \quad (10)$$

$$y = r \cos \phi \sin \lambda \quad (11)$$

$$z = r \sin \phi \quad (12)$$

 The angular distance ψ between vectors \mathbf{r} and \mathbf{r}' can be expressed using spherical coordinates

$$\cos \psi = \frac{\mathbf{r} \cdot \mathbf{r}'}{|\mathbf{r}| |\mathbf{r}'|} = \sin \phi \sin \phi' + \cos \phi \cos \phi' \cos(\lambda - \lambda'). \quad (13)$$

154

The following relation can be used in the integral eq. 3

$$|\mathbf{r} - \mathbf{r}'| = \sqrt{|\mathbf{r}|^2 + |\mathbf{r}'|^2 - 2|\mathbf{r}| |\mathbf{r}'| \cos \psi} \quad (14)$$

$$\rho(\mathbf{r}') = \rho(|\mathbf{r}'|, \phi', \lambda') \quad (15)$$

$$dV = |\mathbf{r}'|^2 \cos \phi' dr d\phi d\lambda \quad (16)$$

 The gradient operation expressed using a non-Cartesian basis \mathbf{e}^j is

$$\nabla U = h_j^{-1} \mathbf{e}^j \frac{\partial U}{\partial x^j} \quad (17)$$

155

 where h_j are the normalization coefficients which for spherical coordinates are $h_r = 1$, $h_\phi = r$, and $h_\lambda = r \cos \phi$.

156

157

The double gradient operation in dyadic notation becomes

$$\begin{aligned} \nabla \nabla U &= h_i^{-1} \mathbf{e}^i \frac{\partial}{\partial x^i} \left(h_j^{-1} \mathbf{e}^j \frac{\partial U}{\partial x^j} \right) \\ &= h_i^{-1} \mathbf{e}^i \left(\mathbf{e}^j \frac{\partial h_j^{-1}}{\partial x^i} \frac{\partial U}{\partial x^j} + h_j^{-1} \frac{\partial \mathbf{e}^j}{\partial x^i} \frac{\partial U}{\partial x^j} + h_j^{-1} \mathbf{e}^j \frac{\partial^2 U}{\partial x^i \partial x^j} \right). \end{aligned} \quad (18)$$

158

 The derivatives of the basis vectors $\mathbf{e}^i \rightarrow (\mathbf{e}_r, \mathbf{e}_\phi, \mathbf{e}_\lambda)$ (radial outward, north, east direction) with respect to spherical coordinates $x^i \rightarrow (r, \phi, \lambda)$:

159

$$\frac{\partial(\mathbf{e}_r, \mathbf{e}_\phi, \mathbf{e}_\lambda)}{(r, \phi, \lambda)} = \begin{pmatrix} 0 & \mathbf{e}_\phi & \mathbf{e}_\lambda \cos \phi \\ 0 & -\mathbf{e}_r & -\mathbf{e}_\lambda \sin \phi \\ 0 & 0 & -\mathbf{e}_r \cos \phi + \mathbf{e}_\phi \sin \phi \end{pmatrix} \quad (19)$$

160

2.2 Global spherical harmonic analysis and topographic sources

161

 The scalar Green function G can be expressed using spherical harmonics

$$G(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{r} \sum_{n=0}^{\infty} \frac{1}{2n+1} \left(\frac{r'}{r} \right)^n \sum_{m=-n}^n Y_{n,m}(\hat{\mathbf{r}}) Y_{n,m}^*(\hat{\mathbf{r}}') \quad (20)$$

162 where $\mathbf{r} = r\hat{\mathbf{r}}$, $\mathbf{r}' = r'\hat{\mathbf{r}}'$, $\hat{\mathbf{r}}' = [\cos\phi' \cos\lambda', \cos\phi' \sin\lambda', \sin\phi']^T$.

163 We substitute this equation in eq. 3 together with eqs 15 and 16.

$$\begin{aligned}
 U &= \gamma \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{1}{2n+1} \left(\frac{1}{r}\right)^{n+1} Y_{n,m}(\hat{\mathbf{r}}) \times \\
 &\times \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} \rho(\hat{\mathbf{r}}') Y_{n,m}^*(\hat{\mathbf{r}}) \cos\phi d\phi d\lambda \int_{R_0+h_1}^{R_0+h_2} r'^{n+2} dr
 \end{aligned} \quad (21)$$

164 Approximating the radial integral by the first three terms of Taylor series, we obtain
 165

$$\begin{aligned}
 U &= \gamma \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{R_0^{n+3}}{2n+1} \left(\frac{1}{r}\right)^{n+1} Y_{n,m}(\hat{\mathbf{r}}) \times \\
 &\times \int_{-\pi/2}^{\pi/2} \int_{-\pi}^{\pi} F(\hat{\mathbf{r}}') Y_{n,m}^*(\hat{\mathbf{r}}) \cos\phi d\phi d\lambda
 \end{aligned} \quad (22)$$

where $F(\hat{\mathbf{r}}')$ is defined as

$$F = \frac{\rho}{R_0} (h_2 - h_1) + \frac{(n+2)}{R_0^2} (h_2^2 - h_1^2) \rho + \frac{(n+2)(n+1)}{R_0^3} (h_2^3 - h_1^3) \rho. \quad (23)$$

166 Here, $h_1(\phi, \lambda)$, $h_2(\phi, \lambda)$ describe the bottom and top boundary topography of the
 167 spherical layer with density $\rho(\phi, \lambda)$, R_0 is the reference radius.

168 $F(\hat{\mathbf{r}}')$ can be expanded in spherical harmonics with coefficients $F_{n,m}$:

$$F(\hat{\mathbf{r}}') = \sum_{n=0}^{\infty} \sum_{m=-n}^n F_{n,m} Y_{n,m}(\hat{\mathbf{r}}') \quad (24)$$

169 Substituting eq. (24) into eq. (22) and using the orthogonality property of spherical
 170 harmonics, we obtain

$$U(r, \hat{\mathbf{r}}) = \gamma R_0^2 \sum_{n=0}^{\infty} \sum_{m=-n}^n \frac{4\pi}{2n+1} \left(\frac{R_0}{r}\right)^{n+1} F_{n,m} Y_{n,m}(\hat{\mathbf{r}}) \quad (25)$$

171 The external gravitational potential in geocentric spherical coordinates can be represented
 172 in terms of surface spherical harmonics:

$$U(r, \hat{\mathbf{r}}) = \frac{\gamma M}{R} \sum_{n=0}^{\infty} \sum_{m=-n}^n \left(\frac{R}{r}\right)^{n+1} \bar{C}_{n,m} Y_{n,m}(\hat{\mathbf{r}}) \quad (26)$$

173 where $M = 4\pi\rho_E R^3/3$ is the total mass of the Earth with the average density of
 174 ρ_E , R is the reference radius, and $\bar{C}_{n,m}$ are fully normalized spherical harmonic coefficients.
 175

176 The Stokes coefficients for the gravitational potential can be obtained by equating
 177 these two equations:

$$\bar{C}_{n,m} = \frac{3}{\rho_E (2n+1)} \left(\frac{R_0}{R}\right)^{n+3} F_{n,m}. \quad (27)$$

178 The first and second spatial derivatives of the gravitational potential with respect
 179 to spherical coordinates can be obtained in the spectral domain. In particular, the first
 180 and second radial derivatives are

$$\frac{\partial U}{\partial r} = \frac{\gamma M}{R^2} \sum_{n=0}^{\infty} \sum_{m=-n}^n (n+1) \left(\frac{R}{r}\right)^{n+2} \bar{C}_{n,m} Y_{n,m}(\hat{\mathbf{r}}) \quad (28)$$

$$\frac{\partial^2 U}{\partial r^2} = \frac{\gamma M}{R^3} \sum_{n=0}^{\infty} \sum_{m=-n}^n (n+2)(n+1) \left(\frac{R}{r}\right)^{n+3} \bar{C}_{n,m} Y_{n,m}(\hat{\mathbf{r}}) \quad (29)$$

181 The radial-latitudinal cross-derivative is

$$\frac{\partial^2 U}{\partial r \partial \phi} = \frac{\gamma M}{R^2} \sum_{n=0}^{\infty} \sum_{m=-n}^n (n+1) \left(\frac{R}{r}\right)^{n+2} \bar{C}_{n,m} D_{\phi} Y_{n,m}(\hat{\mathbf{r}}). \quad (30)$$

182 This expression involves differentiation of spherical harmonics $D_{\phi} Y_{n,m}$ which can
 183 be obtained by standard recursion relations.

184 The physical components of the gravity gradient tensor can be obtained by sub-
 185 stituting the derivatives with respect to the spherical coordinates into eq. 18. The gra-
 186 dient operation applied twice provides the gravity gradient tensor expressed in a local
 187 coordinate frame :

$$\begin{aligned} \nabla \nabla U(\mathbf{r}, \mathbf{r}') &= \nabla \left(\frac{\partial U}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial U}{\partial \phi} \mathbf{e}_{\phi} + \frac{1}{r \cos \phi} \frac{\partial U}{\partial \lambda} \mathbf{e}_{\lambda} \right) = \frac{\partial^2 U}{\partial r^2} \mathbf{e}_r \mathbf{e}_r + \left(\frac{1}{r^2} \frac{\partial^2 U}{\partial \phi^2} + \frac{1}{r} \frac{\partial U}{\partial r} \right) \mathbf{e}_{\phi} \mathbf{e}_{\phi} \\ &+ \left(\frac{1}{r^2 \cos^2 \phi} \frac{\partial^2 U}{\partial \lambda^2} + \frac{1}{r} \frac{\partial U}{\partial r} - \frac{\sin \phi}{r^2 \cos \phi} \frac{\partial U}{\partial \phi} \right) \mathbf{e}_{\lambda} \mathbf{e}_{\lambda} + \\ &+ \left(\frac{1}{r} \frac{\partial^2 U}{\partial \phi \partial r} - \frac{1}{r^2} \frac{\partial U}{\partial \phi} \right) \mathbf{e}_{\phi} \mathbf{e}_r + \left(\frac{1}{r} \frac{\partial^2 U}{\partial \phi \partial r} - \frac{1}{r^2} \frac{\partial U}{\partial \phi} \right) \mathbf{e}_r \mathbf{e}_{\phi} \\ &+ \left(\frac{1}{r \cos \phi} \frac{\partial^2 U}{\partial \lambda \partial r} - \frac{1}{r^2 \cos \phi} \frac{\partial U}{\partial \lambda} \right) \mathbf{e}_{\lambda} \mathbf{e}_r + \left(\frac{1}{r \cos \phi} \frac{\partial^2 U}{\partial \lambda \partial r} - \frac{1}{r^2 \cos \phi} \frac{\partial U}{\partial \lambda} \right) \mathbf{e}_r \mathbf{e}_{\lambda} \\ &+ \left(\frac{1}{r^2 \cos \phi} \frac{\partial^2 U}{\partial \lambda \partial \phi} + \frac{\sin \phi}{r^2 \cos^2 \phi} \frac{\partial U}{\partial \lambda} \right) \mathbf{e}_{\lambda} \mathbf{e}_{\phi} + \left(\frac{1}{r^2 \cos \phi} \frac{\partial^2 U}{\partial \lambda \partial \phi} + \frac{\sin \phi}{r^2 \cos^2 \phi} \frac{\partial U}{\partial \lambda} \right) \mathbf{e}_{\phi} \mathbf{e}_{\lambda} \end{aligned}$$

188 2.3 Gravity gradient kernels

189 Depending on application, the integral can be practical to evaluate either in Carte-
 190 sian or in spherical coordinates. The tensor Green functions describing the gravity gra-
 191 dients in Earth-centered reference frame is (e.g. Martinec (2014))

$$\nabla \nabla G(\mathbf{r}, \mathbf{r}') = -\frac{1}{|\mathbf{r} - \mathbf{r}'|^3} \left[\mathbf{I} - \frac{3(\mathbf{r} - \mathbf{r}') \otimes (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} \right]. \quad (32)$$

192 The comparison of model results with the GOCE data requires the coordinate trans-
 193 formation according to the traditional in geophysics sign convention for the gravity gra-
 194 dients. In particular, the radial gravity gradient anomaly is assumed positive for a pos-
 195 itive mass anomaly in the local coordinate frame (x-north, y-west and z-up).

196 The zero-order approximation for the forward problem (Wild-Pfeiffer, 2008) which
 197 is equivalent to the sum of point masses is found sufficiently accurate for the geometry

198 of our problem. The geocentric radius for each layer R is the is referenced to the cen-
 199 ter of mass of each volume element. Using eq. (32) together with eqs (13)-(14), the Green's
 200 function for the radial gravity gradient can be written

$$G_{rr} = \frac{\partial^2 G}{\partial r^2} = -\frac{1}{|\mathbf{r} - \mathbf{r}'|^3} + \frac{3(r - r' \cos \psi)^2}{|\mathbf{r} - \mathbf{r}'|^5}. \quad (33)$$

201 The Green function corresponding to the gravity anomaly on the sphere is

$$G_r = \frac{r - r' \cos \psi}{|\mathbf{r} - \mathbf{r}'|^3}. \quad (34)$$

The integral eq. (6) written in the discrete matrix form for the gravity gradient tensor is

$$\mathbf{d} = \mathbf{G}\mathbf{m} \quad (35)$$

202 where \mathbf{d} is the data vector, \mathbf{G} is the system matrix and \mathbf{m} is the density vector.

203 The conversion of gravity gradient tensor in the local Cartesian system spherical
 204 coordinates (LNOF) to the x-, y-, z- tensor components in global Cartesian system (ECEF)
 205 can be performed by tensor rotation:

$$\mathbf{d}' = \mathbf{Q}^T \mathbf{d} \mathbf{Q}, \quad (36)$$

206 where $\mathbf{Q}(\phi, \theta)$ is the transformation matrix (Bouman et al., 2013).

207 2.4 Solution of the inverse problem

208 We assume a linear model that connects data and model parameters in the form
 209 of eq. (35). The Gaussian probability distribution for the data can be written

$$p(\mathbf{d}) \propto \exp\left(-\frac{1}{2\sigma_d^2}(\mathbf{G}\mathbf{m} - \mathbf{d})^T \boldsymbol{\Sigma}_d^{-1}(\mathbf{G}\mathbf{m} - \mathbf{d})\right) \quad (37)$$

210 with data correlation function $\boldsymbol{\Sigma}_d$ and variance σ_d^2 .

211 We apply following *a priori* constraints as spatial weighting function (Li & Old-
 212 enburg, 1996; Zhdanov et al., 2011)

$$\mathbf{m}_w = \mathbf{W}\mathbf{m}. \quad (38)$$

The Gaussian probability distribution for the model parameters can be expressed in the form

$$p(\mathbf{m}) \propto \exp\left(-\frac{1}{2}(\mathbf{m} - \mathbf{m}_0)^T \mathbf{W}^T \mathbf{C}_w^{-1} \mathbf{W}(\mathbf{m} - \mathbf{m}_0)\right) \quad (39)$$

213 \mathbf{C}_w^{-1} is the covariance of the weighted parameters and \mathbf{m}_0 is the prior density model.

214 We assume that the covariance of weighted parameters is related to the density co-
 215 variance as

$$\mathbf{C}_w = \alpha^{-1} \mathbf{C}_m = \alpha^{-1} \sigma_m^2 \boldsymbol{\Sigma}_m \quad (40)$$

216 where α^{-1} is a coefficient approximately equal to the mean of the squared diag-
 217 onal elements of the weighting matrix \mathbf{W}

$$\alpha^{-1} \approx \frac{1}{N} \sum_{i=1}^N w_i^2, \quad (41)$$

218 Σ_m is the correlation function, σ_m^2 is the variance.

The joint posterior probability can be written in the form

$$p(\mathbf{m}|\mathbf{d}) \propto \exp\left(-\Phi(\mathbf{m})\right) \quad (42)$$

with

$$2\Phi(\mathbf{m}) = \sigma_d^{-2}(\mathbf{G}\mathbf{m} - \mathbf{d})^T \Sigma_d^{-2}(\mathbf{G}\mathbf{m} - \mathbf{d}) + \alpha\sigma_m^{-2}(\mathbf{m} - \mathbf{m}_0)^T \mathbf{W}^T \Sigma_m^{-1} \mathbf{W}(\mathbf{m} - \mathbf{m}_0). \quad (43)$$

219 The mean and the covariance function that maximize the posterior probability can
 220 be written as solution of a least-squares problem. The solution corresponding to the in-
 221 version in data space (Tarantola, 2004):

$$\Delta \mathbf{m}_w = \mathbf{G}_w^\dagger [\mathbf{G}_w \mathbf{G}_w^\dagger + \alpha \mathbf{I}_d]^{-1} \delta \mathbf{d}, \quad (44)$$

$$\tilde{\Sigma}_m = \Sigma_m - \mathbf{G}_w^\dagger [\mathbf{G}_w \mathbf{G}_w^\dagger + \alpha \mathbf{I}_d]^{-1} \mathbf{G}_w \Sigma_m \quad (45)$$

222 where $\Delta \mathbf{m}_w = \mathbf{W}(\mathbf{m} - \mathbf{m}_0)$ are weighted model parameters, $\mathbf{G}_w = \mathbf{G}\mathbf{W}^{-1} =$
 223 $\mathbf{W}^{-1}\mathbf{G}^T$ is the weighted kernel, \mathbf{I}_d is the identity matrix with the size equal to the num-
 224 ber of data points, the data residuals denoted as $\Delta \mathbf{d} = \mathbf{d} - \mathbf{G}\mathbf{m}_0$ and the adjoint weighted
 225 kernel \mathbf{G}_w^\dagger defined as

$$\mathbf{G}_w^\dagger = \frac{\sigma_m^2}{\sigma_d^2} \Sigma_m \mathbf{G}_w^T \Sigma_d^{-1}. \quad (46)$$

226 The solution can also be written in an alternative form in the case of inversion in
 227 the model space:

$$\Delta \mathbf{m}_w = \tilde{\mathbf{G}}_w^\dagger \delta \mathbf{d}, \quad (47)$$

$$\tilde{\Sigma}_m = \Sigma_m [\mathbf{G}_w^\dagger \mathbf{G}_w + \alpha \mathbf{I}_m]^{-1} \quad (48)$$

228 where $\tilde{\mathbf{G}}_w^\dagger = \frac{\sigma_m^2}{\sigma_d^2} \tilde{\Sigma}_m \mathbf{G}_w^T \Sigma_d^{-1}$ and \mathbf{I}_m is the identity matrix with the size equal to
 229 the number of model parameters.

230 The ensemble of random realization corresponding to the posterior probability den-
 231 sity function can be obtained using the Cholesky decomposition of the posterior covari-
 232 ance matrix \mathbf{C}_m

$$\mathbf{m}_{ens} = \Delta \mathbf{m} + \mathbf{L}^T \xi. \quad (49)$$

233 Here, $\Delta \mathbf{m}$ is the solution for the mean density distribution, ξ is a vector of mutu-
 234 ally independent random numbers with zero mean and unit variance and \mathbf{L} is the ma-
 235 trix of Cholesky factors such as $\mathbf{C}_m = \mathbf{L}^T \mathbf{L}$.

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2.5 Data and model covariance matrices

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Assuming a stationary Gaussian random process, the covariance matrix \mathbf{K} is related to the variogram $\gamma(h)$ estimated at the distance h between a pair of points as

$$\mathbf{K}(h) = \mathbf{K}(0) - \gamma(h) = \sigma_d^2 - \gamma(h), \quad (50)$$

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where σ_d^2 is the data variance. The variogram, estimated using N grid points at the spherical distance h , can be expressed as

$$\gamma(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} (\delta v(x_i + h) - \delta v(x_i))^2, \quad (51)$$

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where $\delta v(x)$ is the parameter variation with respect to the mean value.

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The uncertainty of the Moho depth dominates the uncertainty of the residual gravity signal. We neglect other factors might contribute to the uncertainty, and obtain the data covariance matrix using the covariance for the Moho depth \mathbf{C}_s and the surface Green function \mathbf{G}_s at the regional average radial distance

$$\tilde{\mathbf{C}}_d = \mathbf{G}_s \mathbf{C}_s \mathbf{G}_s^T. \quad (52)$$

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The normalization is required to ensure that patches with the same spherical surface area have the same probability:

$$\mathbf{C}_d = \frac{1}{\cos \phi} \tilde{\mathbf{C}}_d. \quad (53)$$

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The prior information about the length scale and spatial variability of the density field can be incorporated using the covariance matrix. For the model parameter covariance inside the sphere, we assume the statistical model by Kolyukhin and Minakov (2020):

$$\mathbf{C}_m = \sigma_m^2 \boldsymbol{\Sigma}_\Omega(\phi, \lambda) \boldsymbol{\Sigma}_r(r), \quad (54)$$

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where σ_m^2 is the model variance, $\boldsymbol{\Sigma}_\Omega(\phi, \lambda)$ and $\boldsymbol{\Sigma}_r(r)$ are the angular and the radial correlation functions, respectively. The correlation functions can be obtained using the variogram method. There are a number of functions that can be used to approximate empirical variogram (Terdik et al., 2015; Lantuéjoul et al., 2019). In this work, the angular covariance is approximated using the inverse distance model (Terdik et al., 2015).

$$\boldsymbol{\Sigma}_\Omega(\phi, \lambda) = (1 + a^2 - 2a \cos \psi)^{-1/2}. \quad (55)$$

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Here, the correlation length depends on the parameter $|a| < 1$.

The variogram in the radial direction is approximated using an exponential-type covariance (Monin & Yaglom, 1975) (their eq. 11.20)

$$\boldsymbol{\Sigma}_r(r) = \exp(-b_1 |\mathbf{r}|) \cos b_2 |\mathbf{r}|, \quad (56)$$

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with the correlation length defined by the parameters b_1 and b_2 . The sensitivity of S-wave velocities and density to temperature changes, inferred from empirical data, can be used to obtain the model constraints in terms of spatial correlations.

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2.6 Spatial weighting and depth resolution

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The function \mathbf{W} acts as a stabilizing functional for the inverse problem and provides depth weighting to each parameter according its contribution to the data points used in the inversion (Zhdanov, 2015). The integrated sensitivity of the data at the observation plane S to variation of the model parameter k can be expressed as

$$\mathbf{W}^T \mathbf{W} = \text{diag} \left(\frac{\|\delta \mathbf{d}\|}{\delta m_k} \right) = \text{diag} \left(\sqrt{\iint_S G_k^2 dS} \right). \quad (57)$$

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The shape of the averaged gravity gradient kernel at a point centered at the origin of coordinate eq. (32) is azimuthally symmetric. For analytical demonstration of the form of the weighting function, it is convenient to perform integration in cylindrical coordinates:

$$\mathbf{W}^T \mathbf{W} = \text{diag} \left(\sqrt{\int_0^{2\pi} d\phi \int_0^\infty G_k^2 r dr} \right). \quad (58)$$

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Using the expression for the eigenvalue of the gravity gradient tensor corresponding to a point mass (Pedersen & Rasmussen, 1990), the integral in eq. (58) can be written as

$$2\pi \int_0^\infty G_{ik}^2 r dr = 2\pi \int_0^\infty \frac{2r}{(r^2 + z^2)^3} dr = -\frac{\pi}{(r^2 + z^2)^2} \Big|_0^\infty = \frac{\pi}{z^4} \quad (59)$$

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where $r = \sqrt{x^2 + y^2}$ is the radial distance from the origin to the observation point. After the square root is applied twice, the model weighting coefficients become proportional to the inverse distance from the observation point to the point mass:

$$w_i \propto 1/z_i. \quad (60)$$

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Such spatial weighting suppresses model variation in the shallow part of the model (with respect to the prior model) and enhances model variation in the deeper part of the model.

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To better understand the density imaging using satellite gradiometry data, it is useful to analyze properties of the integrated gravity gradient kernel. The principles of potential field imaging (Zhdanov et al., 2011) can be illustrated on the example of vertical gradient U_{zz} . The integrated kernel is directly related to the migration density field if the data represent a boxcar function:

$$K_{zz} = \int_0^{2\pi} d\phi \int_0^{r_0} \frac{r}{(r^2 + z^2)^{3/2}} \left(\frac{3z^2}{r^2 + z^2} - 1 \right) dr. \quad (61)$$

283

This definite integral equals to

$$K_{zz} = \frac{2\pi r_0^2}{(r_0^2 + z^2)^{3/2}}. \quad (62)$$

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The maximum of the kernel is located at the surface before the weights in eq. (60) are applied:

$$K_{zz} = \frac{2\sqrt{\pi}r_0^2 z^2}{(r_0^2 + z^2)^{3/2}}. \quad (63)$$

286 The kernel has a larger geometrical spreading with depth for wider gravity gradi-
 287 ent anomalies. The maximum of this weighted kernel and corresponding maximum of
 288 the migration density field can be found at the extreme point:

$$\frac{\partial K_{zz}}{\partial z} = \frac{2\sqrt{\pi}r_0^2 z (2r_0^2 - z^2)}{(r_0^2 + z^2)^{5/2}} = 0. \quad (64)$$

From where, the predicted maximum of imaged density field is related to the ra-
 dius of the integration region as

$$z = \sqrt{2}r_0. \quad (65)$$

289 For the 2D case, using analytical integration in the complex plane, Zhdanov (2015)
 290 has shown that the gravity migration density distribution has a maximum at the loca-
 291 tion of the point mass. Similarly, it can also be shown numerically for the case of 3D ge-
 292 ometry.

293 2.7 Numerical implementation of the gravity gradient inversion

294 A least squares solution in the form of eq. (44) can be obtained using an iterative
 295 solution technique (Liang et al., 2014; Barnoud et al., 2016) such as the method of con-
 296 jugate gradients and LSQR (Paige & Saunders, 1982). For three dimensional problems,
 297 the system matrix quickly grows and this approach becomes computationally challeng-
 298 ing. Alternatively, we can use the formulation of the inversion in the data space eq. (44),
 299 (45). In this case, the matrix to be inverted is of the data size and can be performed us-
 300 ing the singular value decomposition (ChARRIERIAU & CHOUTEAU, 2003). Moreover, assum-
 301 ing that the data are uncorrelated, we can modify the probability function of model pa-
 302 rameters by incorporating new data, such as additional measurements, or combine dif-
 303 ferent gravity gradient components. Applied successively to each data point, this method
 304 does not require inversion of large matrix, and, therefore, can be numerically efficient.
 305 The corresponding least-squares solution is based on eqs (44),(45) (see Tarantola (2004)).
 306 Using our notation it can be written as

$$\mathbf{m}_w^{(k+1)} = \mathbf{m}_w^{(k)} + H^{-1}\mathbf{q}\delta d_k \quad (66)$$

$$\mathbf{C}_m^{(k+1)} = \mathbf{C}_m^{(k)} - H^{-1}\mathbf{q}\mathbf{q}^T \quad (67)$$

$$\delta d_k = d_k - \mathbf{G}_k \mathbf{W}^{-1} \mathbf{m}_w^{(k)} \quad (68)$$

$$\mathbf{q} = \sigma_d^{-1} \mathbf{C}_m^{(k)} \mathbf{G}_k \mathbf{W}^{-1} \quad (69)$$

$$H = \alpha + \mathbf{G}_k \mathbf{W}^{-1} \mathbf{q} \quad (70)$$

307 The k index denotes current data point with the mean d_k and variance σ_d . \mathbf{G}_k is
 308 the system matrix eq. (35) with the number of rows corresponding to the number of data
 309 components (a row vector for single-component data). The memory requirements can
 310 be substantially reduced by noticing the local nature of gravity gradient kernels. There-
 311 fore, only significant \mathbf{G}_k elements can be selected. We found that model parameters be-
 312 yond 600-700 km distance from the observation point have a very small contribution to
 313 the data, and, thus, corresponding matrix elements of \mathbf{G}_k and \mathbf{C}_m can be ignored with-
 314 out a substantial change of the solution. The vector \mathbf{q} is analogous to the adjoint op-
 315 erator \mathbf{G}^\dagger (eq. (46)). The matrix H reduces to the scalar for single-component data H
 316 (or a small square matrix with the size of the number of data components). Note that
 317 the mean weighted density $\mathbf{m}_w^{(k)}$ and the covariance matrix $\mathbf{C}_m^{(k)}$ are updated at each it-
 318 eration k . The final density model $\mathbf{m} = \mathbf{W}^{-1} \mathbf{m}_w$ is obtained after the last data point

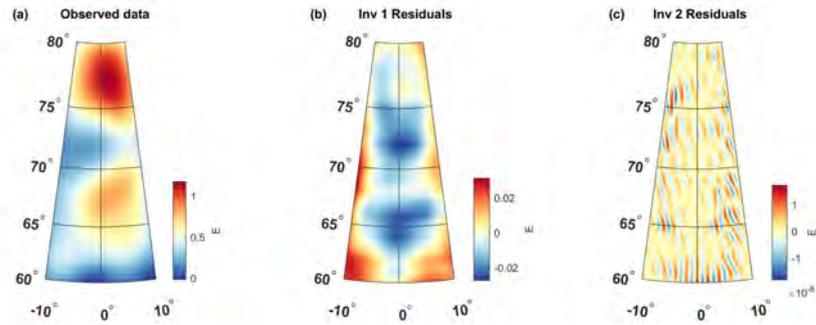


Figure 4. Reconstructed synthetic data using a spherical random density model. (a) synthetic input data (radial gravity gradient); (b) the data residuals obtained using the LSQR damped least squares inversion method; (c) the data residuals obtained using the recursive least squares inversion method with the constrained covariance model.

319 has been assimilated. Equation (66) allows for a rapid density imaging method similar
 320 to the potential field migration suggested by Zhdanov et al. (2011).

321 2.8 Synthetic tests

322 The 3D synthetic density model represents a spherical shell model with the lateral
 323 extent of $20^\circ \times 20^\circ$ and the bottom at the top mantle transition zone (410 km depth). The
 324 model is parameterized using 20 layers comprised of spherical prisms with a 0.5-degree
 325 resolution. We simulate the density anomalies in the model as a Gaussian random field
 326 with zero mean and covariance determined by eqs (54)-(55). The description of the numerical
 327 method for the random field simulation inside the sphere can be found in Meschede
 328 and Romanowicz (2015) and Kolyukhin and Minakov (2020). The parameters defining
 329 the covariance model were selected according to the empirical correlation functions (Fig.
 330 10) estimated using the seismic tomography model for the northeast Atlantic region by
 331 Rickers et al. (2013); Fichtner et al. (2018). We calculate the radial gravity gradient signal
 332 (Fig. 4a) corresponding to the random density model (Fig. 5a) using eqs (6) and (33).
 333 The density distribution was reconstructed using the two methods described in section
 334 2.7.

335 The first modeling approach we have used is the LSQR method with diagonal co-
 336 variance matrices ($\sigma_d = \pm 10 \text{ s}^{-1}$, $\sigma_m = \pm 10 \text{ kgm}^{-3}$) and the zero prior mean density
 337 anomaly. An optimal damping parameter was found based on the standard L-curve cri-
 338 terion (Aster et al., 2018). The data residuals and reconstructed model are shown in Fig.
 339 4b and Fig. 5b. The inversion recovers the lateral position, depth to the center of mass
 340 and average intensity of density anomalies in the model. The depth smearing limits the
 341 resolution of fine structures in the model.

342 The second method we have applied is the recursive least squares inversion in the
 343 data space with the full model covariance matrix and the diagonal data covariance ma-
 344 trix. The simulation results are in Fig. 4c and Fig. 5c. The constraints on spatial cor-
 345 relations in the model allows recovering not only average position (center of mass) of the
 346 density anomalies by also their correct aspect ratio. The spatial correlation controls the
 347 shape, relative strength and depth of individual density anomalies.

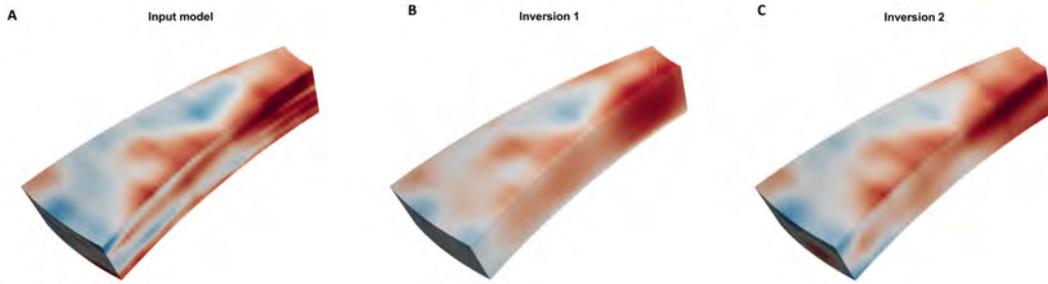


Figure 5. Reconstructed synthetic spherical random density model. (a) synthetic input model. The covariance model is defined by eqs (55),(56) with $a = 0.94$, $b_1 = 0.03$, and $b_2 = 0.1$. (b) the model obtained using the LSQR damped least squares inversion method. (c) the model obtained using the recursive least squares inversion method with the constrained covariance model.

3 Results

3.1 Gravity and gravity gradient signals of lithospheric layers

We assume that the total gravity signal in the North Atlantic consists of the following main components: 1) topography (elevation and bathymetry) and the associated Bouguer correction; 2) ice thickness variation; 3) sedimentary thickness variation, constrained by multichannel seismic data; 4) crustal thickness and density variations, constrained by wide-angle seismic data; 5) lithospheric thickness variation due to stretching and subsequent cooling, constrained by crustal age grid (Fig. 2); and 6) density variation in the upper mantle. The long-wavelength signal due to lower-mantle density variations was neglected since it is found to be small in gravity gradients compared to this signal in the geoid and the gravity anomaly field (see Fig. 3).

The topography and bathymetry data were extracted from the international GEBCO2020 bathymetry and topography data including the ice thickness model over Greenland <https://www.gebco.net> (Fig. 2). The topography/Bouguer correction is performed using the reduction density of 2850 kg m^{-3} . The density of ice is assumed 970 kg m^{-3} . The global sediment thickness grid is combined using the marine sedimentary thickness by Straume et al. (2019) and the CRUST1.0 sediment thickness on land (Laske et al., 2013; Szwillus et al., 2019). Regional sedimentary thickness and crustal thickness data are based on the seismic reflection and refraction database compiled during NAGTEC project <http://www.nagtec.org> (Funk et al., 2017). The assumed sediment density is 2400 kg m^{-3} . The average density of crystalline crust follows the results of statistical interpolation by Szwillus et al. (2019). The density variation within the crustal layer is found to have a second-order effect compare to the crustal thickness variation. The lithospheric cooling correction (Fig. 7c,d) is computed using a pure shear lithospheric extension model (McKenzie, 1978) and the ocean age grid (Gaina, Nasuti, et al., 2017).

We have estimated spherical harmonic coefficients for each crustal density layer using global spherical harmonic analysis (Sneeuw, 1994; Wiczcerek, 2007). Then, we calculated the gravitational potential (Stokes) coefficients from which the gravitational potential and its functionals can be obtained (Novák & Grafarend, 2006). The residual gravity and gravity gradient anomalies correspond to the observed data after the effects of each individual crustal layers has been subtracted (Fig. 8).

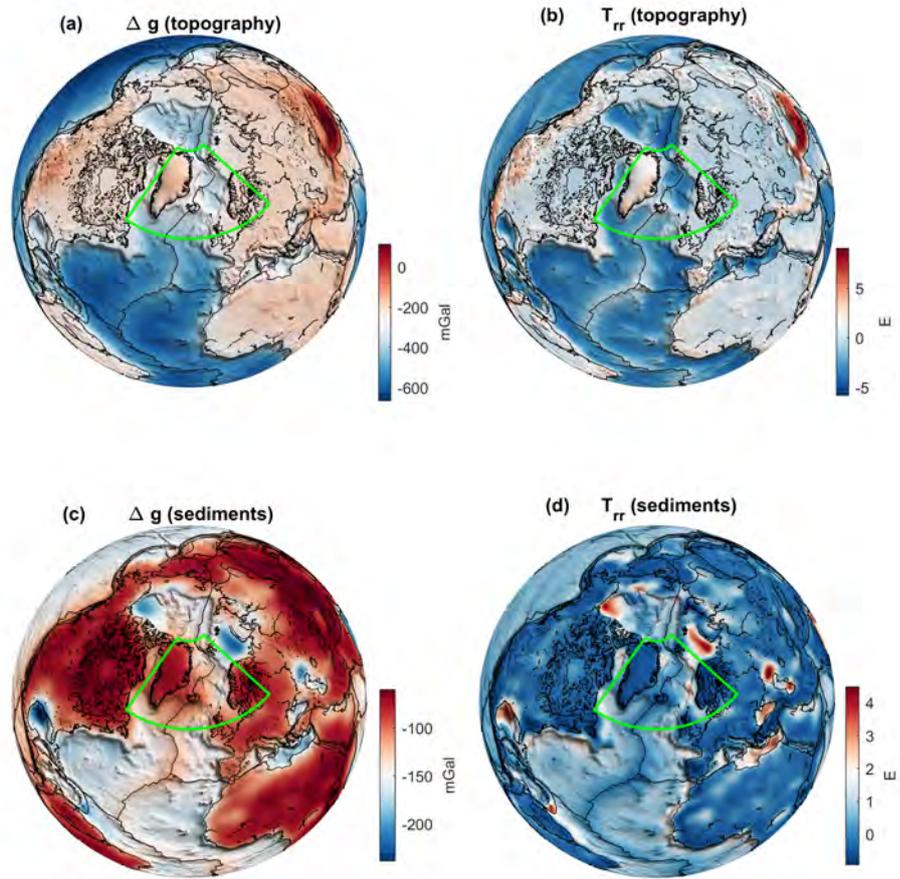


Figure 6. Gravity and radial gravity gradient anomaly due to the variation of topography (a,b) and sediment thickness (c,d) at the height of 220 km. The sector indicates the northeast Atlantic study region.

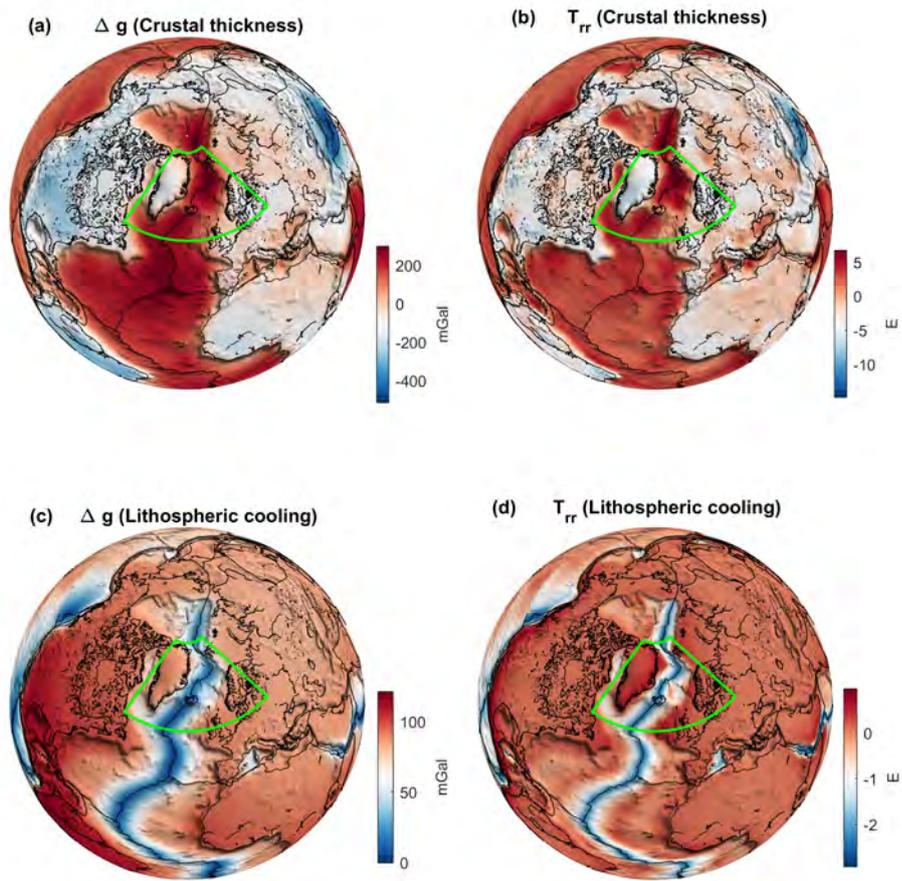


Figure 7. Gravity and radial gravity gradient anomaly due to the variation of crustal thickness (a,b) and oceanic crustal age (c,d) at the height of 220 km. The sector indicates the northeast Atlantic study region.

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3.2 Residual gravity and gravity gradient signal

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The goal of the following analysis is to extract from the observed gravity data the gravity signal corresponding to the 3D heterogeneous density structure of the lithosphere and sub-lithospheric upper mantle. We subtract from the observed data in Fig. 1 the signal of the crust including the topography correction and the thermal density signal due to lithospheric cooling (Fig. 7).

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The residual gravity and radial gravity gradient anomalies emphasize the effects of dense and cold continental roots and low-density regions adjacent to the Iceland hotspot region. The gravity effect of localized lithospheric density anomalies is more pronounced in residual gravity gradient anomalies than in the total field. The range of variation is from about -100 mGal to 75 mGal and $\pm 2-3$ E, for the gravity and the gravity gradient, respectively.

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The obtained residual gravity gradients (Fig. 8) can be linked to the density variation unaccounted by the 3D reference model. The amplitude values of the residual gradients ($\pm 2 - 3$ E) is about twice of the observed gradients, and the crustal correction constitutes about 2/3 of the total signal. A rough estimate of the gravity gradient signal associated with a 100-km size spherical density anomaly due to a temperature change of 100 K located in a middle upper mantle would correspond to about 1 E.

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The interpretation of the residual signal is most transparent in the case of the radial gravity gradient (Fig. 8). The lithospheric and upper mantle signal is more pronounced in the residual gravity gradient signal (Fig. 8b,d) than in the residual gravity anomalies (Fig. 8a,c). The residual signal shows a correlation with the upper mantle seismic velocity anomalies in the global tomography model by Schaeffer and Lebedev (2013). In particular, at the depth of 80 km (Fig. 8d) in the oceanic, both to the north and south of Iceland, and within cratonic regions. The negative residual signal at the east Greenland margin, the south Norway region and northern British Isles implies a low-density lithosphere at depth. The Fennoscandian craton appears colder and thicker compared to the Greenland lithosphere in both seismic tomography model and gravity data. Note that the observed data in Figs 1 and 3 show anti-correlation with the seismic anomalies (see also Sebera et al. (2017)).

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3.3 Statistical characterization of input data and prior information

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The non-uniqueness of the inverse problem can be addressed using various approaches to incorporate prior information. In our case, the largest uncertainty in the data (residual gravity gradient signal) arises from the uncertainty of the crustal thickness due to non-homogeneous coverage of wide-angle seismic data. This prior information is incorporated in the inversion using the data covariance matrix \mathbf{C}_d . Assuming a linear model between data and model parameters, the variance of crustal thickness can be translated to the data variance (Fig. 9) using eq. (52). We find the probability distribution for the crustal thickness following the geostatistical method described in Szwillus et al. (2019). Since the full original dataset is not available, we extracted the actual Moho depth values from corresponding published grids (Funck et al., 2017; Mooney, 2015; Szwillus et al., 2019) along the profile coordinates with a step of 10 km, assuming that the values at the data locations have not been biased by the interpolation in the regional grid. Then, we applied a spherical kriging interpolation to the obtained dataset.

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The data covariance matrix \mathbf{C}_d was obtained from the Moho variance grid using eq. (52) and the gravity gradient kernel eq. (33). For simplicity, we consider only diagonal elements of this matrix and imply that the data points are independent. This assumption is not generally required but allows for an efficient numerical implementation. The diagonal elements of $\mathbf{C}_d^{-1/2}$ (standard deviation) shown in Fig. 9 imply the largest variance over southwestern Greenland ($\sigma_d^{1/2} > 1$ Eotvos). The passive margin of Nor-

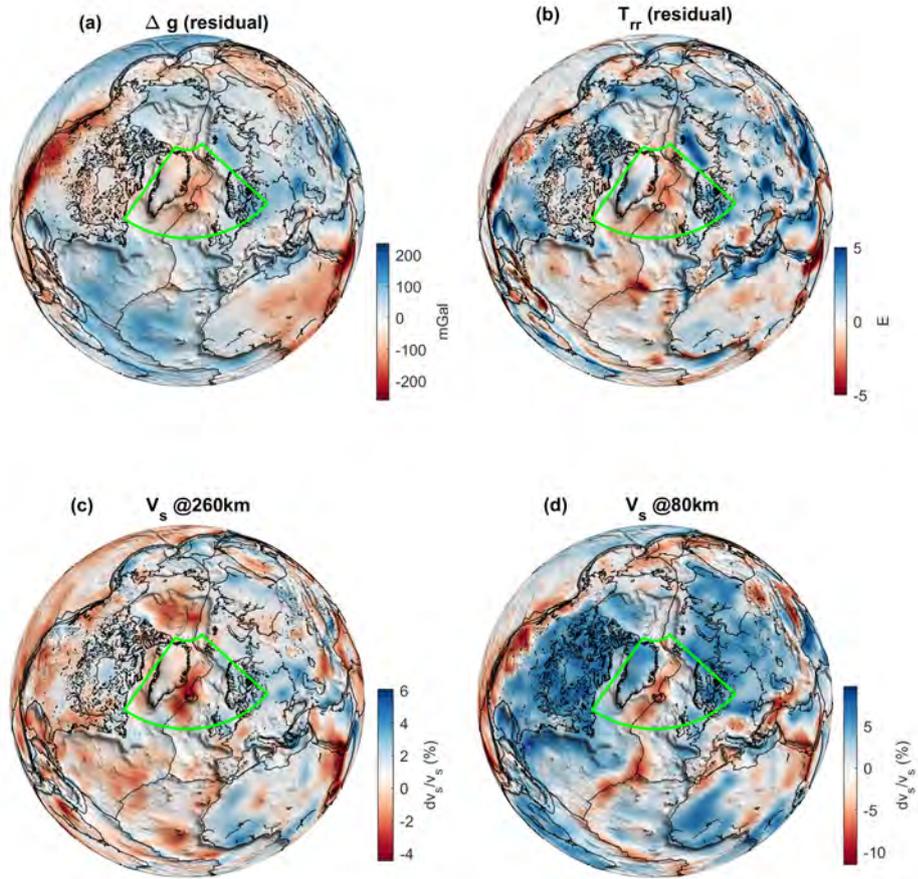


Figure 8. The residual gravity and radial gravity gradient (a,b) and seismic shear velocity perturbation at the depth of 260 km (c) and 80 km (d) in the global tomography model by Schaeffer and Lebedev (2013). The sector indicates the northeast Atlantic study region.

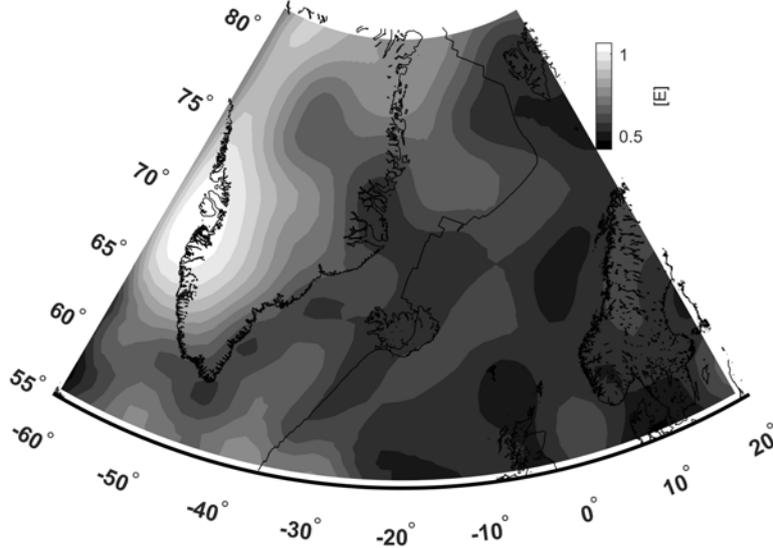


Figure 9. Data uncertainty (square root of the diagonal data covariance matrix \mathbf{C}_d)

429 way is densely covered by seismic profiles and has small data uncertainty ($\sigma_d^{1/2} < 0.5$
 430 Eotvos).

431 The model covariance matrix \mathbf{C}_m can be obtained using the variogram method de-
 432 scribed in section 2.5. We applied this method to the seismic shear velocity variation in
 433 the regional tomography model by Rickers et al. (2013); Fichtner et al. (2018) which has
 434 a better spatial resolution compare to global models. We assume that the spatial cor-
 435 relations of seismic velocity and density anomalies are similar. Fig. 10 shows the radial
 436 correlation function (Σ_r), estimated for a bin size of 20, 30 and 40 points, at the depth
 437 of 50-410 km, after the 1D mean has been removed. The estimated correlation becomes
 438 negative beyond a radial distance of about 150 km. This type of spatial variation can
 439 be approximated in the analytic form by a combination of exponential and cosine func-
 440 tions (Monin & Yaglom, 1975). We have also estimated the correlation depending on the
 441 spherical distance up to 0.5 rad (or about 3000 km) at four different depth intervals be-
 442 tween 65 km and 265 km depth. The angular correlation function (Σ_Ω) can be repre-
 443 sented by the inverse distance model (Lantuéjoul et al., 2019) with the coefficient a be-
 444 tween 0.9 and 0.99 depending on the depth.

445 3.4 Inversion of residual gravity gradients

446 The density model was parameterized as a spherical shell with a lateral grid resolu-
 447 tion of 50-70 km and the depth resolution of about 20 km. The single-component in-
 448 version was performed using the residual radial gravity gradient signal (T_{rr}) shown in
 449 Fig. 11. The range of the signal is ± 3 Eotvos. In the inversion setup, we assume a zero
 450 density variation as a prior model. The predicted mean density model is presented for
 451 the depth of 150 km (Fig. 13).

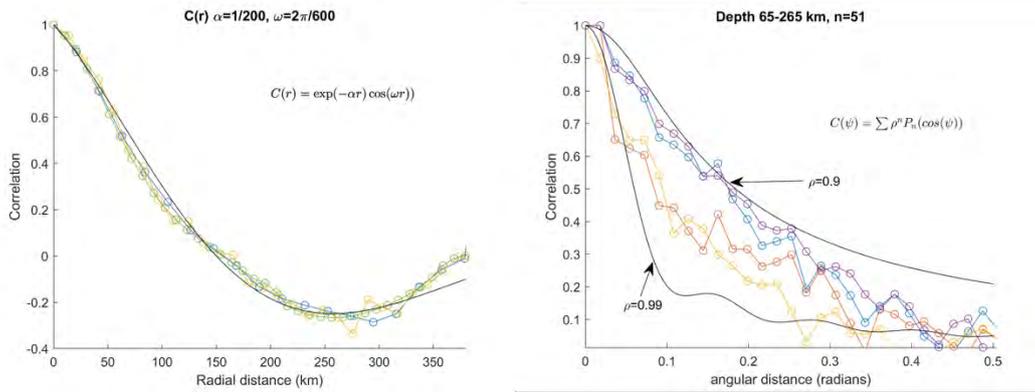


Figure 10. Empirical radial (a) and angular (b) correlation functions estimated using the seismic S-wave tomography model and the variogram method. (a) the color indicates various bin sizes (20, 30 and 40 data points). (b) the color indicates the correlation function estimated at four different depth intervals (65-115 km, 115-165 km, 165-210 km and 210-265 km); the bin size is 30 points.

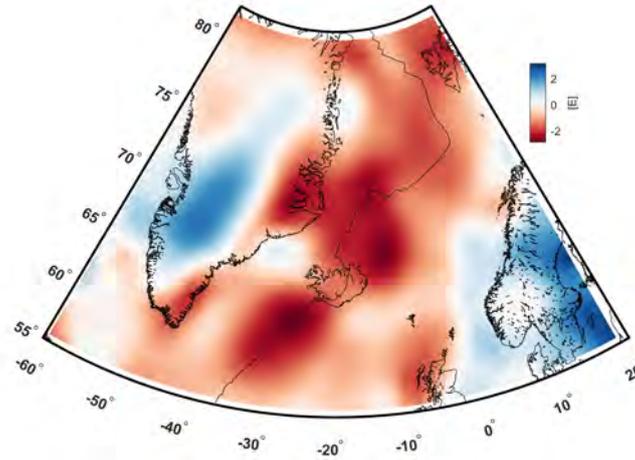


Figure 11. Residual gravity gradient anomalies (T_{rr}). The coastlines and mid-Atlantic ridge axis are shown.

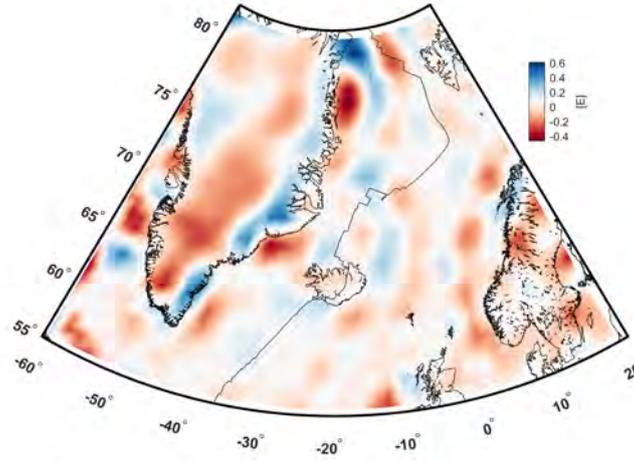


Figure 12. The misfit of predicted gravity gradient signal (T_{rr}) based on the final density model. The coastlines and mid-Atlantic ridge axis are shown.

452 The calculated data misfit shows no systematic pattern (Fig. 12). The range of the
 453 misfit is about ± 0.5 Eotvos which is generally within the data uncertainty $2\sigma_d^{1/2}$ (cf. Fig.
 454 9).

455 The general pattern of the density perturbation reflects the distribution of resid-
 456 ual anomalies in Fig. 13. The predicted negative density anomalies in the upper man-
 457 tle correlate with a wider region along mid-ocean ridges where seamount volcanism may
 458 have been active since the Oligocene (ca 30 Ma). In addition, the thinned continental
 459 crust of Rockall Plateau, where older seamounts were emplaced (ca. 50-60 Ma), is un-
 460 derlain by a low-density upper mantle (Fig. 13). The most intense negative mantle
 461 density anomaly (about -40 kg m^3) at the west Greenland margin corresponds to the early
 462 Cenozoic location of the Iceland hotspot (Torsvik et al., 2015). The Greenland-Iceland-
 463 Faeroe ridge is underlain by a positive density anomaly in the shallow lithosphere. The
 464 negative density anomalies are observed underneath the Caledonian deformation front
 465 in northern British Isles and southern Norway. The mass deficit under the central-east
 466 Greenland margin and across Greenland is expressed in the density model at middle up-
 467 per mantle depths.

468 The comparison with regional high-resolution seismic tomography model (V_{SH}) by
 469 Rickers et al. (2013); Fichtner et al. (2018), shown at the same depth, indicate a sim-
 470 ilar correlated pattern of positive and negative anomalies. The negative anomalies are
 471 located along the mid-Atlantic ridge, and to a lesser extent under northern British Isles
 472 and the Norwegian margin. The positive anomalies are below the cratonic parts of Green-
 473 land and Fennoscandia. The dissimilarities between the tomography and gravity mod-
 474 els at a particular depth can be partly related to the non-uniqueness of the inverse grav-
 475 ity problem such as along the Iceland-Faeroe Ridge and at the west Greenland margin
 476 (Fig. 13 and Fig. 14). A more detailed discussion on the predicted mantle density vari-
 477 ation with its relation to crustal structure and seismic velocities along three regional tran-
 478 sects follows in the next chapter.

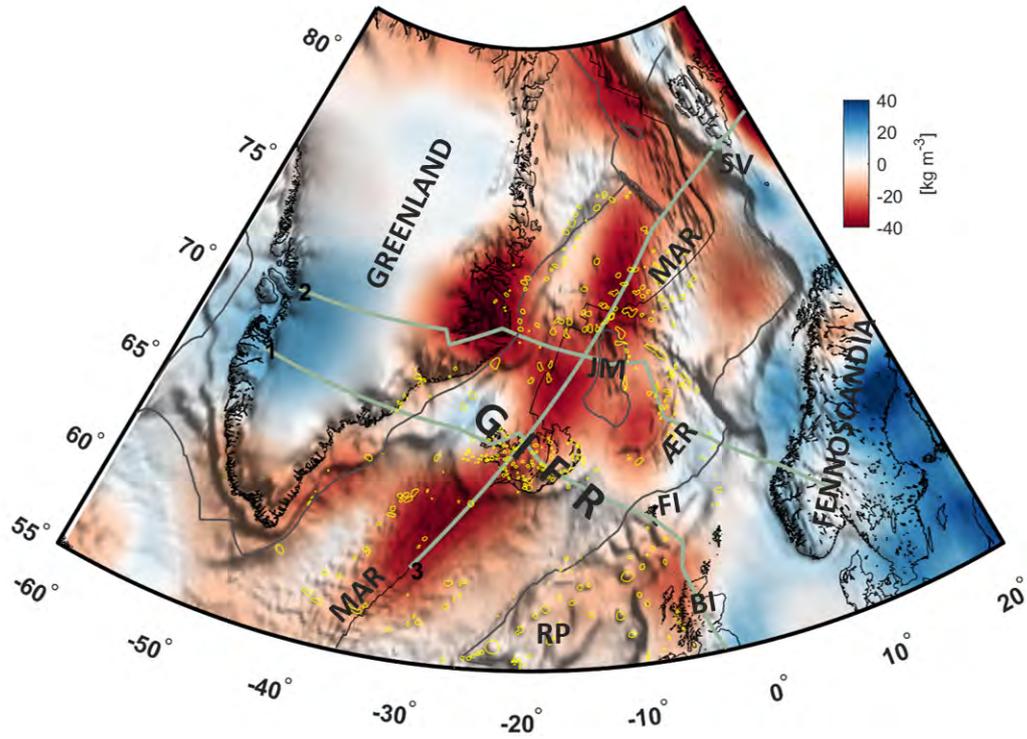


Figure 13. Density anomalies at 150-km depth based on inversion of the residual radial gravity gradient field. The grey lines indicate the location of the model transects. The volcanic centers and seamount-like features identified by Gaina, Blichke, et al. (2017) are indicated by yellow contours. The coastlines, continent-ocean boundaries and the mid-Atlantic ridge axis are shown. \AA R - \AA gir Ridge; BI - British Isles; FI - Faeroe Islands; GIFR - Greenland-Iceland-Faeroe Ridge; JM - Jan Mayen Microcontinent; MAR - Mid-Atlantic Ridge; RP - Rockall Plateau; SV - Svalbard.

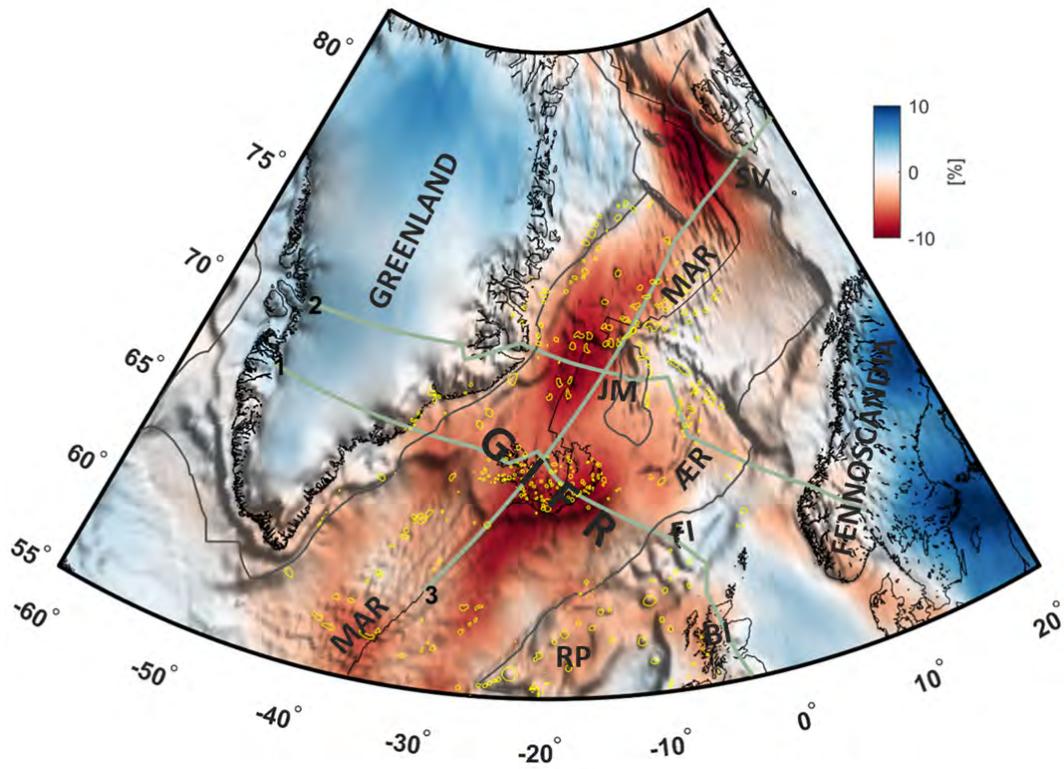


Figure 14. Velocity anomalies at 150-km depth based on tomography model by Rickers et al. (2013); Fichtner et al. (2018). The grey lines indicate the location of the model transects. The volcanic centers and seamount-like features identified by Gaina, Blischke, et al. (2017) are indicated by yellow contours. The coastlines, continent-ocean boundaries and the mid-Atlantic ridge axis are shown. ÆR - Ægir Ridge; BI - British Isles; FI - Faeroe Islands; GIFR - Greenland-Iceland-Faeroe Ridge; JM - Jan Mayen Microcontinent; MAR - Mid-Atlantic Ridge; RP - Rockall Plateau; SV - Svalbard.

4 Discussion

4.1 Mantle density and seismic velocity anomalies along lithospheric transects

Several regional seismic tomography studies have shown an irregular-shape low-velocity seismic anomaly in the upper mantle in the northeast Atlantic region resolved in both S-wave (Pilidou et al., 2005; Legendre et al., 2012; Rickers et al., 2013; Fichtner et al., 2018; Lebedev et al., 2018) (Fig. 14) and P-wave velocity models (Bijwaard & Spakman, 1999; Jakovlev et al., 2012; Hosseini et al., 2020), and can be linked to the Cenozoic Iceland plume activity. The anti-correlation of the seismic velocity and long-wavelength gravity anomalies have previously been discussed by Jones et al. (2002); Rickers et al. (2013); Sebera et al. (2017). Our results are in agreement with their conclusion that the long-wavelength positive gravity anomalies (and corresponding dynamic topography) are associated with the low-density material in the asthenosphere.

The regional S-wave tomography model by Rickers et al. (2013); Fichtner et al. (2018) is based on full-waveform inversion of surface and body waves, and has previously been used to infer geodynamic processes in the northeast Atlantic region (Schoonman et al., 2017). Here, we compare the S-wave velocity anomalies in the tomography model with our density model (Fig. 13) along three lithospheric-scale transects. Each synthetic transect is characterized by good constraints on crustal structure based on controlled-source seismic data. The synthetic transects, whenever it is possible, follow available seismic lines and illuminate key tectonic features of the study area. The transects are shown for the upper 300 km, the region where most of density variation resides.

4.1.1 Profile 1

The west-east Profile 1 (Fig. 15) runs across Greenland (0-750 km), along the Greenland-Iceland-Faeroe Ridge (GIFR) (750-2100 km) and northern British Isles (2100-3000 km) where it intersects the main Caledonian suture zone (Barton, 1992). The profile crosses the thick and cold Greenland craton where crustal thickness is mainly constrained by receiver function data (Dahl-Jensen et al., 2003). Further east, the profile runs along the western portion of GIFR with thick high-velocity igneous or transitional crust (Korenaga et al., 2000; Yuan et al., 2020). The crustal thickness of the mainly volcanic Iceland Plateau reaches about 40 km, as it was estimated from the receiver function analyses (Kumar et al., 2007) and wide-angle profiles by Darbyshire et al. (1998) and Staples et al. (1997). In a regional context, Iceland is part of GIFR which represents a complex region of excessive magmatic crustal accretion due to overlapping rift systems, interlinked rifts and transform zones with a variable uplift and subsidence history (Hjartarson et al., 2017). In such excessively magmatic regions, high-density ultramafic rocks can be emplaced at or above Moho (Richards et al., 2013; Funck et al., 2017), and significantly decrease the density contrast at the crust-mantle interface. The P-wave velocity and density structure along the eastern part of GIFR is apparently similar to the western part; although, the velocity model might be poorly resolved due to short source-receiver offsets.

The lithospheric density images derived using the gravity gradient inversion provide complementary information to seismological data. The thin extended continental crust within the Faeroe Basin (Raum et al., 2005) is underlain by slightly denser upper mantle compared to GIFR to the west and northern British Isles to the east. The Greenland lithosphere has a cold and dense cratonic root to a depth of about 300 km according to both the seismic and gravity data (Fig. 15). The asthenosphere beneath Iceland has a low-velocity and corresponding low-density anomaly of a relatively smaller magnitude (about 15-20 kg m⁻³). At the east Greenland margin, (profile distance 500-800 km or about 40°E) along the profile the low-density anomalies (above 200 km depth) correlates with the region affected by the Cenozoic volcanism related to the emplacement of the North Atlantic Igneous Province (Fig. 13). Similarly, the high-amplitude low-density

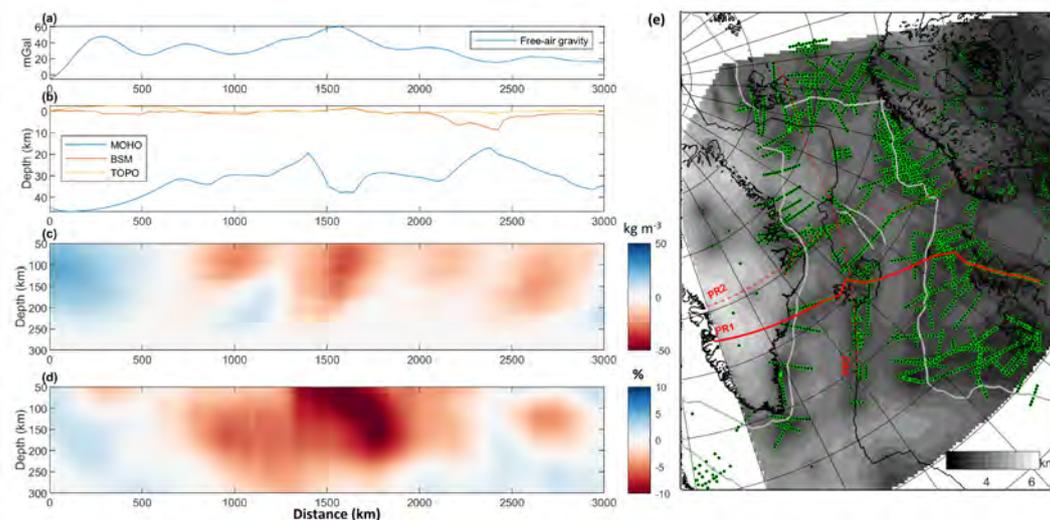


Figure 15. Inversion results along W-E Profile 1 across the northeast Atlantic. (a) Observed free-air gravity anomaly; (b) Crustal geometry: the Moho depth, top basement and topography; (c) density variation with respect to the 3D reference model; (d) seismic shear velocity perturbation in the regional S-wave tomography model (Rickers et al., 2013; Fichtner et al., 2018); (e) the uncertainty of crustal thickness (one standard deviation) with location of seismic refraction profiles (green) and synthetic lithospheric transects (red).

530 anomaly at the northern Britain margin (profile distance 2300-3000 km or about -12°E
 531) corresponds to Paleocene volcanic centers in the Faeroes region. This density anomaly
 532 is outlined by the Caledonian suture zone. A possible explanation for a negative density
 533 anomaly beneath the Caledonian deformation front can be related to thin lithosphere
 534 and/or the presence of trapped oceanic crust which can be rich in plagioclase at elevated
 535 lithospheric temperatures. The lithospheric density structure of GIFR can be related to
 536 ultramafic melts crystallized at or below the Moho in combination with fragments of con-
 537 tinental lithosphere and/or pyroxenite-rich mantle (Yuan et al., 2020; Foulger et al., 2019).

538 *4.1.2 Profile 2*

539 Profile 2 (Fig. 16) generally follows the previously compiled lithospheric transect
 540 across the North Atlantic by Mjelde et al. (2008). The central and east Greenland litho-
 541 sphere have a contrasting density structure in the model. In the upper lithosphere, the
 542 P-wave velocity of thick continental crust thickness of central-east Greenland (> 35 km)
 543 was constrained based on the analysis of broadband seismic data (Kraft et al., 2019). The
 544 transition to low-density mantle beneath east Greenland margin in Fig. 16b is associ-
 545 ated with the shallow lithosphere-asthenosphere boundary in the seismic tomography
 546 model (Fig. 16c). The hyper-extended continental crust of Jan Mayen microcontinent
 547 (1700 km distance) is underlain by a low-density asthenosphere. This may explain a rel-
 548 atively elevated topography of Jan Mayen (Tan et al., 2017, 2018). The upper mantle
 549 beneath the extinct Ægir spreading ridge (A. Breivik et al., 2014) has coincident low-
 550 density and low-velocity anomalies (profile distance 2000 km). The shallow lithosphere
 551 of the continental margin of Norway appears with a similar positive anomalous density
 552 as the Greenland lithosphere whereas the seismic velocities are relatively low here.

553 As in Profile 1, the correlation of the lithospheric low-density anomalies with the
 554 distribution of Cenozoic volcanism is observed along Profile 2. The density image sug-

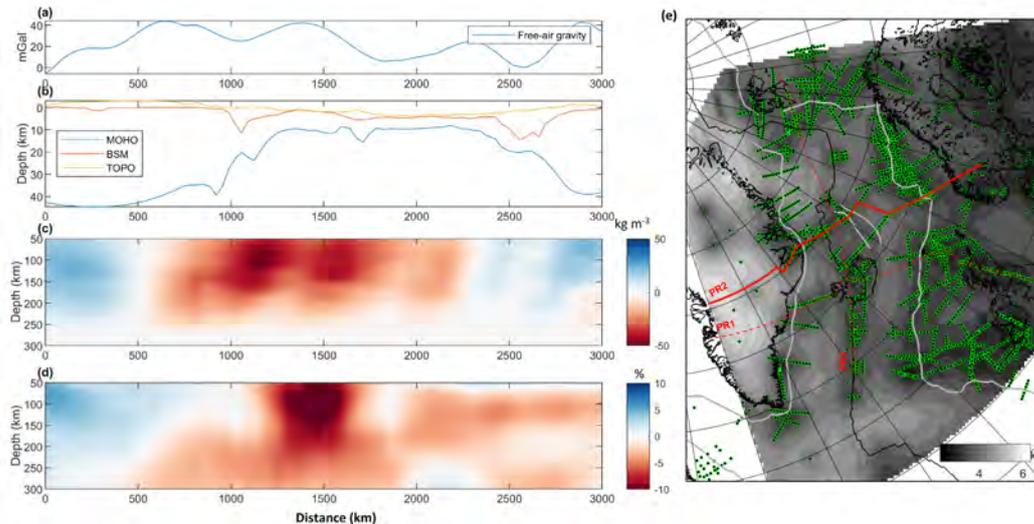


Figure 16. Inversion results along W-E Profile 2 across the northeast Atlantic. (a) Observed free-air gravity anomaly; (b) Crustal geometry: the Moho depth, top basement and topography; (c) density variation with respect to the 3D reference model; (d) seismic shear velocity perturbation in the regional S-wave tomography model (Rickers et al., 2013; Fichtner et al., 2018); (e) the uncertainty of crustal thickness (one standard deviation) with location of seismic refraction profiles (green) and synthetic lithospheric transects (red).

555 gests that the low-density mantle anomaly beneath the East Greenland margin and the
 556 Jan Mayen region has the same deep asthenospheric source. The density and seismic ve-
 557 locity structure suggests branching of a deep thermal anomaly in the shallow upper man-
 558 tle towards east Greenland and the mid-Atlantic Ridge.

559 4.1.3 Profile 3

560 Profile 3 approximately follows the Mid-Atlantic Ridge (Fig. 17), across Iceland
 561 (500-1100 km) and Jan Mayen microcontinent (1500-1600 km) and ends at the passive
 562 margin of Svalbard. The segmentation of igneous crustal thickness along Profile 3 can
 563 be associated with the alternation of low-density and low-shear velocity anomalies in the
 564 asthenosphere. This variation can be linked to the excess crustal accretion at the spread-
 565 ing ridge influenced by the Iceland hotspot (A. J. Breivik et al., 2008; Tan et al., 2018;
 566 Ito, 2001). The low density anomaly is obtained in the mantle both north and south of
 567 Iceland. A deep-seated density anomaly north of Iceland might extend over large dis-
 568 tance in the shallow asthenosphere towards Svalbard margin where thin lithosphere is
 569 predicted using various geophysical data (Vagnes & Amundsen, 1993; Minakov, 2018;
 570 Selway et al., 2020). The intense low-velocity in the upper 100 km beneath the thick ig-
 571 neous crust of Iceland (Gudmundsson, 2003) does not correspond a similar low-density
 572 anomaly in Fig. 17. This result should be interpreted with caution since it might also
 573 reflect the insufficient resolution in the shallow lithosphere beneath Iceland using the single-
 574 component linear gravity gradient inversion we have applied to produce the density im-
 575 age in Fig. 17c. Incorporating other gravity gradient components and/or additional geo-
 576 physical data can be helpful to further constrain the density structure in this region.

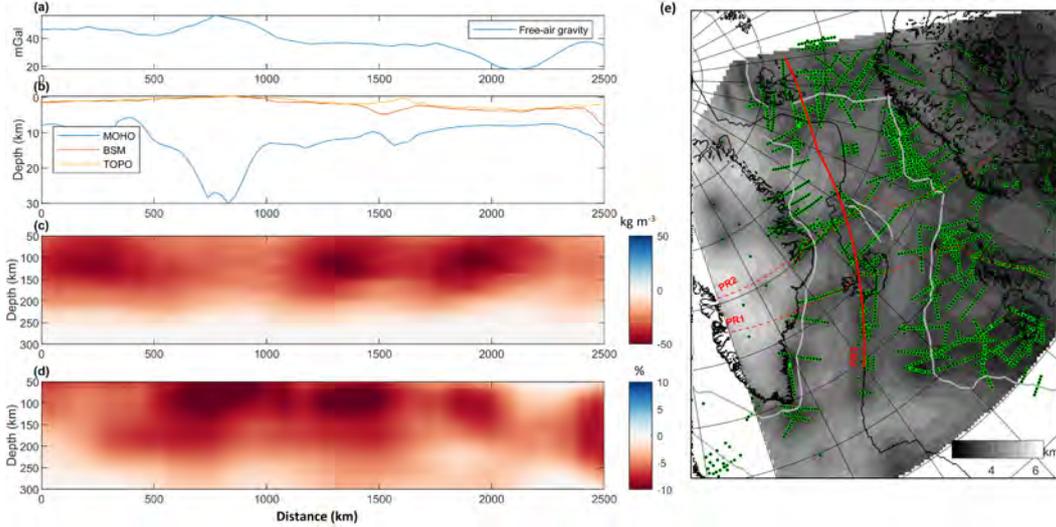


Figure 17. Inversion results along S-N Profile 3 across the northeast Atlantic. (a) Observed free-air gravity anomaly; (b) Crustal geometry: the Moho depth, top basement and topography; (c) density variation with respect to the 3D reference model; (d) seismic shear velocity perturbation in the regional S-wave tomography model (Rickers et al., 2013; Fichtner et al., 2018); (e) the uncertainty of crustal thickness (one standard deviation) with location of seismic refraction profiles (green) and synthetic lithospheric transects (red).

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4.2 Relation between density and seismic velocity anomalies

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The density structure of the upper mantle is an important parameter for numerical modeling of the lithosphere evolution and for understanding the present-day distribution of lithospheric stresses. The geophysical properties of the upper mantle can be estimated using mineral physics calculations along the lithospheric geotherm e.g. (Stixrude & Lithgow-Bertelloni, 2005). The relation between the seismic velocity and density variations can be established based on their temperature partial derivatives ($\delta\rho/\delta T$, $\delta v_s/\delta T$). The conversion coefficient ($\delta\rho/\delta v_s$) is about 0.2 for adiabatic mantle and a realistic range of chemical composition (Karato, 2008). The deviation of the actual relation between the density anomaly and seismic velocity perturbation from the theoretical value 0.2 increases as the local geotherm deviates from the mantle adiabat.

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The joint probability density of the mean density perturbation ($d\rho/\rho_0$) and the seismic velocity perturbation (dv/v_0) for the three selected profiles (shown in Fig. 18) indicates that the theoretical relation $\delta\rho/\delta v_s \approx 0.2$ is recovered for a young oceanic lithosphere for the velocity perturbation -3 to +2 %. For a more pronounced negative velocity anomalies (-3% to -8%) the maximum of joint probability distribution shifts toward smaller $d\rho/\rho_0$ values. This can be interpreted in terms of presence of melt since its direct effect on density is negligible compared to the attenuation of seismic shear velocities.

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4.3 Model resolution and uncertainty

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The diagonal elements of the posterior covariance matrix provide variance of the resulting density model. Fig. 19 indicates the maximum variance reduction at the depth of about 150 km. The prior model covariance is assumed constant of $400 \text{ kg}^2\text{m}^{-6}$. The maximum variance reduction is about $250 \text{ kg}^2\text{m}^{-6}$. The variance reduction with depth

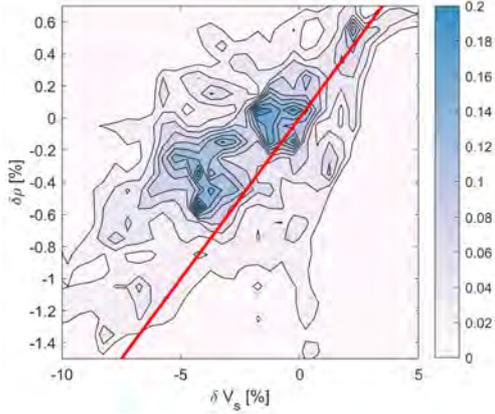


Figure 18. The joint probability density function for the seismic velocity variation and density variation (mean model expressed as a percentage) in the upper mantle. The depth range is 50-250 km. The reference mantle density is 3400 kg m^{-3} . The red line corresponds to the theoretical density-velocity conversion coefficient for adiabatic mantle $\partial_T \rho / \partial_T v = 0.2$.

601 reflects the shape of the weighted integrated kernel in eq. (63). The largest sensitivity
 602 is located at the depths of 100-150 km, which makes the method sensitive to the vari-
 603 ation of the lithosphere-asthenosphere boundary geometry.

604 Our probabilistic inversion approach implies that the density variation in the tar-
 605 get region is a result of a Gaussian process. The estimated mean realization of this pro-
 606 cess is shown in Fig. 13. A way to evaluate the density model parameter space is to gen-
 607 erate an ensemble of random realizations using the posterior covariance. This approach
 608 can help to test various geological hypotheses proposed in recent publications against
 609 interpretation of the GOCE gravity gradient data, such as the composition and nature
 610 of the GIFR lithosphere (Foulger et al., 2019; Yuan et al., 2020). A random realization
 611 can be constructed using Cholesky decomposition of the covariance matrix and a ran-
 612 dom vector eq. (49). Six random models (shown in Fig. 20) are centered at the estimated
 613 mean model whereas the variance is $150\text{-}400 \text{ kg}^2\text{m}^{-6}$ depending on the depth. The full
 614 exploration requires a much larger number of realization. Here, we just demonstrate the
 615 length scales and the general pattern of more robust features such as the anomalous low-
 616 density mantle beneath mid-Atlantic ridge and a high-denser lithosphere of the Fennoscand-
 617 ian craton. The model density variations in the asthenosphere have a sheet-like struc-
 618 ture where the low-density material extends over the oceanic basin towards the passive
 619 margins.

620 5 Conclusions

621 Satellite gravity gradients contain useful information on the density structure of
 622 the crust and upper mantle. In this work, we present a probabilistic linear inversion method
 623 to image the density heterogeneity within the lithosphere and sub-lithospheric upper man-
 624 tle. The prior information is incorporated through the spatial (depth) weighting of the
 625 model and the data and the model covariance functions, estimated using spherical geo-
 626 statistical analysis of independent models based on seismological data. This approach
 627 provides a novel approach for constrained linear inversion of satellite gravity gradient
 628 data in three dimensions.

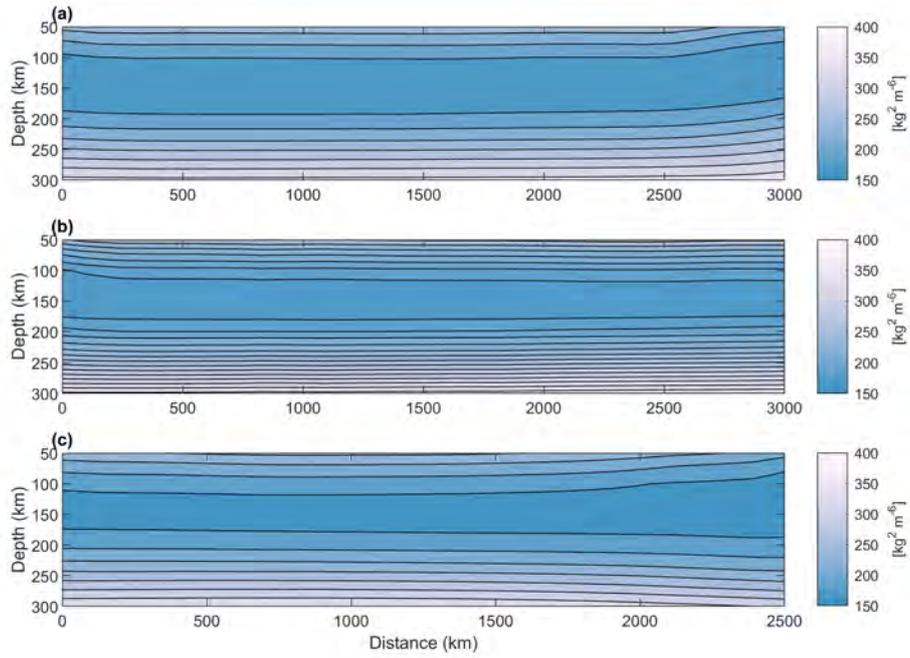


Figure 19. Diagonal elements of the posterior covariance matrix. (a) Profile 1, (b) Profile 2, (c) Profile 3. For location of transects see Fig. 13

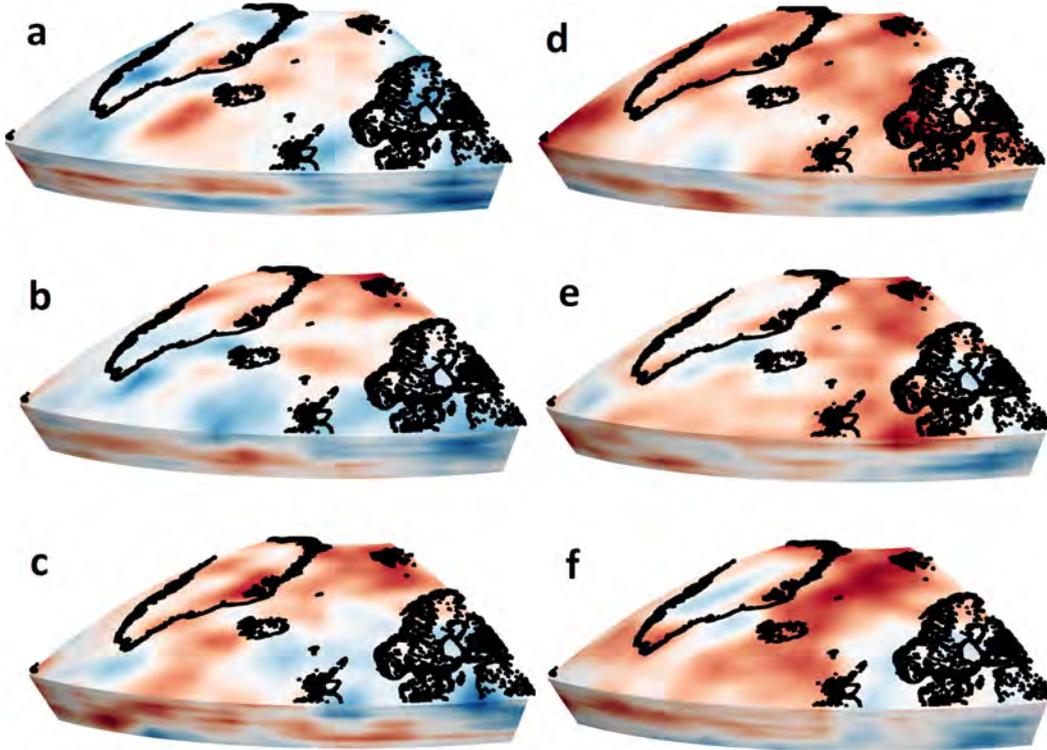


Figure 20. Ensemble of six random realizations generated with the Cholesky decomposition of the posterior covariance matrix. The color scale is from -50 to 50 kg m^{-3} .

The following density features has been resolved in our model for the northeast Atlantic upper mantle. A low-density asthenosphere north and south of Iceland (20-40 kg m⁻³) correlate with the distribution of Cenozoic seamounts and seamount-like features of the ocean floor. No strong low-density anomaly is observed under the present-day location of Iceland. The lithosphere beneath the Greenland-Iceland-Faeroe Ridge appears on average denser relative to the background mantle. The predicted density variation in the upper mantle is generally consistent with seismic velocity anomalies implying a mostly thermal origin of density heterogeneities.

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