

Probing lateral density variations in the crust from gravity and topography: applications to the Moon and Mars

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ABSTRACT

We present a constraint matrix to be used in the determination of gravity field models from spacecraft tracking data that uses information from topography and that allows for the direct determination of lateral variations in crustal density. Our approach is based on a matrix formulation of Bouguer corrections using a spherical harmonics expansion for density. This formulation also allows to directly determine the spherical harmonics coefficients for density in the crust from a set of gravity coefficients. We validate this by comparison with an approach using localization and show that both methods results in comparable density maps. We then apply the constraint matrix on a test case using

lunar data from before the Gravity Recovery and Interior Laboratory (GRAIL) mission, and compare this with results from GRAIL, showing that we can obtain density results similar to those from GRAIL data. We also apply this constraint to the determination of the gravity field of Mars. While our results for Mars tentatively suggest a hemispherical density contrast separated by the north-south dichotomy, the resolution of Martian gravity is currently too low to robustly determine large-scale density variations.

Keywords: The Moon (1692), Mars (1007)

1. INTRODUCTION

The density of the crust of a planetary body is an important parameter for geophysical studies into the planet’s formation and evolution. Remote sensing data can map the crust’s composition from which the density can be inferred but it ultimately provides only direct information about the surface. Bulk crustal density for planetary bodies is then often adopted based on composition and assumed densities. The high resolution of the gravity field models from the Gravity Recovery and Interior Laboratory (GRAIL) mission (Zuber et al. 2013), combined with high-resolution topography from the Lunar Orbiter Laser Altimeter (LOLA) instrument (Smith et al. 2017) onboard the Lunar Reconnaissance Orbiter (LRO), and the high correlations between the two, meant that it was possible to unambiguously determine the crustal density (Wieczorek et al. 2013). This showed that the Moon’s crust has a lower density than assumed, which was also suggested by a study prior to GRAIL using lower-resolution data (Huang & Wieczorek 2012). In addition, the combination of GRAIL and LOLA has allowed the mapping of lateral and vertical density variations of the Moon’s crust based on localization techniques (Wieczorek et al. 2013; Besserer et al. 2014; Han et al. 2014; Wahl & Oberst 2019; Wahl et al. 2020; Goossens et al. 2020).

In Goossens et al. (2017) we presented a constraint for the determination of a gravity field model from spacecraft tracking data based on topography information that allowed for the direct determination of the average crustal density of a planet. Here, we extend this constraint by taking into account

lateral variations in crustal density. To construct the constraint, we present a matrix formulation that also allows for the direct mapping of the coefficients of an expansion in spherical harmonics of the density variations from a set of gravity field coefficients. We compare the resulting densities from this matrix formulation with densities obtained from localization and show that they result in comparable density maps. We then explore the use of the new constraint to determine lateral crustal density variations from the resulting gravity field model for cases using data from the Moon and Mars.

This paper is structured as follows. We introduce the matrix formulation in Section 2. We validate the determination of densities from gravity field coefficients with GRAIL data in Section 3. We then introduce our constraint in Section 4. We apply this constraint to determine gravity field models of the Moon, based on pre-GRAIL data, and of Mars. Using these resulting gravity field models, we determine and discuss lateral density variations of the crust of the Moon and Mars in Section 5. We end with conclusions in Section 6.

2. METHODS

The standard expression for the gravitational potential U for a planet with a reference radius R and a gravitational parameter GM at a point Q with spherical coordinates radius $r > R$, longitude λ , and latitude ϕ is (Kaula 1966)

$$U(Q) = \frac{GM}{R} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \left(\frac{R}{r}\right)^{l+1} \bar{\nu}_{l,m} \bar{Y}_{l,m}(\phi, \lambda). \quad (1)$$

Here, the function $\bar{Y}_{l,m}(\phi, \lambda)$ is defined as

$$\bar{Y}_{l,m}(\phi, \lambda) = \bar{P}_{l,|m|}(\sin \phi) \begin{cases} \cos m\lambda, & m \geq 0 \\ \sin |m|\lambda, & m < 0 \end{cases}. \quad (2)$$

The functions $\bar{P}_{l,m}(\sin \phi)$ are the associated Legendre functions of degree l and order m , and the bar indicates the standard 4π normalization of this function (Kaula 1966). The coefficients $\bar{\nu}_{l,m}$ are the standard gravity model coefficients (also called Stokes coefficients).

The contribution of topography to gravity can be expressed in spherical harmonics (Wieczorek & Phillips 1998), and it depends on the density of crust, which can be laterally varying. The spherical harmonic coefficients for gravity-from-topography can be expressed as (Wieczorek 2015)

$$\bar{\nu}_{l,m}^{\text{gt}} = \frac{4\pi R^3}{M(2l+1)} \sum_{n=1}^{l+3} \frac{(\rho h^n)_{l,m}}{R^n n!} \frac{\prod_{j=1}^n (l+4-j)}{l+3}, \quad (3)$$

where M is the planet's mass, the superscript “gt” stands for gravity-from-topography, $h(\phi, \lambda)$ is the topography (referenced to a sphere of radius R) expressed in spherical harmonics, and ρ is the density between h and R . The combination of laterally varying density $\rho(\phi, \lambda)$ and topography to the power of n is expressed in spherical harmonics as (Wieczorek 2015)

$$(\rho h^n)_{l,m} = \frac{1}{4\pi} \int_{\Omega} [\rho(\phi, \lambda) h^n(\phi, \lambda)] \bar{Y}_{l,m}(\phi, \lambda) d\Omega, \quad (4)$$

where Ω is a sphere. We note that ρ is assumed to be varying laterally here but not vertically; this has implications for the interpretation of gravity and densities that we discuss later.

If we express the density variations in spherical harmonics (with a maximum degree of L_{max}) as well,

$$\rho(\lambda, \phi) = \sum_{l=0}^{L_{\text{max}}} \sum_{m=-l}^{m=l} \alpha_{l,m} \bar{Y}_{l,m}(\phi, \lambda), \quad (5)$$

then the orthogonality of the $\bar{Y}_{l,m}(\phi, \lambda)$ functions means that the gravity-from-topography coefficients from eq. (3) can be expressed as a linear combination of the density spherical harmonic coefficients $\alpha_{l,m}$. In other words, we can construct a matrix $\mathbf{G}$ such that a vector of gravity-from-topography coefficients $\mathbf{x}$ can be represented by a sub-space projection of the type

$$\mathbf{x} = \mathbf{G}\boldsymbol{\alpha}, \quad (6)$$

where $\boldsymbol{\alpha}$ is the vector of density spherical harmonic coefficients. We note that $M_x = \dim(\mathbf{x}) > M_{\alpha} = \dim(\boldsymbol{\alpha})$. The columns of $\mathbf{G}$ consist of vectors of gravity-from-topography coefficients from eq. (3) where the density $\rho(\phi, \lambda)$ is computed for only one spherical harmonic mode per column (*i.e.*, using $\alpha_{l,m} = 1.0$). This matrix $\mathbf{G}$ will be the basis of our new constraint that we discuss in Section 4.

We can also extract α from $\mathbf{x}$. We note that $\mathbf{G}$ is not a square matrix, and its QR -decomposition is given as

$$\mathbf{G} = \mathbf{Q}\mathbf{R}, \quad (7)$$

with $\mathbf{Q}$ being a real matrix of size $M_x \times M_\alpha$ (*i.e.*, $\mathbf{Q} \in \mathcal{R}^{M_x \times M_\alpha}$) having orthonormal columns and $\mathbf{R}$ being a real matrix of size $M_\alpha \times M_\alpha$ (*i.e.*, $\mathbf{R} \in \mathcal{R}^{M_\alpha \times M_\alpha}$) being an upper-triangular matrix. Then, we define $\mathbf{G}_\perp$ as a matrix such that $\mathbf{G}_\perp^\top \mathbf{G} = \mathbf{0}$ whose QR -decomposition is given by

$$\mathbf{G}_\perp = \mathbf{Q}_\perp \mathbf{R}_\perp, \quad (8)$$

with $\mathbf{Q}_\perp \in \mathcal{R}^{M_x \times M_x - M_\alpha}$ having orthonormal columns such that $\mathbf{Q}_\perp^\top \mathbf{Q} = \mathbf{0}$ and $\mathbf{R}_\perp \in \mathcal{R}^{M_x - M_\alpha \times M_x - M_\alpha}$ is an upper-triangular matrix. The matrix $\mathbf{G}_\perp$ completes $\mathbf{G}$ for a full-rank transformation of $\mathbf{x}$ into α which spans the columns of $\mathbf{G}$ and an additional set β which spans the columns of $\mathbf{G}_\perp$. As such

$$\mathbf{x} = \begin{bmatrix} \mathbf{G} & \mathbf{G}_\perp \end{bmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad (9)$$

and we note that

$$\begin{bmatrix} \mathbf{G} & \mathbf{G}_\perp \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{R}^{-1} \mathbf{Q}^\top \\ \mathbf{R}_\perp^{-1} \mathbf{Q}_\perp^\top \end{bmatrix}. \quad (10)$$

From eq. (9) and (10) it follows that

$$\begin{aligned} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} &= \begin{bmatrix} \mathbf{R}^{-1} \mathbf{Q}^\top \\ \mathbf{R}_\perp^{-1} \mathbf{Q}_\perp^\top \end{bmatrix} \mathbf{x}, \\ &= \begin{bmatrix} (\mathbf{G}^\top \mathbf{G})^{-1} \mathbf{G}^\top \\ (\mathbf{G}_\perp^\top \mathbf{G}_\perp)^{-1} \mathbf{G}_\perp^\top \end{bmatrix} \mathbf{x}, \end{aligned} \quad (11)$$

which means that α can be extracted from $\mathbf{x}$.

3. VALIDATION OF THE MATRIX FORMULATION WITH GRAIL GRAVITY

Before we construct the new constraint based on $\mathbf{G}$, we validate the matrix formulation by using it to extract densities directly from a set of gravity field model coefficients. The first validation of

eq. (11) consisted of generating $\mathbf{x}$ directly from eq. (3) for a given set of density spherical harmonics $\boldsymbol{\alpha}$, and then applying eq. (11) to recover $\boldsymbol{\alpha}$. We confirmed that we can recover the density coefficients perfectly. We also note here already that in order to apply eq. (11) one does not need the entire set of gravity field coefficients of $\mathbf{x}$. In other words, one can band-limit this to a certain range of spherical harmonic degrees: the density can be extracted, for example, using only the higher degrees, which makes sense since at higher degrees gravity is expected to be mostly following topography. Of course when doing so the matrix $\mathbf{G}$ needs to be dimensioned accordingly.

We next validate the matrix formulation with data from GRAIL. Laterally varying density has been determined from GRAIL using localization and the effective density method (Wieczorek et al. 2013; Besserer et al. 2014; Han et al. 2014; Wahl & Oberst 2019; Wahl et al. 2020; Goossens et al. 2020). The effective density $\rho_{\text{eff}}(l)$ is defined as (Wieczorek et al. 2013)

$$\rho_{\text{eff}}(l) = \frac{S_{g_{\text{obs}}, g_{\text{topo}}}}{S_{g_{\text{topo}}, g_{\text{topo}}}}, \quad (12)$$

where g_{obs} is observed gravity and g_{topo} is gravity-from-topography with a constant, uniform crustal density. The cross-power per degree $S_{a,b}(l)$ between two functions with spherical harmonic coefficients $a_{l,m}$ and $b_{l,m}$ is defined as

$$S_{a,b}(l) = \sum_{m=-l}^{m=l} a_{l,m} b_{l,m}. \quad (13)$$

Local effective density spectra can be obtained through localization using Slepian functions (Wieczorek & Simons 2005, 2007). Here, we follow earlier work (Wieczorek et al. 2013; Goossens et al. 2020), and we use localization with a cap radius of 15° and a spectral bandwidth of $L_{\text{win}} = 58$ which allows us to use 30 tapers. We use the GRGM1200B model (Goossens et al. 2020) together with LOLA topography to generate gravity-from-topography with a unit density, and we localize the effective density spectrum on a global grid spaced every 5° . We determine the average density by averaging the localized effective density spectrum over the degree range $l = 150 - 310$ (Wieczorek et al. 2013). We then transform this global map of densities into spherical harmonics of degree and order 50. We also determine the density directly from eq. (11) using the same degree range for gravity, for different density expansions (degree and order 5, 12, and 50).

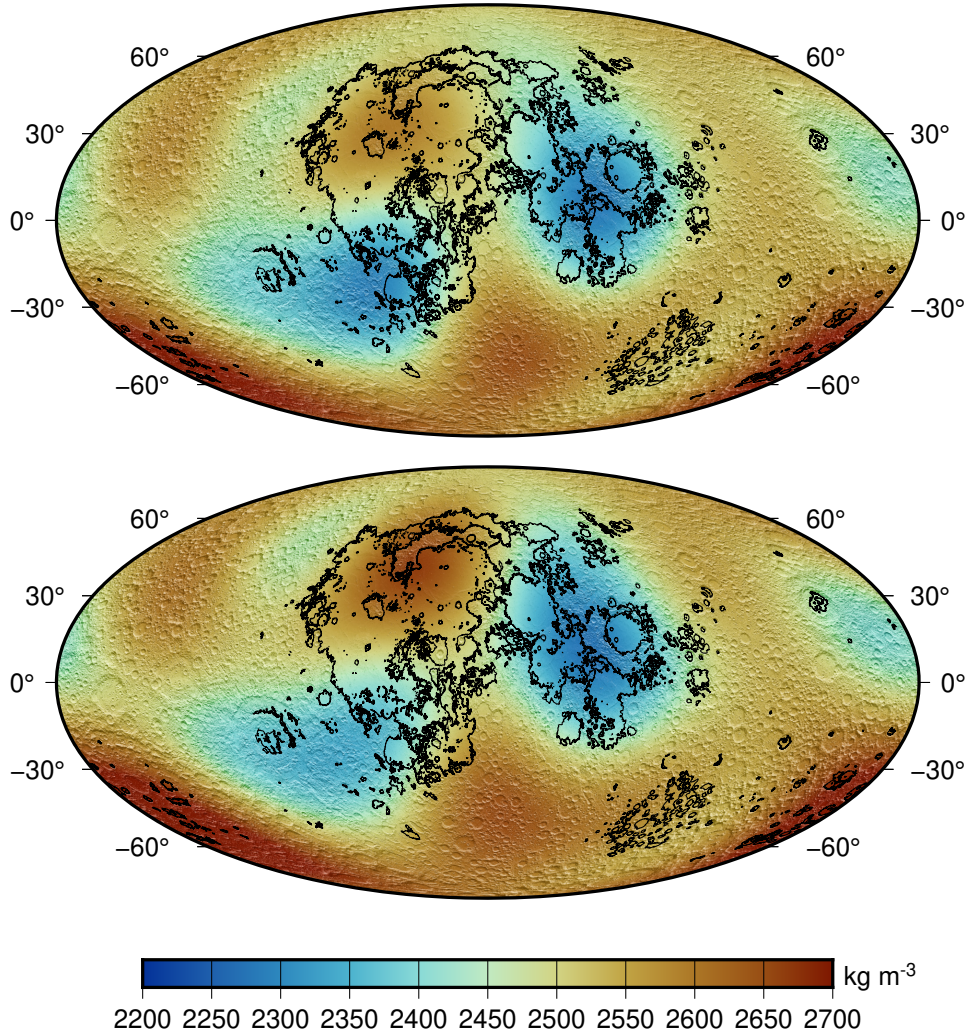


Figure 1. Density of the Moon’s crust determined from effective density and localization (top) and from the matrix formulation (bottom). Both maps are from a degree and order 5 spherical harmonic expansion of density (see text). The map is in a Mollweide projection centered on the nearside. The map is shaded by topography and we indicate the locations of the mare areas.

We show both density maps at degree 5 in Figure 1. The map from the matrix formulation resembles that of the localization method very closely. For both maps, the mean and range of the densities is very close, with density varying between 2275 and 2770 kg m^{-3} . Correlations per degree between the two spherical harmonic models are larger than 0.95 up to degree 4, and 0.72 for degree 5. We also highlight that both maps clearly outline a density anomaly in the South Pole-Aitken (SPA) basin, which can also be (partly) seen in the GRAIL results for the crust (Wieczorek et al. 2013), noting

that SPA is also associated with a large mass excess in the mantle (James et al. 2019), extending to depths that our crustal density results do not probe. This indicates that the matrix formulation can readily determine large scale density variations without the need for localization, which requires the tuning of several parameters (cap radius and window bandwidth to determine the number of tapers). The matrix method does require the construction of $\mathbf{G}$ which becomes more costly as the maximum degrees for gravity and density increase. For a gravity field up to degree and order 660, constructing $\mathbf{G}$ took 40 minutes for a degree and order 5 density model, 8.7 hours for a degree and order 20 density model, and ~ 2 days for a degree and order 50 density model. This can readily be sped up with parallelization, and $\mathbf{G}$ can be stored to probe multiple models, for example using different degree ranges.

It should also be noted that the matrix formulation as implemented does not account for vertical variations of density, for example caused by porosity variations. The slope of the effective density spectrum can be interpreted as a density change with depth (Wieczorek et al. 2013; Han et al. 2014; Besserer et al. 2014). For the matrix formulation that extracts density coefficients directly from gravity coefficients, *i.e.*, eq. (11), there is no such sensitivity. It determines the average density of the crust, similar to averaging the effective density spectrum over a range of degrees. We implicitly assume that the averaging of the effective density spectrum over a large enough range of degrees results in an estimate of the average density of the crust; this will likely only hold if the lower degree is not too high (*i.e.*, starting the averaging at a high degree would likely only give the average density of the upper part of the crust). This lack of sensitivity to vertical variations may account for some of the differences between densities derived from the matrix formulation and those determined using the effective density method, as discussed below.

If we increase the degree and order of the extracted density maps, the spectral power of the density spherical harmonics obtained with the matrix formulation increases, resulting in, eventually, unrealistically high densities. We show this for several expansions in Figure 2, where the power per degree $P(l)$ is defined as

$$P(l) = \sqrt{\frac{1}{2l+1} \sum_{m=-l}^{m=l} \alpha_{l,m}^2}. \quad (14)$$

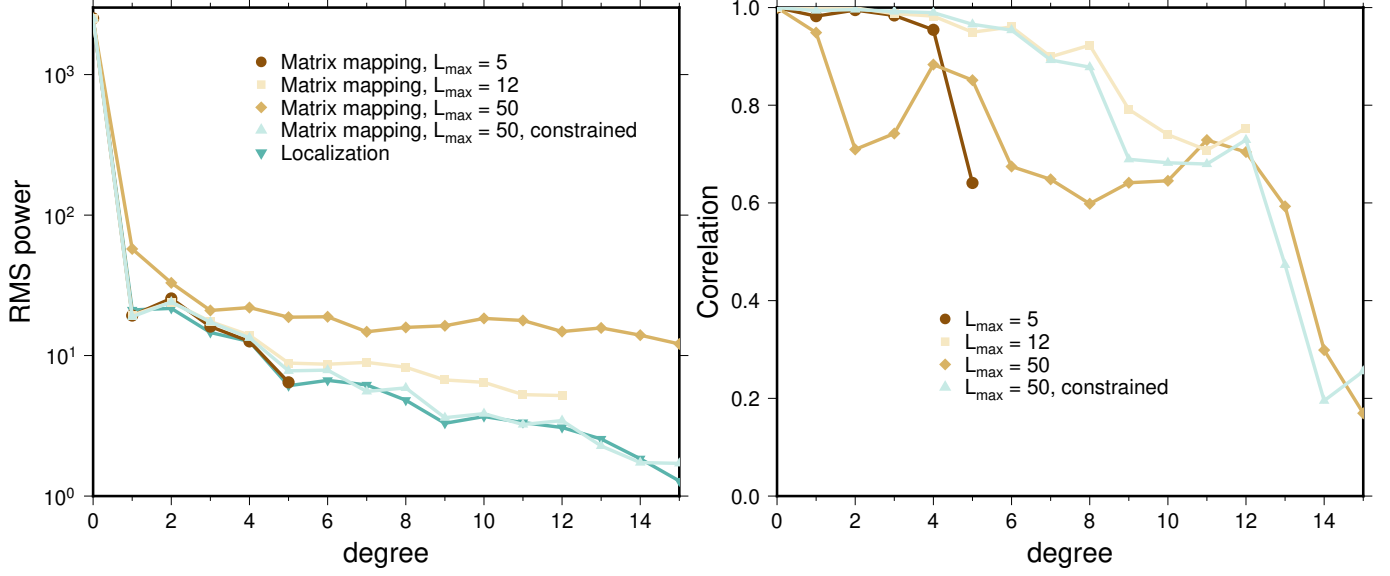


Figure 2. Power per degree for several spherical harmonic expansions of density of different maximum degree and order, using either localization or the matrix mapping (left), and correlations between these models and the model obtained through localization (right).

However, it should also be noted that the crustal density map from localization is limited in resolution due to the localization cap size of 15° and spacing of 5° , which results in an effective resolution of degree and order 12. At that degree correlations between the localization model and the matrix method models are still above 0.6 as can be seen in Figure 2. We show the density models of degree and order 12 in Figure 3 (top). The stronger amplitudes in the model from the matrix method are apparent: while the densities from the localization model vary between 2110 and 2760 kg m^{-3} , those from the matrix formulation have a range between 1170 and 3870 kg m^{-3} . We note that the density signal is strongest over the mare areas, where gravity and topography correlate not as well as in other locations and where gravity cannot be entirely explained by topography (see also below). The density map from the localization method is smoother, even though both have the same spherical harmonics resolution. This can also be deduced from Figure 2 where the matrix formulation degree and order 12 model has higher power than the density model from the localization.

At degree and order 50, the power of the density model from the matrix method does not decrease much per degree, and this results in unrealistically high densities. This may indicate a limit in the matrix formulation but perhaps also a limit in resolution for the density that we can determine from

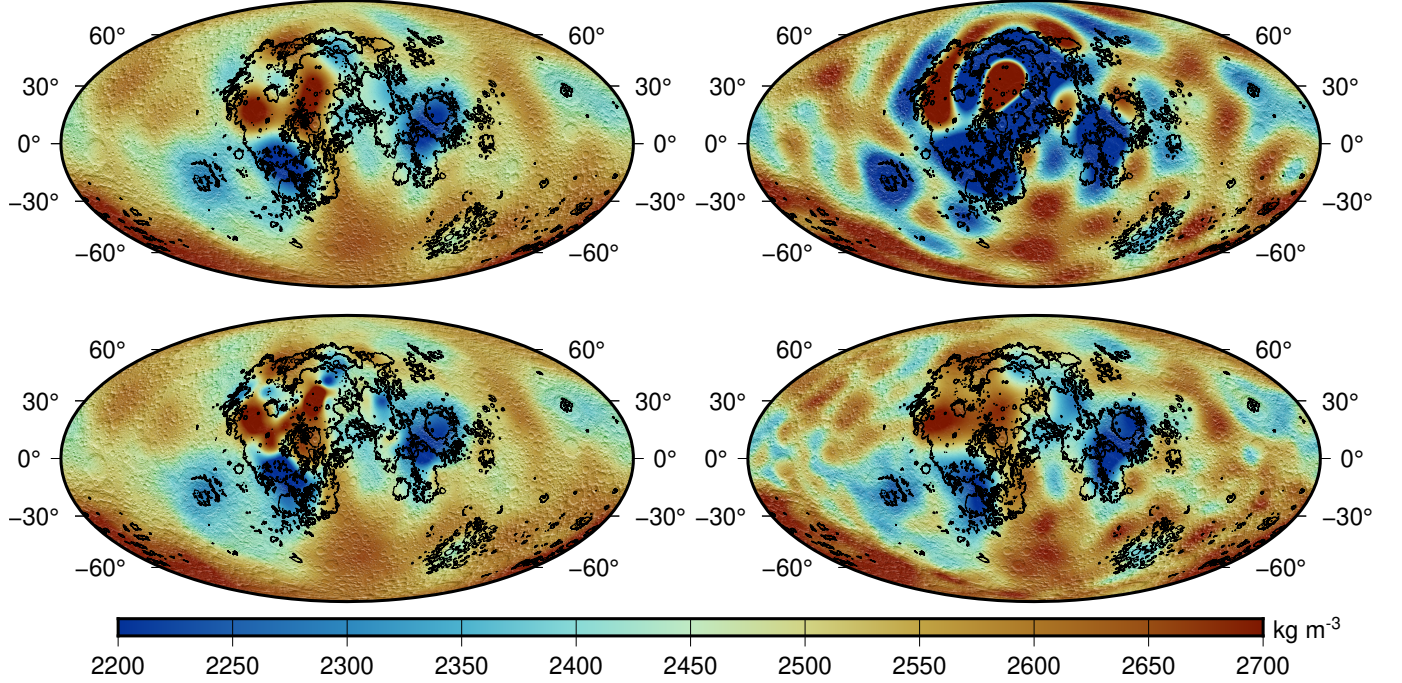


Figure 3. Density of the Moon’s crust in spherical harmonics of degree and order 12 (top) and 50 (bottom). We show maps based on localization (left) and the matrix method (right). The map for the degree and order 50 density model from the matrix formulation used a damping constraint (see text). The maps have the same projection and properties as Figure 1.

the gravity field. While we transformed the density map from the localization method to degree and order 50, its actual resolution is limited due to choices for the localization, as stated before. When comparing the density maps from localization in Figure 3 (left) between the degree and order 12 (top) and 50 (bottom) expansions, we note that most of the signal is captured by the degree and order 12 map. The range for the degree and order 50 map is larger, with densities between 2000 and 3200 kg m^{-3} vs densities between 2100 and 2800 kg m^{-3} for the degree and order 12 map, but the mean and standard deviation are nearly the same for the two. We again note that both models clearly highlight the SPA density anomaly.

When determining the density from eq. (11), one can also apply a constraint to dampen the power in the higher degrees; this is expected in order to maintain realistic densities from higher degree and

order expansions. The mapping of the density from gravity can then be written as

$$\boldsymbol{\alpha} = (\mathbf{G}^T \mathbf{G} + \mathbf{K})^{-1} \mathbf{G}^T \mathbf{x}, \quad (15)$$

where $\mathbf{K}$ is a constraint matrix. We construct one similar to a Kaula-type constraint used in gravity field determination (Kaula 1966) where the diagonals of $\mathbf{K}$ have entries l^4/D^2 , with D a constant. When constructing a constraint like this, we leave the $\alpha_{0,0}$ term (the constant density term that describes the average density of the crust) unconstrained. We show such a density map in Figure 3 (bottom right) using a value $D = 5 \times 10^{11}$ which was obtained by varying the constant D and evaluating the solutions for their power and correlations with the localized expansion. The density model from the matrix method is again comparable to that from the localization method. The range of densities is closer between the models than was the case for the degree and order 12 models. The densities from the localization method vary between 2000 and 3200 kg m⁻³ while those from the constrained matrix formulation vary between 2000 and 2800 kg m⁻³. Of course, the constraint was chosen empirically to reasonably match the power in the density from the localization method.

Finally, we stress that the differences between the two methods are mostly located over the mare areas. We show the differences in density between the degree and order 12 and 50 expansions of the two methods in Figure 4, where it is clear that the differences outside the mare areas are much smaller. The mean and root-mean-square (RMS) of the differences over the nearside (using values inside a circle centered on the nearside with a radius of 80°) between the two degree and order 12 density maps are -94 and 283 kg m⁻³ and those over the farside (using values inside a circle centered on the farside with a radius of 80°) are -0.18 and 61 kg m⁻³, respectively. The mean and RMS over the nearside of the density differences for the degree and order 50 maps are 7 and 59 kg m⁻³ and those over the farside 0.57 and 39 kg m⁻³, respectively. While the dynamic range of densities in some of the models is thus large, this is mostly due to unreasonable densities in the area where a direct comparison of gravity and topography is already more problematic. The mare areas thus require a separate treatment, and can, for example, be left out as was done in earlier analysis (*e.g.*, Wieczorek et al. 2013), or use separate modeling (*e.g.*, Gong et al. 2016; Broquet & Andrews-Hanna 2024a,b).

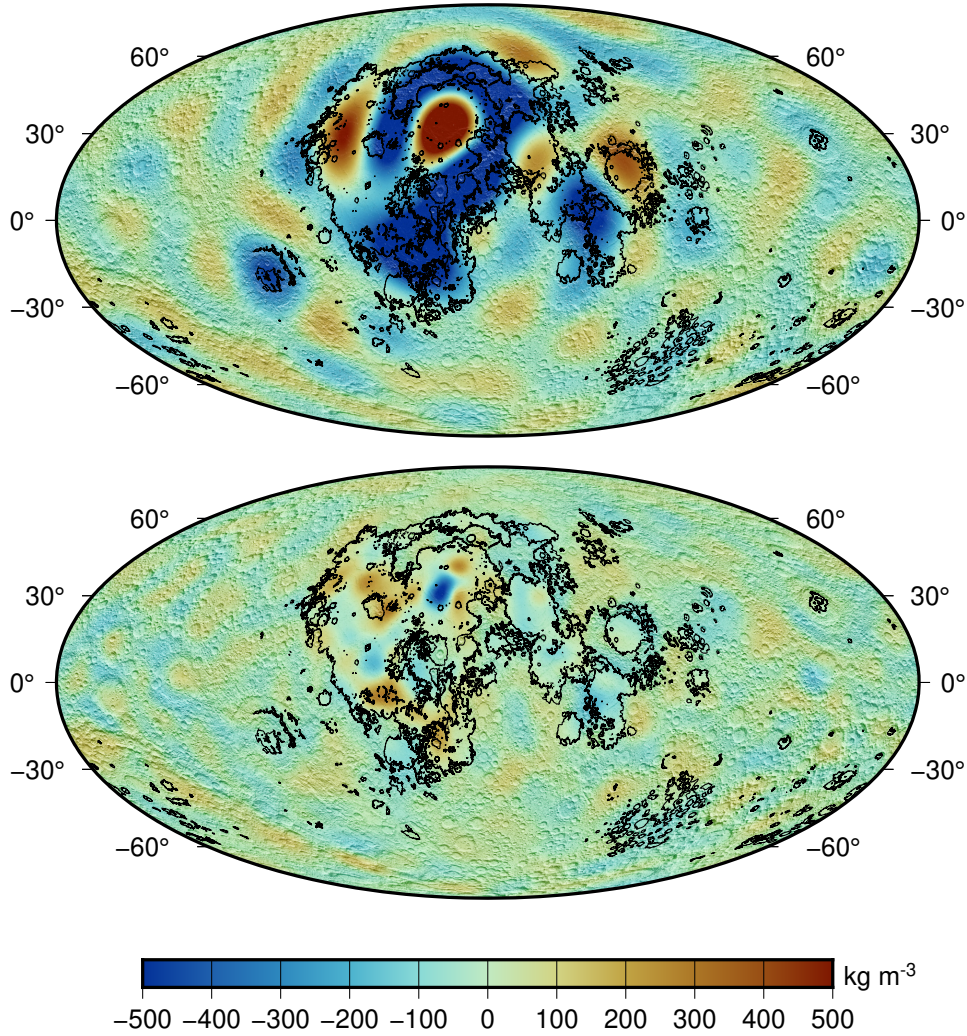


Figure 4. Differences in density between the localization models and the densities based on the matrix method from Figure 3. The differences for the degree and order 12 model are on the top and those for the degree and order 50 model (using the constrained density map) on the bottom. The maps have the same projection and properties as Figure 1.

Due to the use of an additional constraint, the differences in density between the degree and order 50 models are smaller than those between the degree and order 12 models.

4. THE RM-S CONSTRAINT

The matrix formulation can also be used to construct a constraint to be used when determining gravity field models from spacecraft tracking data. Previously we derived a constraint based on topography information that allowed the direct estimation of the average crustal density from tracking

data (Goossens et al. 2017). With the matrix approach presented here we can now extend this to include the entire set of density spherical harmonics $\boldsymbol{\alpha}$; the previous constraint only included $\alpha_{0,0}$ and can be considered a sub-set of this new constraint. Because we left one parameter free to estimate, the previous constraint matrix was not full-rank and we called it “rank minus 1” (RM1). We call this new constraint “rank minus S ” (RM- S) with S degrees of freedom, being the number of density coefficients.

In order to construct the constraint, we seek to minimize a cost function $J(\mathbf{x})$ with respect to the gravity model parameter vector $\mathbf{x}$ given by

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{d} - \mathbf{a}(\mathbf{x}))^T \mathbf{W} (\mathbf{d} - \mathbf{a}(\mathbf{x})) + \frac{1}{2} \lambda (\mathbf{x}_a - \mathbf{x})^T \mathbf{P} (\mathbf{x}_a - \mathbf{x}), \quad (16)$$

where $\mathbf{d}$ is a data vector, $\mathbf{a}(\mathbf{x})$ is a non-linear model of parameter vector $\mathbf{x}$, $\mathbf{W}^{-1}$ is a data noise covariance matrix, $\mathbf{x}_a$ is an *a priori* preferred model parameter state vector with attendant covariance matrix $\mathbf{P}^{-1}$, and damping parameter λ . In order to find the minimum, we employ a Gauss-Newton (GN) estimator whose k -th iteration is given by

$$\begin{cases} \Delta \mathbf{x}_k = (\mathbf{A}_k^T \mathbf{W} \mathbf{A}_k + \lambda \mathbf{P})^{-1} (\mathbf{A}_k^T \mathbf{W} \mathbf{r}_k + \lambda \mathbf{P} (\mathbf{x}_a - \mathbf{x}_k)), \\ \mathbf{x}_{k+1} = \mathbf{x}_k + \Delta \mathbf{x}_k, \end{cases} \quad (17)$$

where $\mathbf{r}_k = \mathbf{d} - \mathbf{a}(\mathbf{x}_k)$ and $\mathbf{A}_k = \frac{\partial \mathbf{a}}{\partial \mathbf{x}_k}$ are the residual vector and the Jacobian matrix, respectively, at the nominal state $\mathbf{x}_k$ of the k -th iteration. Here, $\mathbf{x}_k$ is again the vector with coefficients of a spherical harmonic expansion of the gravity field (and other parameters that are estimated from the data), the matrix $\mathbf{A}_k$ is the matrix with partial derivatives of the measurements with respect to the estimated parameters for iteration k , the matrix $\mathbf{W}$ is the data weight matrix, the vector $\mathbf{r}_k$ contains the data residuals, and $\mathbf{P}$ is the constraint applied in the inversion. In subsequent applications we perform only one GN iteration, but we keep the subscript k for completeness. We now construct this constraint $\mathbf{P}$.

With the definitions of $\mathbf{G}$ and $\mathbf{G}_\perp$ and their QR -decomposition as in eq. (7) and (8), the constraint matrix $\mathbf{P}$ is defined such that

$$\mathbf{P} = \mathbf{G}_\perp \mathbf{G}_\perp^T. \quad (18)$$

This is the most general form of a symmetric positive semi-definite matrix of rank $M_x - M_\alpha$ whose null space is spanned by $\mathbf{G}$. This means that $\mathbf{R}_\perp$ is a free parameter to be determined.

The vector space spanned by the columns of $\mathbf{Q}_\perp$ must contain the complex effects other than those from a low-degree spherical harmonic expansion of ρ spanned by $\mathbf{Q}$. While these effects are encoded by $\mathbf{R}_\perp$, it is beyond the scope of the present paper to investigate them and so we set $\mathbf{R}_\perp = \mathbf{I}$, which in some sense indicates “minimal assumptions” about these complex effects. However, it will be shown in the appendix that as $\lambda \rightarrow \infty$, then the solution becomes invariant to the choice of $\mathbf{R}_\perp$.

In terms of the constraint nomenclature “RM- S ”, the R stands for $\text{rank}(\mathbf{A}_k) = M_x$ and $S = M_\alpha$. Since as $\lambda \rightarrow \infty$ we want $\mathbf{x}$ to only be non-zero in the sub-space spanned by $\boldsymbol{\alpha}$, then $\mathbf{x}_a = \mathbf{0}$. In other words, the constraint suppresses that part of the solution $\mathbf{x}_k$ in the sub-space $\mathbf{G}_\perp$ and allows it to exist in the sub-space for $\boldsymbol{\alpha}$, with the values of $\boldsymbol{\alpha}$ determined by the data. We show in Appendix A that as $\lambda \rightarrow \infty$, $\mathbf{x}_{k+1} = \mathbf{G}\boldsymbol{\alpha}_{k+1}$.

Finally, we note that the constraint matrix $\mathbf{P}$ as given in eq. (18) can be formed from $\mathbf{G}$ directly instead of from $\mathbf{G}_\perp$. Because we choose $\mathbf{R}_\perp = \mathbf{I}$, we can write eq. (18) as $\mathbf{P} = \mathbf{Q}_\perp \mathbf{Q}_\perp^T$. Considering again the full-rank transformation as given in eq. (9) and that $\mathbf{G}_\perp^T \mathbf{G} = \mathbf{0}$ (*i.e.*, $\mathbf{G}_\perp$ is the null space of $\mathbf{G}^T$), we can also write

$$\begin{aligned} \mathbf{P} &= \mathbf{Q}_\perp \mathbf{Q}_\perp^T \\ &= \mathbf{I} - \mathbf{Q} \mathbf{Q}^T \\ &= \mathbf{I} - \mathbf{G} (\mathbf{G}^T \mathbf{G})^{-1} \mathbf{G}^T. \end{aligned} \quad (19)$$

5. DENSITY VARIATIONS FOR THE MOON AND MARS

We now apply the RM- S constraint matrix to a data system $\mathbf{N}$ expressed as a normal equation system together with its right-hand side $\mathbf{y}$ to estimate a set of gravity coefficients $\mathbf{x}$ from tracking

data following

$$\mathbf{x} = (\mathbf{N} + \lambda \mathbf{P})^{-1} \mathbf{y}, \quad (20)$$

where λ is the constraint factor. We determine this factor empirically by inspecting the resulting power spectrum for the density coefficients and by inspecting correlations with either an existing gravity solution (such as GRGM1200B for the Moon) or with gravity-from-topography. For the latter we use a constant density for the crust. Because our solutions are constrained towards gravity-from-topography with laterally varying density, this means that correlations between our solution and constant-density gravity-from-topography will not be exactly unity even for large values of λ , despite the use of the same topography in eq. (4). Nevertheless, we use this as it serves as a good proxy.

We also note that we can use two different ways to determine lateral density variations in the crust from an RM- S constrained gravity field model: by using the matrix formulation or the localization method. The advantage of the latter is that we could in principle extract vertical density variation information from the gravity field, similar to earlier work, provided that the constraint is not applied too strongly (which would be similar to applying the earlier RM1 constraint so strongly that the resulting effective density spectrum shows a constant density for all degrees).

5.1. Results for the Moon

We used the data matrix from the SGM150J model, a model using SELENE and historical tracking data that included farside tracking and had a global resolution of degree and order ~ 70 (Goossens et al. 2011). In our earlier work we showed that with this pre-GRAIL data set and the RM1 constraint we obtain the same bulk density for the Moon’s crust as the GRAIL result (Goossens et al. 2017). We apply the RM- S constraint starting at degree $l = 50$ for the gravity solution, for different maximum degrees of the density expansion. We estimate gravity solutions of degree and order 150. We construct the constraint for degree and order 5 and 12 density models.

To determine the value for the constraint factor λ we computed solutions with λ varying from 10^{11} to 10^{26} , and evaluated these solutions by computing correlations with GRGM1200B, which is

independent and entirely determined by data up to degree ~ 660 . Compared to the earlier RM1 solutions where the constraint factor $\lambda_{\text{RM1}} = 1$ resulted in solutions with high correlations with gravity-from-topography (Goossens et al. 2017, 2020), we have to use larger values for λ here because of the different construction of the constraint: we simply need larger values for λ for the constraint to take effect.

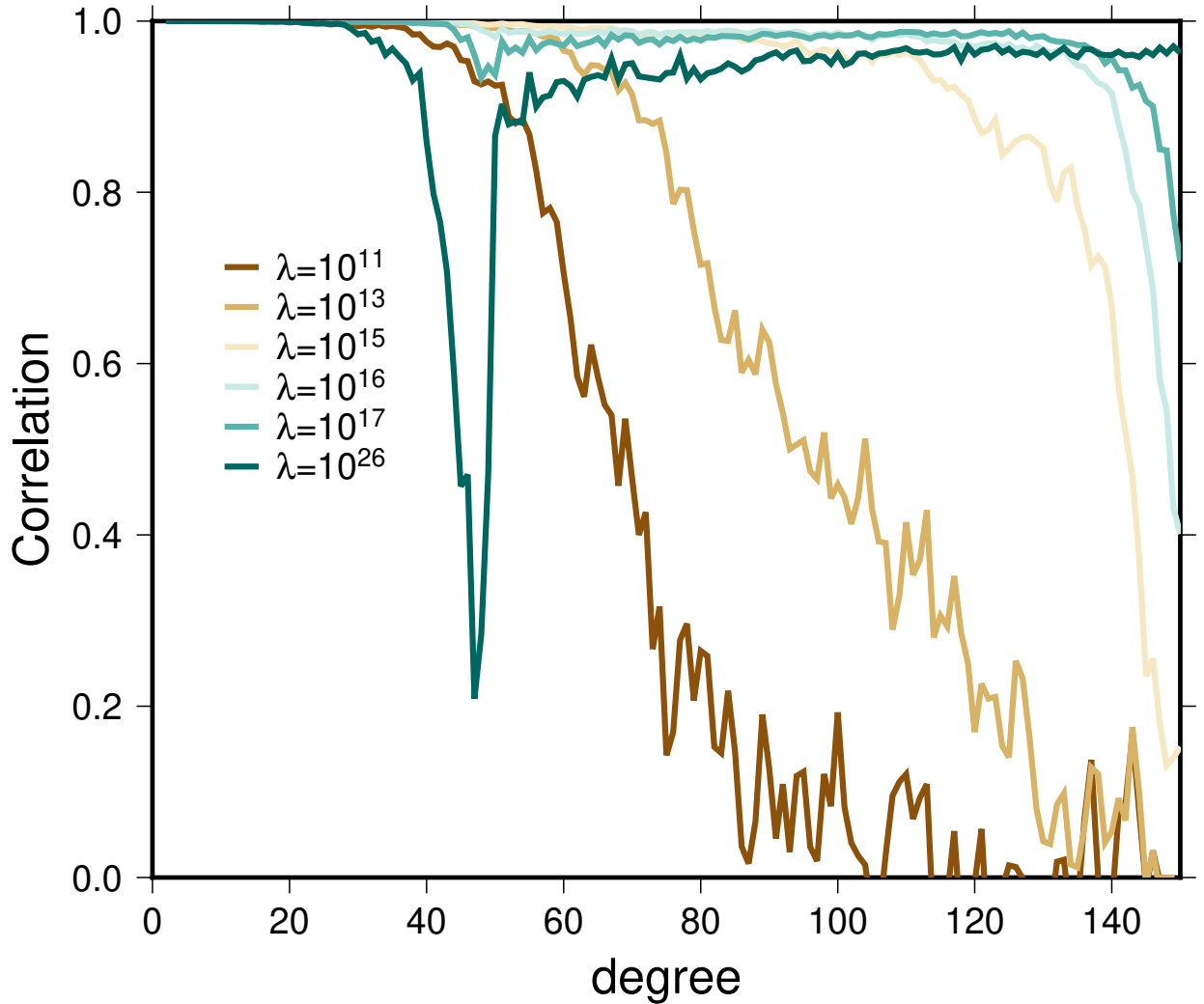


Figure 5. Correlations between RM- S constrained solutions and GRGM1200B for different constraint factors λ . The RM- S solutions use the SGM150J data matrix where the constraint is applied from degree 50 for a degree and order 5 density model.

We show these correlations in Figure 5 where we applied an RM- S constraint using a degree and order 5 expansion for the density. From this figure we find that $\lambda = 10^{16}$ produces solutions with high correlations over most of the degree range. For larger values of λ we find artifacts in the correlations around the degree from which the constraint was applied. This was also the case for the RM1 constraint, although it should be noted that those artifacts did not show in the effective density spectra for such solutions (Goossens et al. 2017).

The range of constraint factors λ that we tested span many orders of magnitude. As with any constraint, its effect on the solution strongly depends on this factor. Apart from the correlations mentioned above, we also inspected the resulting gravity field models and their power, as well as the power in the degree and order 5 density models extracted using the matrix formulation. The gravity field model and its power show some variations but not much for $\lambda > 10^{16}$. The density models (see also below) do show variations in power, with the lowest power for density extracted from models with factors around $\lambda = 10^{16}$.

We show results for the lunar crustal density from the solution with $\lambda = 10^{16}$ and the RM- S constraint for a degree and order 5 density model in Figure 6. We used the degree range $l = 70 - 150$ to extract the density from the gravity model, making use of the extended resolution of the model due to the constraint (compared to the global resolution of degree 70 for the normal SGM150J model). We compare the results we obtain from the RM- S constrained model with those obtained from localization using the GRGM1200B model. We used the same gravity degree range $l = 70 - 150$ to average the effective density spectra for the GRGM1200B model (the same spectra as we used for the results shown in Figure 1). To extract a density model from the RM- S model, we applied localization or we used the matrix formulation to extract a degree and order 5 model. Both are shown together with the results from the GRGM1200B model. For the localization applied to the RM- S model, we used 1 taper instead of 30 because of the lower resolution of the model. Because we use a windowing bandwidth of 20, we average the resulting effective density spectra between degrees 70 and 130.

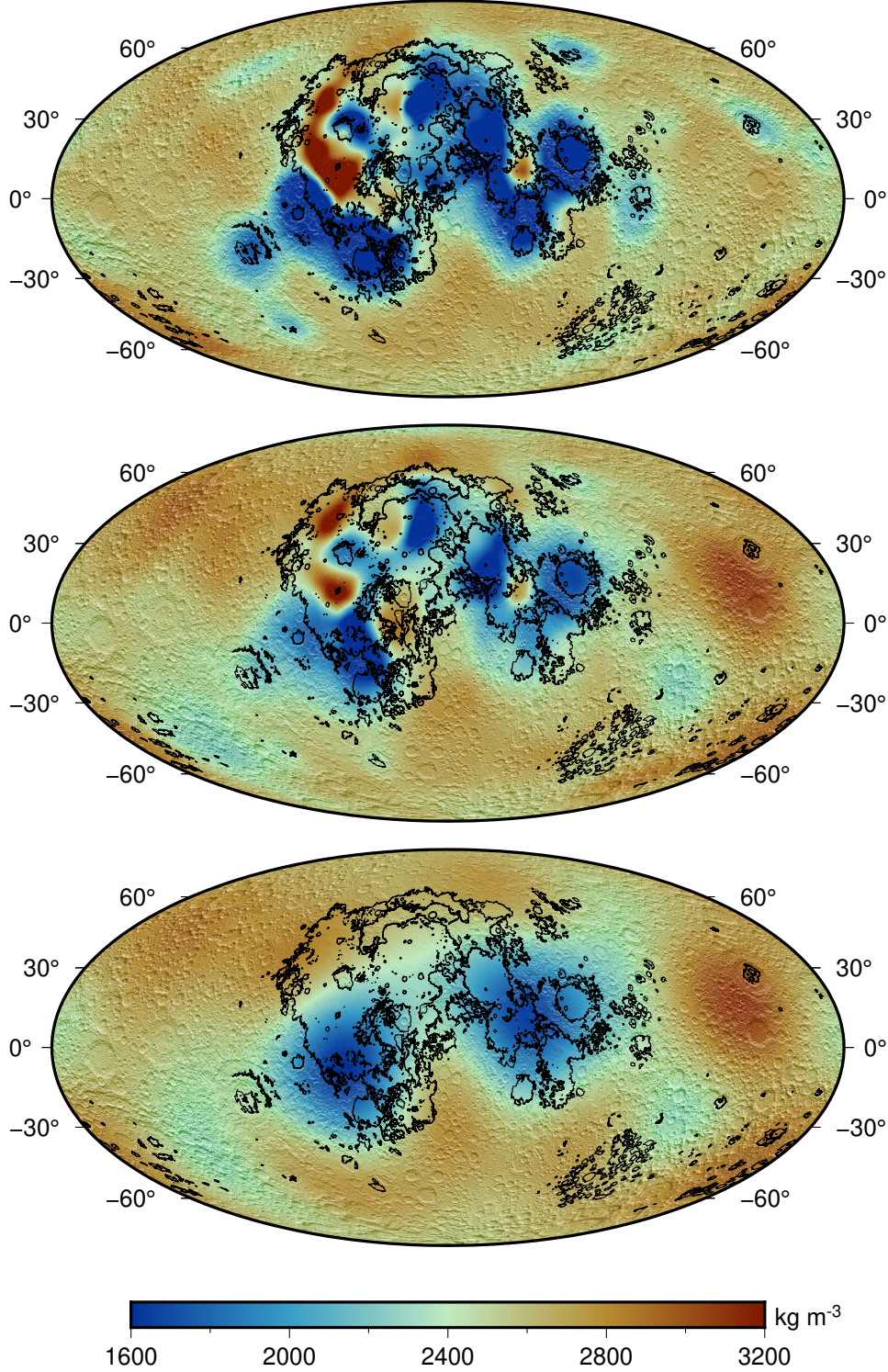


Figure 6. Crustal density variations for the Moon from localization using the GRGM1200B model (top), from an RM- S constrained model using a degree and order 5 density model to construct the constraint based on pre-GRAIL data, using localization (middle), and for a degree and order 5 density model using the matrix formulation (bottom). We used the gravity degree range $l = 70 - 150$. The RM- S model used a constraint factor of $\lambda = 10^{16}$ and a density expansion of degree and order 5. The maps have the same projection and properties as Figure 1.

As can be seen in Figure 6 the results from the RM- S solution on the pre-GRAIL data set using localization are close to those from GRGM1200B. The densities from the RM- S constrained model (using either localization or the matrix formulation) show the same overall large-scale pattern, with higher amplitudes in some parts for the RM- S localization results. The dynamic range for the densities obtained from localization of the GRM1200B model is 200 to 4200 kg m⁻³, that for the RM- S constrained densities from localization 800 to 3300 kg m⁻³, and that for the RM- S constrained model using the matrix formulation 1600 to 3100 kg m⁻³. The latter clearly shows a more subdued signal, with densities that overall appear more reasonable. The strongest signals are again over the mare areas, and this is also where the largest differences occur. The means and standard deviations around the mean for all 3 densities maps are close. This shows that with the new constraint we can extract density variations even from a lower-resolution data set.

We are limited by the resolution of the input data set, and we thus cannot use the higher gravity degree range (> 150) that was used to determine the Moon’s crustal density. Values for the densities in Figure 6 are larger than those in Figure 1 which used the degree range $l = 150 - 310$. In part this may be because, in general, lower degrees reflect greater depths (Bowin 1986; Goossens & Smith 2023) and thus, perhaps, larger densities. On the other hand, the density anomaly in SPA that we highlighted in Figures 1 and 3 is now less pronounced. While present it is smaller in amplitude and appears with an offset from the center of SPA. This is the case for all maps, including the result using the GRGM1200B model, and this may be related to the degree range we need to use. These lower degrees may also still be affected by flexure (Wieczorek et al. 2013), yet earlier results with the RM1 constraint showed that despite the lower degree range we can still obtain the same result for the average density of the crust as from a GRAIL model. The RM- S derived spherical harmonic models for the density shown here also have an average density (the $\alpha_{0,0}$ term of eq. (5)) of around 2520 kg m⁻³, the same as the GRAIL derived value.

We show results from an RM- S model that used a degree and order 12 density expansion in the construction of the constraint in Figure 7. We compare density results from localization and from the matrix formulation. Both maps in Figure 7 are similar but the densities from the matrix method

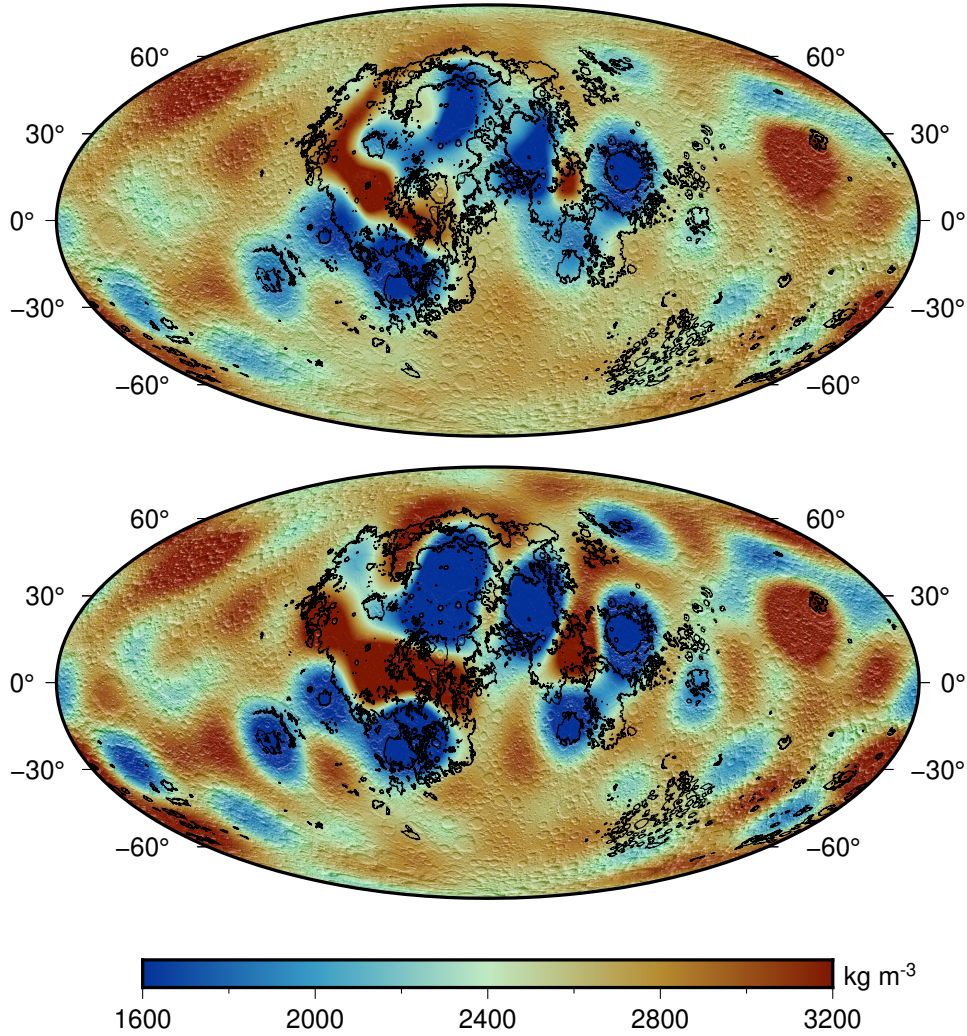


Figure 7. Crustal density variations for the Moon from an RM- S constrained model using a degree and order 12 density model to construct the constraint, based on pre-GRail data, using localization (top), and for a degree and order 12 density model using the matrix formulation (bottom). We used the gravity degree range $l = 70 - 150$. The RM- S model used a constraint factor of $\lambda = 10^{16}$ and a density expansion of degree and order 12. The maps have the same projection and properties as Figure 1.

are generally higher. The range for the densities from localization is 500 to 4200 kg m $^{-3}$ and that for the densities using the matrix formulation is even larger at -1000 to 4600 kg m $^{-3}$. Yet, again the mean is similar for all models and the largest values occur over the mare areas. The map from the localization is similar to that using the RM- S solution based on a degree and order 5 density

expansion (Figure 6), whereas that from the matrix formulation clearly shows stronger amplitudes, also in parts outside of the mare areas.

There is also an influence of the start degree used in either the averaging of the effective density spectra or when using the matrix formulation to extract densities. We obtain more realistic density variations when we use a higher starting degree to extract the density from the gravity model, *e.g.*, 80 versus 70. Yet overall, the patterns remain the same, indicating we can extract density variations.

Finally, we note that if we extract a density model from an RM1 constrained gravity model (in this case, with the matrix method), we find a solution that in general shows smaller variations in lateral density. We show this in Figure 8. This is to be expected because the RM1 model is constructed to match gravity-from-topography with a constant density. The stronger the constraint is applied (expressed as the constraint factor λ_{RM1}), the fewer variations we expect. Figure 8 shows that this is the case. But even for the mildly constrained solution using $\lambda_{\text{RM1}} = 1$, the density variations are smaller than those obtained with the RM-*S* constraint as shown in Figures 6 and 7. The range for the densities from the RM1 model using $\lambda = 1$ is 1900 to 2770 kg m⁻³ whereas that for the RM1 model using $\lambda = 100$ is 2300 to 2750 kg m⁻³. This shows that the RM-*S* constraint indeed allows multiple degrees of freedom to extract density variations. Applying this constraint to the GRAIL data set at full resolution is left for future work. We anticipate that this could improve the higher degrees of the gravity field model as well as studies of the Bouguer gravity to investigate sub-surface density variations by accounting for lateral density variations in the Bouguer correction.

5.2. Results for Mars

For Mars we used the data system of the GMM-3 Mars gravity model (Genova et al. 2016). This is a gravity field model of degree and order 120 based on the tracking of Mars Global Surveyor, Mars Odyssey, and Mars Reconnaissance Orbiter. Like in our earlier work (Goossens et al. 2017), we use an expanded data set where the partial derivatives of the tracking data with respect to the gravity model coefficients for Mars Reconnaissance Orbiter were generated for a degree and order 150 model. We apply the RM-*S* constraint starting at degree $l = 40$.

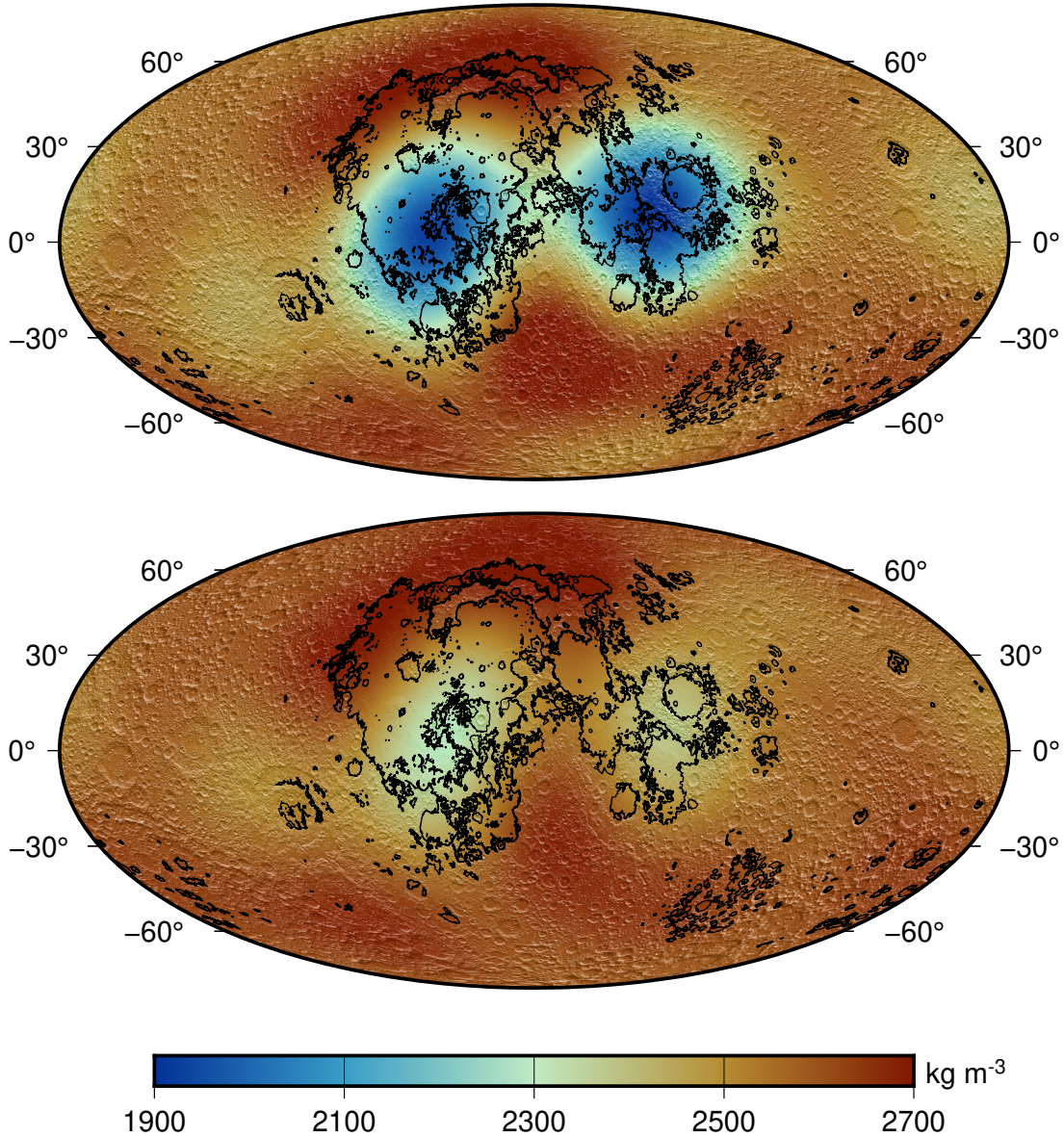


Figure 8. Crustal density variations for the Moon extracted with the matrix method from an RM1-constrained model based on the SGM150J data matrix, using $\lambda_{RM1} = 1$ (top) or $\lambda_{RM1} = 100$ (bottom). We used the gravity degree range $l = 70 - 150$, and the density models are of degree and order 5. The maps have the same projection and properties as Figure 1.

Because we lack a constraint-free gravity solution up to high degree and order for Mars to compare our solutions with, we determine the constraint factor λ by comparing correlations with gravity-from-topography, using a constant density for the crust. We show such correlations in Figure 9. Correlations generally increase with increasing λ . However, for a large value such as $\lambda = 10^{27}$

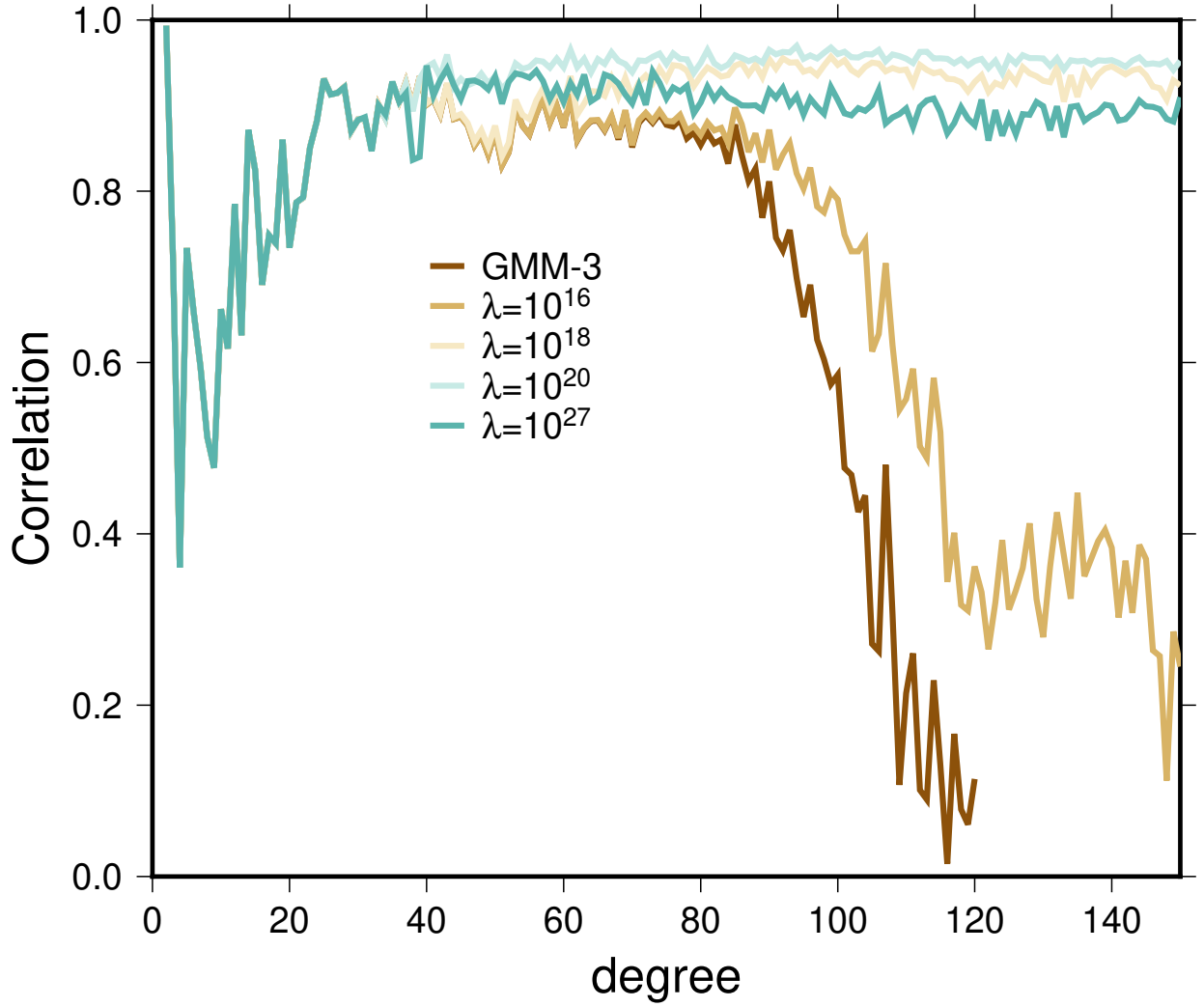


Figure 9. Correlations between RM- S constrained solutions and gravity-from-topography using a constant density for the crust. The RM- S solutions use the GMM-3 data matrix where the constraint is applied from degree 40 for a degree and order 5 density model. Correlations for the GMM-3 model are also shown.

correlations start dropping. While this is expected, we also find that the power in the density harmonics increases with increasing λ , as shown in Figure 10 (left). We thus choose to focus on solutions using $\lambda = 10^{20}$. We extracted the density coefficients using the gravity degree range $l = 40 - 150$ but we found that using a higher degree range such as $l = 80 - 150$ results in very similar density models.

We show the resulting crustal density maps in Figure 11, using either localization (top) or the matrix method (middle) for degree and order 5 models. If we change some of the parameters such

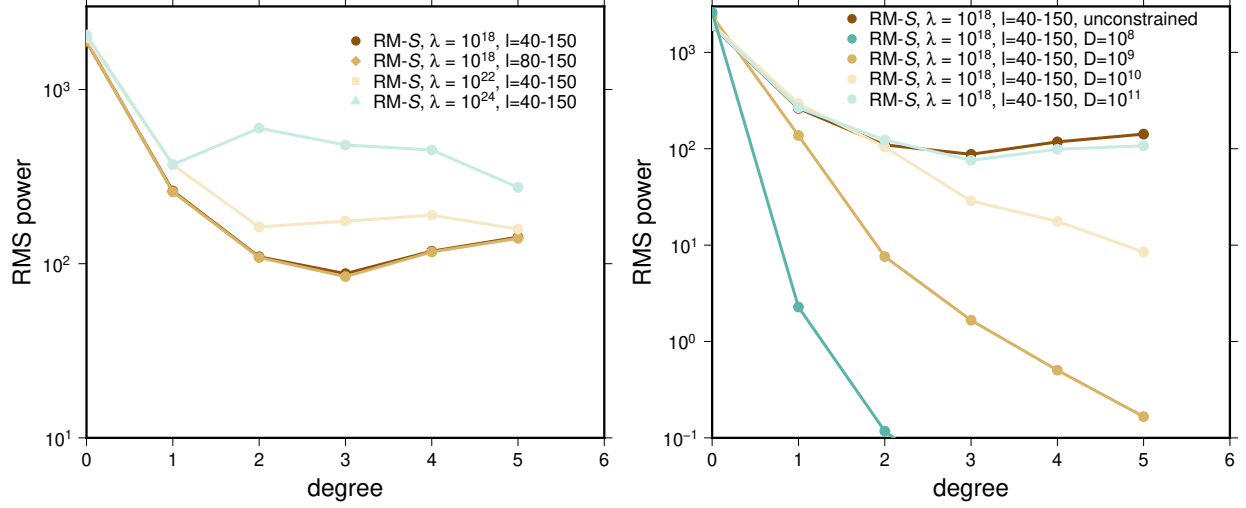


Figure 10. Power per degree for density models of the crust of Mars, derived from RM-S constrained Mars gravity models with different values for λ (left) and for density solutions following eq. (15) using different additional constraint values for D (right).

as the range from which to extract the density coefficients, or the degree from which the constraint is applied, the pattern remains the same. The maps shows high density values over the volcanic complexes, which is to be expected, and over the north. Yet the values are unrealistically high or low. The range for the densities from localization is -860 to 7700 kg m^{-3} and that for the densities from the matrix method is 200 to 4300 kg m^{-3} .

As explained earlier, we can smooth the resulting density model by applying an additional constraint when extracting the density coefficients, following eq. (15). Decreasing the factor D decreases the power in the density coefficients, which is shown in Figure 10. This results in more realistic values of the density but this also biases the density values towards lower values. Nonetheless, by suppressing the power in the higher degrees of the density expansion, the longer wavelength signal (but not the amplitude) remains preserved, hinting at the possibility of density variations in Mars' crust. We show such a model in Figure 11 (bottom). The range in densities is now much reduced: they vary between 2000 and 2850 kg m^{-3} .

Due to the choice of the additional smoothing only the lowest degree signal is retained in Figure 11 (bottom). However, this signal is common among all the solutions we investigated; it is just strongly

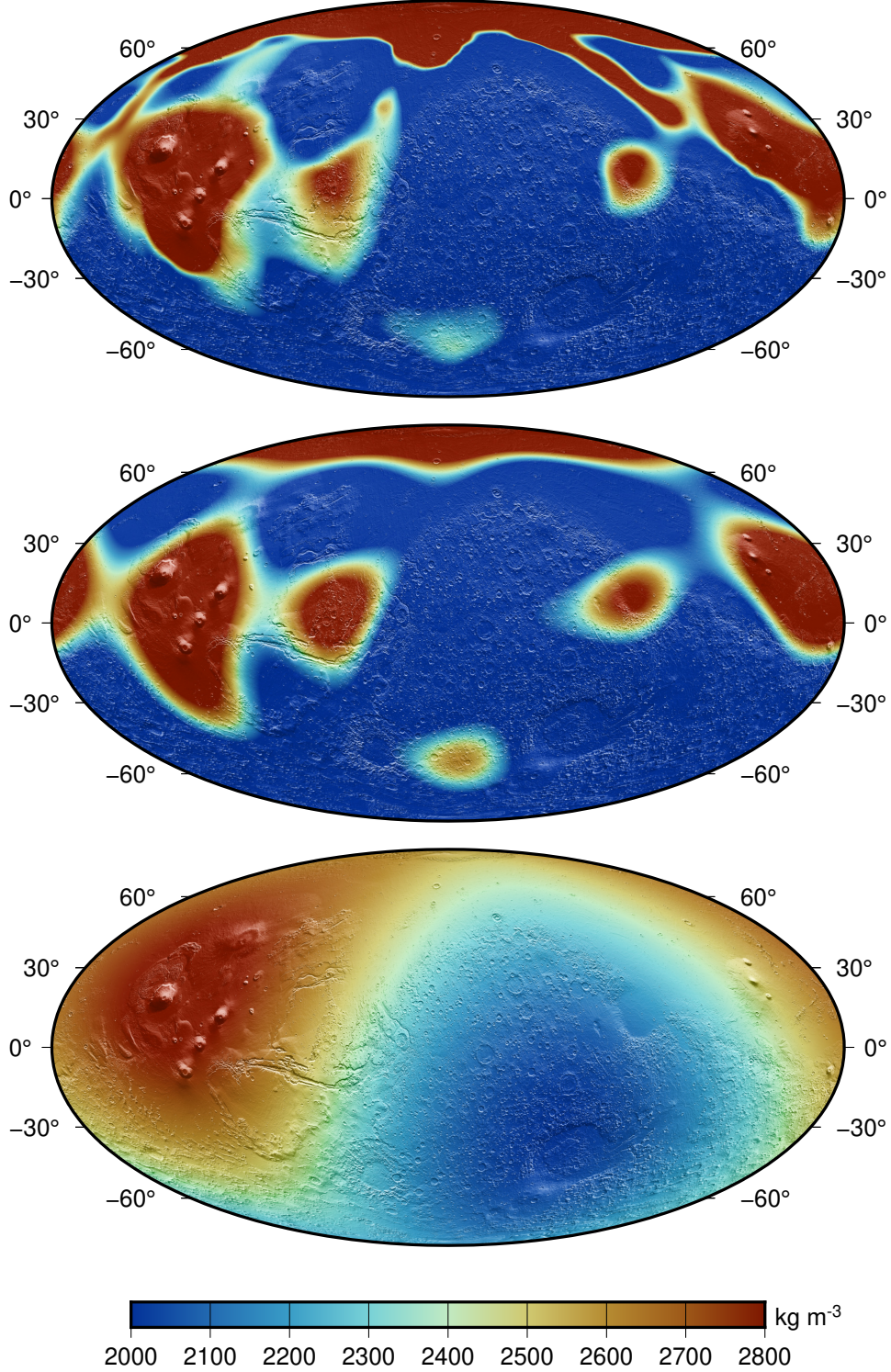


Figure 11. Crustal density variations for Mars based on an RM- S constrained model with $\lambda = 10^{20}$ and a density expansion of degree and order 5 used to construct the constraint. We show densities based on localization (top; see text for details), based on the matrix method (middle), and based on the matrix method with an additional smoothing constraint using $D = 10^9$ (bottom). The map is in a Mollweide projection centered on zero longitude, shaded by topography.

pronounced for the solution using $D = 10^9$ because the higher degree signals are suppressed. The signal clearly shows north-south differences in density. It also correlates well with the crustal dichotomy boundary, for example when comparing the degree-1 terms of this density model with a spherical harmonics expansion for the crustal dichotomy (Wieczorek 2023). Different densities for the north and south, divided by the dichotomy, have been considered when constructing crustal thickness maps for Mars from gravity and topography, with the north having a higher density than the south (Wieczorek et al. 2022). The effect of such varying densities in the crust is a more uniform crustal thickness (Goossens et al. 2017; Wieczorek et al. 2022).

Recent analyses of seismic data combined with gravity used a model with a uniform density crust (Drilleau et al. 2024). This was in turn based on the analysis of surface waves which found best-fitting models that have a density contrast between the north and south $\leq 200 \text{ kg m}^{-3}$ (Kim et al. 2023). While this suggests that the densities are close, this still allows a difference in crustal density between the north and south. Our results for Mars are tentative since the gravity models are at (or even still below) the edge of sufficient resolution to confidently extract density variations. Yet they indicate that large-scale density variations are possible, and interestingly show that these variations are compatible with being divided by the dichotomy.

Crustal density variations can be determined unambiguously from gravity and topography when gravity and topography correlate highly, and when there are no sub-surface density anomalies that also correlate with topography, as can occur at lower degrees due to flexure, or at higher degrees in the presence of volcanic infilling of depressions or due to impact-generated porosity beneath craters. In such a case, the admittance (which is the transfer function between gravity and topography) is independent of flexure effects (Wieczorek et al. 2013), and the admittance value is then determined by the crustal density. We used the thin-plate model of Turcotte et al. (1981) to compute admittance as a function of elastic thickness (a proxy for the mechanical thickness of the lithosphere) for Mercury, Venus, and Mars, with the goal to find the approximate degree for which the admittance can be used to determine the density. For simplicity we assumed a mantle density of 3500 kg m^{-3} , a crustal thickness of 35 km, and a crustal density of 2700 kg m^{-3} for all three planets. In addition, we used

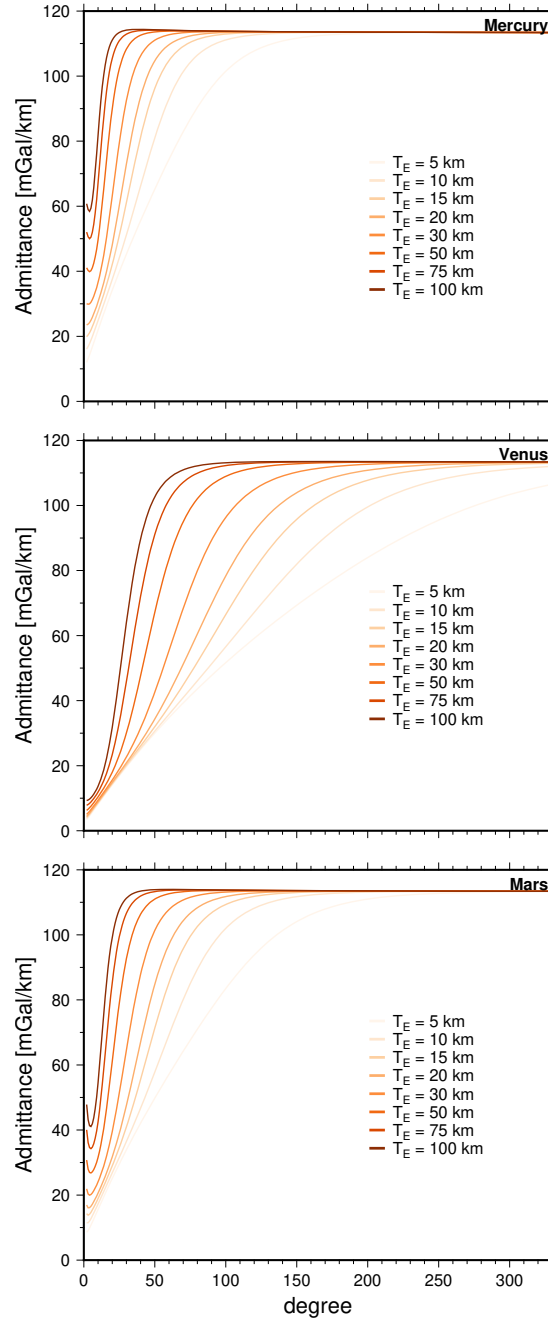


Figure 12. Theoretical admittance for Mercury (top), Venus (middle), and Mars (bottom), using the model of [Turcotte et al. \(1981\)](#), for various values of elastic thickness T_E (for a fixed value of crustal thickness of 35 km). Darker colors indicate larger elastic thicknesses. The degree where the curves become mostly independent of elastic thickness is the degree from which gravity and topography should correlate highly.

a Young's modulus of 100 GPa and a Poisson ration of 0.25. The results are shown in [Figure 12](#), and it can be clearly understood that the degree for which admittance becomes independent of

elastic thickness is lower for smaller planets. While this depends on the elastic thickness, assuming values larger than 20 km, for Mercury the degree would approximately be between 30 and 60, for Venus between 100 and 200, and for Mars between 40 and 90. This would suggest perhaps that the current resolution of Mars models might be sufficient, yet our results clearly show this is not the case. Elastic thickness for Mars may be low in many places (Audet 2014) which would require higher resolution gravity. Data from the BepiColombo mission to Mercury should result in gravity field models with a global resolution between degree 30 and 50 (Iess et al. 2021; Genova et al. 2021), and data from the VERITAS mission to Venus should result in models with a resolution larger than degree 160 (Giuliani et al. 2025). Both will thus be good candidates to apply our constraint method to determine lateral variations in crustal density. Applying this method to the full GRAIL data may also result in improved, high-resolution estimates of the density of the lunar crust.

6. CONCLUSIONS

We have presented a constraint for gravity field determination based on spacecraft tracking data, that uses information from topography and that allows for the direct determination of spherical harmonic coefficients describing lateral density variations in the crust. The constraint is based on a matrix formulation of the Bouguer correction, which can also be used to directly determine lateral density variations from gravity field coefficients. We validated this matrix formulation using GRAIL models, showing that we obtain similar densities as those obtained using localization methods. We then introduced the new constraint matrix and we show that the scale factors for the spherical harmonics terms of the density function are determined by the data, not the constraint. When we apply this constraint to a pre-GRAIL data set, we showed that we obtain the same density variations as we obtain from a GRAIL model. However, we have to use a lower range of gravity degrees because we are limited by the resolution of the pre-GRAIL data set. We also applied this constraint to a data system from Mars tracking data. For Mars, we do not have a GRAIL-like model to test our results against, and the Mars models are currently only at the edge or even below the resolution to confidently determine density variations. Our Mars results are thus tentative but they hint at

the possibility of large-scale density variations for Mars, separated by the dichotomy, with higher densities for the north, as well as over the volcanic complexes.

We note that results from our constraint cannot be a substitute for missing data. It cannot extend resolution beyond what is present in the current data. But it can extract information that may otherwise be suppressed when other regularization, such as a Kaula rule, is used. This constraint may prove useful in the future for planets such as Mercury and Venus when higher resolution gravity field models become available, or to apply to the GRAIL data set at its full resolution.

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APPENDIX

A. THE RM- S CONSTRAINT AND $\lambda \rightarrow \infty$

Here we show the behavior of the $\Delta \mathbf{x}_k$ correction term as $\lambda \rightarrow \infty$, that is, as the influence of the constraint increases. For brevity let us define $\mathbf{N}_k = \mathbf{A}_k^T \mathbf{W} \mathbf{A}_k$ and $\mathbf{y}_k = \mathbf{A}_k^T \mathbf{W} \mathbf{r}_k$. Let us also assume that $\mathbf{N}_k$ is invertible such that it has a Cholesky decomposition of $\mathbf{N}_k = \mathbf{L}_k \mathbf{L}_k^T$, where $\mathbf{L}_k$ is a lower-

triangular matrix. Using the Sherman-Morrison-Woodbury formula, we now rewrite $\Delta \mathbf{x}_k$ as

$$\begin{aligned}
\Delta \mathbf{x}_k &= (\mathbf{N}_k + \lambda \mathbf{G}_\perp \mathbf{G}_\perp^\text{T})^{-1} (\mathbf{y}_k - \lambda \mathbf{G}_\perp \mathbf{G}_\perp^\text{T} \mathbf{x}_k), \\
&= (\mathbf{N}_k + \lambda \mathbf{G}_\perp \mathbf{G}_\perp^\text{T})^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \left[\mathbf{N}_k^{-1} - \mathbf{N}_k^{-1} \mathbf{G}_\perp (\lambda^{-1} \mathbf{I} + \mathbf{G}_\perp^\text{T} \mathbf{N}_k^{-1} \mathbf{G}_\perp)^{-1} \mathbf{G}_\perp^\text{T} \mathbf{N}_k^{-1} \right] (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \mathbf{L}_k^{-\text{T}} \left[\mathbf{I} - \mathbf{L}_k^{-1} \mathbf{G}_\perp (\lambda^{-1} \mathbf{I} + \mathbf{G}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \mathbf{L}_k^{-1} \mathbf{G}_\perp)^{-1} \mathbf{G}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \right] \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k.
\end{aligned} \tag{A1}$$

We now take the limit as $\lambda \rightarrow \infty$

$$\begin{aligned}
\Delta \mathbf{x}_k &= \mathbf{L}_k^{-\text{T}} \left[\mathbf{I} - \mathbf{L}_k^{-1} \mathbf{G}_\perp (\mathbf{G}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \mathbf{L}_k^{-1} \mathbf{G}_\perp)^{-1} \mathbf{G}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \right] \\
&\quad \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \mathbf{L}_k^{-\text{T}} \left[\mathbf{I} - \mathbf{L}_k^{-1} \mathbf{Q}_\perp \mathbf{R}_\perp (\mathbf{R}_\perp^\text{T} \mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \mathbf{L}_k^{-1} \mathbf{Q}_\perp \mathbf{R}_\perp)^{-1} \mathbf{R}_\perp^\text{T} \mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \right] \\
&\quad \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \mathbf{L}_k^{-\text{T}} \left[\mathbf{I} - \mathbf{L}_k^{-1} \mathbf{Q}_\perp \mathbf{R}_\perp \mathbf{R}_\perp^{-1} (\mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \mathbf{L}_k^{-1} \mathbf{Q}_\perp)^{-1} \mathbf{R}_\perp^{-\text{T}} \mathbf{R}_\perp^\text{T} \mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \right] \\
&\quad \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \mathbf{L}_k^{-\text{T}} \left[\mathbf{I} - \mathbf{L}_k^{-1} \mathbf{Q}_\perp (\mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \mathbf{L}_k^{-1} \mathbf{Q}_\perp)^{-1} \mathbf{Q}_\perp^\text{T} \mathbf{L}_k^{-\text{T}} \right] \\
&\quad \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k.
\end{aligned} \tag{A2}$$

and note that the quantity in the square brackets is not only independent of $\mathbf{R}_\perp$, but is also a projection matrix onto the null of the column space of $\mathbf{L}_k^{-1} \mathbf{Q}_\perp$ or onto the column space of its orthogonal complement, which is just $\mathbf{L}_k^\text{T} \mathbf{G}$. Thus, we can rewrite this as

$$\begin{aligned}
\Delta \mathbf{x}_k &= \mathbf{L}_k^{-\text{T}} \left[\mathbf{L}_k^\text{T} \mathbf{G} (\mathbf{G}^\text{T} \mathbf{L}_k \mathbf{L}_k^\text{T} \mathbf{G})^{-1} \mathbf{G}^\text{T} \mathbf{L}_k \right] \mathbf{L}_k^{-1} (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k) - \mathbf{x}_k, \\
&= \mathbf{G} \boldsymbol{\alpha}_{k+1} - \mathbf{x}_k, \\
\mathbf{x}_{k+1} &= \mathbf{G} \boldsymbol{\alpha}_{k+1},
\end{aligned} \tag{A3}$$

where eq. (A3) is indeed in the same form as eq. (6) and

$$\begin{aligned}
\boldsymbol{\alpha}_{k+1} &= (\mathbf{G}^T \mathbf{N}_k \mathbf{G})^{-1} \mathbf{G}^T (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k), \\
&= (\mathbf{G}^T \mathbf{A}_k^T \mathbf{W} \mathbf{A}_k \mathbf{G})^{-1} \mathbf{G}^T \mathbf{A}_k^T \mathbf{W} (\mathbf{r}_k + \mathbf{A}_k \mathbf{x}_k), \\
&= (\mathbf{G}^T \mathbf{A}_k^T \mathbf{W} \mathbf{A}_k \mathbf{G})^{-1} \mathbf{G}^T \mathbf{A}_k^T \mathbf{W} (\mathbf{r}_k + \mathbf{A}_k \mathbf{G} \boldsymbol{\alpha}_k).
\end{aligned} \tag{A4}$$

The last line in eq. (A4) is valid when $\lambda \rightarrow \infty$ for the entire GN iterative process leading to $\mathbf{x}_k = \mathbf{G} \boldsymbol{\alpha}_k$ for all k .

Considering the full rank transformation from eq. (9) it follows that

$$\begin{aligned}
\Delta \mathbf{x}_k &= (\mathbf{N}_k + \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T)^{-1} (\mathbf{y}_k - \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T \mathbf{x}_k), \\
\begin{bmatrix} \Delta \boldsymbol{\alpha}_k \\ \Delta \boldsymbol{\beta}_k \end{bmatrix} &= \begin{bmatrix} \mathbf{R}^{-1} \mathbf{Q}^T \\ \mathbf{R}_\perp^{-1} \mathbf{Q}_\perp^T \end{bmatrix} (\mathbf{N}_k + \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T)^{-1} \begin{bmatrix} \mathbf{Q} \mathbf{R}^{-T} \mathbf{Q}_\perp \mathbf{R}_\perp^{-T} \\ \mathbf{G}^T \\ \mathbf{G}_\perp^T \end{bmatrix} (\mathbf{y}_k - \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T \mathbf{x}_k), \\
&= \left\{ \begin{bmatrix} \mathbf{G}^T \\ \mathbf{G}_\perp^T \end{bmatrix} (\mathbf{N}_k + \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T) \begin{bmatrix} \mathbf{G} & \mathbf{G}_\perp \end{bmatrix} \right\}^{-1} \\
&\quad \begin{bmatrix} \mathbf{G}^T \\ \mathbf{G}_\perp^T \end{bmatrix} (\mathbf{y}_k - \lambda \mathbf{G}_\perp \mathbf{G}_\perp^T \mathbf{x}_k), \\
&= \begin{bmatrix} \mathbf{G}^T \mathbf{N}_k \mathbf{G} & \mathbf{G}^T \mathbf{N}_k \mathbf{G}_\perp \\ \mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G} & \mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G}_\perp + \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \end{bmatrix}^{-1} \\
&\quad \begin{bmatrix} \mathbf{G}^T \mathbf{y}_k \\ \mathbf{G}_\perp^T \mathbf{y}_k - \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \boldsymbol{\beta}_k \end{bmatrix}.
\end{aligned} \tag{A5}$$

The partitioned solution for $\Delta\alpha_k$ is then

$$\begin{aligned} \Delta\alpha_k = & \left\{ \mathbf{G}^T \mathbf{N}_k \mathbf{G} - \mathbf{G}^T \mathbf{N}_k \mathbf{G}_\perp \left[\mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G}_\perp + \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \right]^{-1} \mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G} \right\}^{-1} \\ & \left\{ \mathbf{G}^T \mathbf{y}_k - \mathbf{G}^T \mathbf{N}_k \mathbf{G}_\perp \left[\mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G}_\perp + \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \right]^{-1} \right. \\ & \left. \left(\mathbf{G}_\perp^T \mathbf{y}_k - \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \beta_k \right) \right\}. \end{aligned} \quad (\text{A6})$$

Taking the limit as $\lambda \rightarrow \infty$

$$\begin{aligned} \Delta\alpha_k &= (\mathbf{G}^T \mathbf{N}_k \mathbf{G})^{-1} \mathbf{G}^T [\mathbf{y}_k + \mathbf{N}_k \mathbf{G}_\perp \beta_k], \\ \alpha_{k+1} &= (\mathbf{G}^T \mathbf{N}_k \mathbf{G})^{-1} \mathbf{G}^T [\mathbf{y}_k + \mathbf{N}_k \mathbf{G}_\perp \beta_k] + \alpha_k, \\ &= (\mathbf{G}^T \mathbf{N}_k \mathbf{G})^{-1} \mathbf{G}^T [\mathbf{y}_k + \mathbf{N}_k (\mathbf{G} \alpha_k + \mathbf{G}_\perp \beta_k)], \\ &= (\mathbf{G}^T \mathbf{N}_k \mathbf{G})^{-1} \mathbf{G}^T (\mathbf{y}_k + \mathbf{N}_k \mathbf{x}_k), \end{aligned} \quad (\text{A7})$$

which is equivalent to eq. (A4). The partitioned solution for $\Delta\beta_k$ is then

$$\begin{aligned} \Delta\beta_k &= \left\{ \mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G}_\perp + \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \right\}^{-1} \\ & \left\{ \mathbf{G}_\perp^T \mathbf{y}_k - \lambda (\mathbf{R}_\perp^T \mathbf{R}_\perp)^2 \beta_k - \mathbf{G}_\perp^T \mathbf{N}_k \mathbf{G} \Delta\alpha_k \right\}. \end{aligned} \quad (\text{A8})$$

Taking the limit as $\lambda \rightarrow \infty$

$$\begin{aligned} \Delta\beta_k &= -\beta_k, \\ \beta_{k+1} &= \mathbf{0}, \end{aligned} \quad (\text{A9})$$

which is equivalent to the statement in eq. (A4) that $\mathbf{x}_k = \mathbf{G} \alpha_k$. Eq. (11) can be used to extract α_k from this constrained solution $\mathbf{x}_k$.

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