Mathematical models of the Earth’s density structure and their applications in gravimetric forward modeling

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Abstract: A generalized mathematical model of the Earth’s density structure is presented in this study. This model is defined based on applying the spectral expressions for a 3-D density distribution within the arbitrary volumetric mass layers. The 3-D density model is then converted into a form which describes the Earth’s density structure by means of the density-contrast interfaces between the volumetric mass layers while additional correction terms are applied to account for radial density changes. The applied numerical schemes utilize methods for a spherical harmonic analysis and synthesis of the global density structure models. The developed the Earth’s density models are then defined in terms of the spherical density and density-contrast functions. We also demonstrate how these Earth’s density models can be applied in the gravimetric forward modeling and discuss some practical aspects of representing mathematically density structures within particular components of the Earth’s interior.

Key words: crust, density, gravity, model

1. Introduction

Several Earth’s synthetic models of seismic velocities and/or mass density distribution were developed based on analysis of available seismic data and additional geophysical constraints. Dziewonski et al. (1975) introduced the Parametric Earth Models (PEMs) consisting of piece-wise continuous analytical functions of the radial density and velocity variations defined individually for the oceanic (PEM-O) and continental (PEM-C) lithosphere down to a depth of 420 km while below this depth these two models are
identical. They also provided an averaged function for the whole lithosphere (PEM-A). Dziewonski and Anderson (1981) later presented the Preliminary Reference Earth Model (PREM) which provides information on the seismic velocities and the density structure within the whole Earth’s interior (including the core and mantle) by means of spherically homogenous stratigraphic layers. Kennett and Engdahl (1991) compiled the parameterized velocity model IASP91 that summarized travel time characteristics of main seismic phases. Kennett et al. (1995) compiled the AK135-f model by augmenting the AK135 velocity model with the density and Q-model of Montagner and Kennett (1995). Van der Lee and Nolet (1997) prepared the 1-D averaged model MC35 based on the PEM-C while replacing the high- and low-velocity zones of the PEM-C by a constant S-wave velocity of 4.5 km s\(^{-1}\) within the upper mantle down to a depth of 210 km. Kustowski et al. (2008b) derived the transversely isotropic reference Earth model STW105. More recently, Simmons et al. (2010) developed the GyPSuM tomographic model of the mantle (P and S) seismic velocities and density through a simultaneous inversion of seismic body-wave travel times and geodynamic observables including the free-air gravity anomalies, tectonic plate divergence, dynamic surface topography and the excess ellipticity of the core-mantle boundary. They also incorporated mineral physics constraints in order to link seismic velocities and wave speeds with an underlying hypothesis that temperature is a principal cause of heterogeneities in the non-cratonic mantle. In addition to these studies several other global and regional seismic velocity models were developed. For more details we refer readers to studies, for instance, by Grand et al. (1997), Mégnin and Romanowicz (2000), Grand (2002), Gung and Romanowicz (2004), van der Lee and Frederiksen (2005), Panning and Romanowicz (2006), Houser et al. (2008), Kustowski et al. (2008a, 2008b), Bedle and van der Lee (2009), Panning et al. (2010), Obrebski et al. (2010, 2011), Porritt et al. (2011), James et al. (2011), Lekic and Romanowicz (2011) and Simmons et al. (2012). Summary of these models can also be found in Trabant et al. (2012).

The PEM and PREM models provide 1-D density information only. The Earth’s interior is obviously represented more realistically by synthetic models consisting of stratigraphic layers with a variable depth, thickness and density distribution. Currently available global models provide information on a 3-D density structure only within the crust and upper mantle. Nataf
and Ricard (1996) derived a global model of the crust and upper mantle density structure based on analysis of seismic data and additional constraints such as heat flow and chemical composition. Mooney et al. (1998) compiled the global crustal model with a 5 × 5 arc-deg spatial resolution. The updated global crustal model CRUST2.0 was compiled with a 2 × 2 arc-deg spatial resolution (Bassin et al., 2000). Both models were compiled based on seismic data published until 1995 and a detailed compilation of the ice and sediment thickness. The CRUST1.0 is the most recent version compiled globally with a 1 × 1 arc-deg spatial resolution (Laske et al., 2012). The CRUST1.0 consists of the ice, water, (upper, middle and lower) sediments and (upper, middle and lower) consolidated (crystalline) crustal layers. In addition, the lateral density structure of the upper mantle was incorporated into the CRUST2.0 and CRUST1.0 models. The globally averaged data from active seismic methods and deep drilling profiles were used to predict the sediment and crustal structure where no seismic measurements were available (most of Africa, South America, Greenland and large parts of the oceanic lithosphere) by a generalization to similar geological and tectonic settings. Despite the density distribution within deeper crustal structure over large parts of the world is not yet known with a sufficient resolution and accuracy, there are several global datasets which provide more detailed information on the density distribution within shallower crustal structures. Chen and Tenzer (2015) used such datasets for a compilation of the Earth’s Spectral Crustal Model (ESCM180) with a spectral resolution complete to a spherical harmonic degree of 180 by incorporating more detailed information on the topography, bathymetry, polar ice sheets and geoid surface into the CRUST1.0 model.

In this study a mathematical formalism is developed for describing the Earth’s density structure by means of a 3-D density distribution within stratigraphic mass layers. This description is then modified by means of the density-contrast interfaces. Both formulations are presented in a frequency domain in terms of the spherical density and density-contrast functions. The spectral expressions for describing the Earth’s density structure (given in Sections 2 and 3) are applied in gravimetric forward modeling in Section 4. Some practical aspects of representing the Earth’s lithospheric structures are discussed in Section 5. Summary and concluding remarks are given in Section 6.
2. 2-D Earth’s density model

To begin with we first assume only a lateral density distribution. This density model is applied to describe the geometry and density distribution within an arbitrary volumetric mass layer in a frequency domain. We then present 2-D Earth’s density models described using this spectral representation of the volumetric mass density layers and respective density-contrast interfaces.

2.1. 2-D density layers

The Earth’s density structure is represented by a finite number of volumetric mass layers defined by sets of geometric and density parameters. Adopting the spherical approximation of the Earth, the geometry of each volumetric layer is defined by the heights $U$ and $L$ of the upper and lower bounds respectively, where these heights are stipulated with respect to the Earth’s mean radius $R$. For the upper and lower bounds located below the geoid surface (approximated by the sphere of radius $R$), the parameters $U$ and $L$ become negative. It is worth mentioning that a relative error due to applying the spherical (instead of ellipsoidal) approximation of the Earth is about 0.3% (e.g., Heiskanen and Moritz, 1967).

For the $q$-th volumetric mass layer, a lateral density distribution is defined by:

$$\rho_q(r, \Omega) \cong \rho_q(U_q, \Omega) \; \text{for} \; R + U_q(\Omega) \geq r > R + L_q(\Omega) \; \text{for} \; q = 1, 2, ..., Q, \; (1)$$

where $\rho(U, \Omega)$ is a (nominal) lateral density stipulated at an upper bound $U$ and a location $\Omega$, and $Q$ is a total number of volumetric mass layers applied to describe the Earth’s density structure. A 3-D position is defined in the spherical coordinate system $(r, \Omega)$; where $r$ is the geocentric radius, and $\Omega = (\phi, \lambda)$ denotes the geocentric direction with the spherical latitude $\phi$ and longitude $\lambda$.

Taking into consideration two successive volumetric mass layers $q$ and $q + 1$, the density contrast at their interface is given by:

$$\Delta \rho_{q+1,q}(L_q, \Omega) \equiv \Delta \rho_{q+1,q}(U_{q+1}, \Omega) = \rho_{q+1}(U_{q+1}, \Omega) - \rho_q(U_q, \Omega), \; (2)$$

$$L_q \equiv U_{q+1} \; \text{for} \; q = 1, 2, ..., Q - 1.$$
If we neglect the atmospheric density, the density contrast between the Earth’s atmosphere and the first Earth’s inner density layer \((q = 1)\) are approximately equal: \(\Delta \rho_{1,0}(U_1, \Omega) \approx \rho_1(U_1, \Omega)\). The upper bound is \(U_1 = H\) on land and \(U_1 = 0\) offshore, where \(H\) denotes the topographic height.

### 2.2. Spherical 2-D density and density-contrast functions

Applying methods for a spherical harmonic analysis of the density structure the combined information on the geometry and density distribution within a volumetric mass layer is described by the spherical lower- and upper-bound density functions. These functions including their higher-order terms \(\{q(\rho L)^{(k)}_n, q(\rho U)^{(k)}_n : k = 1, 2, ..., q = 1, 2, ..., Q\}\) are computed based on applying a numerical discretization to the following integral convolutions:

\[
q(\rho L)^{(k)}_n = \frac{2n + 1}{4\pi} \int \int \rho_q(U_q, \Omega') L_q^k(\Omega') P_n(\cos \psi) \, d\Omega' = \\
= \sum_{m=-n}^{n} q(\rho L)^{(k)}_{n,m} Y_{n,m}(\Omega),
\]

(3)

and

\[
q(\rho U)^{(k)}_n = \frac{2n + 1}{4\pi} \int \int \rho_q(U_q, \Omega') U_q^k(\Omega') P_n(\cos \psi) \, d\Omega' = \\
= \sum_{m=-n}^{n} q(\rho U)^{(k)}_{n,m} Y_{n,m}(\Omega),
\]

(4)

where \(Y_{n,m}\) are the (fully-normalized) spherical harmonics of degree \(n\) and order \(m\). The Legendre polynomials \(P_n\) in Eqs. (3) and (4) are computed for the argument of cosine of the spherical distance \(\psi\) between two points \((r, \Omega)\) and \((r', \Omega')\). The infinitesimal surface element on the unit sphere is denoted as \(d\Omega' = \cos \phi' \, d\phi' \, d\lambda'\), and \(\Phi = \{\Omega' = (\phi', \lambda') : \phi' \in [-\pi/2, \pi/2] \land \lambda' \in [0, 2\pi]\}\) is the full spatial angle. The numerical coefficients \(\{q(\rho L)^{(k)}_{n,m}, q(\rho U)^{(k)}_{n,m} : k = 1, 2, ..., q = 1, 2, ..., Q\}\) are generated to a certain degree of spherical harmonics using discrete data of density, height/depth and thickness of a particular structural component of the Earth’s interior.

Substituting Eqs. (3) and (4) to Eq. (2), the spherical density-contrast functions and their higher-order terms \(\{q_{+1,q}(\Delta \rho L)^{(k)}_n : k = 1, 2, ..., q = 1, 2, ..., Q - 1\}\) are introduced by:
Tenzer R.: Mathematical models of the Earth’s density... (67–92)

\[ q+1,L_n^{(k)} = \]
\[
= \frac{2n+1}{4\pi} \int_{\Phi} [\rho_{q+1}(U_{q+1}, \Omega') - \rho_q(U_q, \Omega')] L_q^k(\Omega') P_n(\cos \psi) \, d\Omega' = \]
\[
= \frac{2n+1}{4\pi} \int_{\Phi} \Delta \rho_{q+1,q}(L_q, \Omega') L_q^k(\Omega') P_n(\cos \psi) \, d\Omega' = \]
\[
= \sum_{m=-n}^{n} q+1,q(\rho L)_{n,m}^{(k)} Y_{n,m}(\Omega), \tag{5} \]

where the coefficients \{q+1,q(\rho L)_{n,m}^{(k)} : k = 1, 2, ..., q = 1, 2, ..., Q - 1\} are generated from discrete data of lateral density contrast and height/depth of each density interface. Alternatively, these coefficients can directly be generated from the coefficients \( q(\rho L)_{n,m}^{(k)} \) and \( q+1(\rho U)_{n,m}^{(k)} \) by using the following relation:

\[ q+1,q(\rho L)_{n,m}^{(k)} = q+1(\rho U)_{n,m}^{(k)} - q(\rho L)_{n,m}^{(k)}. \tag{6} \]

As seen in Eq. (5), the spherical density-contrast functions are defined at the lower bounds \( \{L_q : q = 1, 2, ..., Q - 1\} \) of volumetric mass layers. The density contrast at each interface is then computed as the difference between the lateral density values within underlying and overlying layers \( q + 1 \) and \( q \), where the lateral densities are (formally) referenced to the upper bounds \( \{U_q, U_{q+1} : q = 1, 2, ..., Q - 1\} \) of these layers (see Eq. 1).

### 2.3. Earth’s lateral density structure

We now apply the (first-order) spherical density functions \( (\rho L)_n \equiv (\rho L)_{n}^{(1)} \) and \( (\rho U)_n \equiv (\rho U)_{n}^{(1)} \) to describe the Earth’s density structure. From Eqs. (3) and (4), we have:

\[
\sum_{q=1}^{Q} [q(\rho U)_n - q(\rho L)_n] = \frac{2n+1}{4\pi} \int_{\Phi} \rho_1(U_1, \Omega') U_1(\Omega') P_n(\cos \psi) \, d\Omega' + \]
\[
+ \frac{2n+1}{4\pi} \int_{\Phi} [\rho_2(U_2, \Omega') - \rho_1(U_1, \Omega')] L_1(\Omega') P_n(\cos \psi) \, d\Omega' + \]

72
\[
\frac{2n+1}{4\pi} \int_{\Phi} \left[ \rho_3(U_3, \Omega') - \rho_2(U_2, \Omega') \right] L_2(\Omega') P_n(\cos \psi) \, d\Omega' + \\
\vdots
\]

\[
\frac{2n+1}{4\pi} \int_{\Phi} \left[ \rho_Q(U_Q, \Omega') - \rho_{Q-1}(U_{Q-1}, \Omega') \right] L_{Q-1}(\Omega') P_n(\cos \psi) \, d\Omega' - \\
\frac{2n+1}{4\pi} \int_{\Phi} \rho_Q(U_Q, \Omega') L_Q(\Omega') P_n(\cos \psi) \, d\Omega'.
\]

(7)

Substituting from Eq. (2) to Eq. (7), we get:

\[
\sum_{q=1}^{Q} \left[ q(\rho U)_n - q(\rho L)_n \right] = \frac{2n+1}{4\pi} \int_{\Phi} \rho_1(U_1, \Omega') U_1(\Omega') P_n(\cos \psi) \, d\Omega' + \\
\frac{2n+1}{4\pi} \int_{\Phi} \Delta \rho_{2,1}(L_1, \Omega') L_1(\Omega') P_n(\cos \psi) \, d\Omega' + \\
\frac{2n+1}{4\pi} \int_{\Phi} \Delta \rho_{3,2}(L_2, \Omega') L_2(\Omega') P_n(\cos \psi) \, d\Omega' + \\
\vdots
\]

\[
\frac{2n+1}{4\pi} \int_{\Phi} \Delta \rho_{Q,Q-1}(L_{Q-1}, \Omega') L_{Q-1}(\Omega') P_n(\cos \psi) \, d\Omega' - \\
\frac{2n+1}{4\pi} \int_{\Phi} \rho_Q(U_Q, \Omega') L_Q(\Omega') P_n(\cos \psi) \, d\Omega'.
\]

(8)

Taking into consideration definitions of the spherical density and density-contrast functions in Eqs. (3-5), the summation in Eq. (8) becomes:

\[
\sum_{q=1}^{Q} \left[ q(\rho U)_n - q(\rho L)_n \right] = \sum_{m=-n}^{n} \sum_{q=1}^{Q} \rho(U)_{n,m} Y_{n,m}(\Omega) - \\
\sum_{m=-n}^{n} \rho(L)_{n,m} Y_{n,m}(\Omega) + \sum_{q=1}^{Q-1} \sum_{m=-n}^{n} q(\Delta \rho L)_{n,m} Y_{n,m}(\Omega).
\]

(9)
The Earth’s density model in Eq. (9) is defined in terms of the spherical density-contrast coefficients \( \{ q_{+1,q}(\Delta \rho L)_{n,m} : q = 1, 2, ..., Q - 1 \} \) of all interfaces where the (lateral) density contrasts are defined. Moreover, this description also incorporates the coefficients \( q_{=1}(\rho U)_{n,m} \) of the upper bound of the first volumetric layer \( (q = 1) \) and the coefficients \( q_{=Q}(\rho L)_{n,m} \) of the lower bound of the last volumetric layer \( (q = Q) \). As seen in Eq. (9), the description of the Earth’s density structure utilizes only the first-order spherical harmonics \( (\rho L)^{(1)}_{n}, (\rho U)^{(1)}_{n} \) and \( (\Delta \rho L)^{(1)}_{n} \). The higher-order terms of these spherical harmonics (for \( k = 2, 3, ... \)) are applied in expressions for the gravimetric forward modeling of the Earth’s density structure. A discussion of this subject is postponed until Section 4.

We note that if the density structure is described down to the mass center of the Earth, i.e. \( \sum_{m=-n}^{n} Q(\rho L)_{n,m} Y_{n,m}(\Omega) = 0 \), the model in Eq. (9) reduces to:

\[
\sum_{q=1}^{Q} \left[ q_{q}(\rho U)_{n} - q_{q}(\rho L)_{n} \right] = \sum_{m=-n}^{n} (\rho U)_{n,m} Y_{n,m}(\Omega) + \sum_{q=1}^{Q-1} \sum_{m=-n}^{n} q_{+1,q}(\Delta \rho L)_{n,m} Y_{n,m}(\Omega).
\]

(9a)

3. 3-D Earth’s density model

The definitions given in Section 2 are extended here for a more generalized description of the Earth’s density structure by means of a 3-D density distribution function defined for each volumetric mass layer and respective density contrast interfaces. These generalized descriptions are then applied in deriving the 3-D Earth’s density model.

3.1. 3-D density layers

Here we approximated the actual density within an arbitrary volumetric mass layer by a laterally-distributed radial density variation model using the following polynomial function (for each lateral column):
\[ \rho_q(r, \Omega) \cong \rho_q(U_q, \Omega) + q^{\beta}(\Omega) \sum_{i=1}^{I_q} q^{\alpha_i}(\Omega) \left( r - R \right)^i \]  

for \( R + U_q(\Omega) \geq r > R + L_q(\Omega) \quad q = 1, 2, ..., Q \),

where \( \rho_q(U_q, \Omega) \) defines again (see Eq. 1) a nominal value of the lateral density stipulated at an upper bound \( U_q \) and a location \( \Omega \). The radial density change with respect to this nominal density \( \rho_q(U_q, \Omega) \) is described by the parameters \( q^{\beta} \) and \( \{ q^{\alpha_i} : i = 1, 2, ..., I_q \} \), where \( I_q \) is a maximum order of the radial-density function used to describe a radial density change within a particular volumetric mass layer \( q \). Note that the radial density change within each volumetric mass layer is generally described to a different order of \( I_q \). The linear density change, for instance, requires radial-density terms up to the first order while higher-order terms take into consideration also non-linear changes in radial density distribution.

### 3.2. Spherical 3-D density and density-contrast functions

For the 3-D density distribution model in Eq. (10) the spherical lower- and upper-bound density functions and their higher-order terms \( q(\rho L)_{n}^{k+i}, q(\rho U)_{n}^{k+i}: k = 1, 2, ..., i = 0, 1, ..., I_q; q = 1, 2, ..., Q \) in Eqs. (3) and (4) are further modified into the following form (Tenzer et al., 2012a):

\[
q(\rho L)_{n}^{(k+i)} = \begin{cases} 
\frac{2n + 1}{4\pi} \int_{\phi} \int_{\Omega'} \rho_q(U_q, \Omega') L_q^{k}(\Omega') P_n(\cos \psi) \, d\Omega' = \\
= \sum_{m=-n}^{n} q(\rho L)_{n,m}^{(k+i)} Y_{n,m}(\Omega) & i = 0 \\
\frac{2n + 1}{4\pi} \int_{\phi} \int_{\Omega'} q^{\beta}(\Omega') q^{\alpha_i}(\Omega') L_q^{k+i}(\Omega') P_n(\cos \psi) \, d\Omega' = \\
= \sum_{m=-n}^{n} q(\rho L)_{n,m}^{(k+i)} Y_{n,m}(\Omega) & i = 1, 2, ..., I_q
\end{cases}
\] (11)

and
From Eqs. (11) and (12), the respective spherical density-contrast functions and their higher-order terms \( \{ q^{(k+i)}(\Delta \rho L)_n \} \) are found to be:

\[
q^{(k+i)}(\Delta \rho L)_n = \sum_{m=-n}^{n} q^{(k)}(\rho U)_{n,m}(\Omega) \quad i = 0 \\
= \sum_{m=-n}^{n} q^{(k+i)}(\rho U)_{n,m}(\Omega) \quad i = 1, 2, ..., I_q.
\]

(12)

For \( i = 0 \), the coefficients \( \{ q^{(k+i)}(\Delta \rho L)_n \} \) are computed according to Eq. (6). The radial density change of two successive volumetric mass layers is then described by the parameters \( \Delta \beta \) and \( \{ \Delta \alpha_i : i = 1, 2, ..., I_q \} \) in Eq. (13) as follows:

\[
\begin{align*}
\Phi_n \int_{\Omega'} q^{(k+i)}(\rho U) (\Omega') P_n(\cos \psi) \, d\Omega' = \\
&= \sum_{m=-n}^{n} q^{(k+i)}(\Delta \rho L)_{n,m}(\Omega) \quad i = 0 \\
&= \sum_{m=-n}^{n} q^{(k+i)}(\Delta \rho L)_{n,m}(\Omega) \quad i = 1, 2, ..., I_q.
\end{align*}
\]

(13)
\[ q_{+1,q} \Delta \beta (\Omega') = q_{+1, \beta} (\Omega) - q \beta (\Omega') \quad q = 1, 2, ..., Q - 1, \quad (14) \]

and

\[ q_{+1,q} \Delta \alpha_i (\Omega') = q_{+1, \Delta \alpha_i} (\Omega) - q \Delta \alpha_i (\Omega') \quad i = 1, 2, ..., I_q; \quad q = 1, 2, ..., Q - 1. \quad (15) \]

The spherical density-contrast functions in Eq. (13) are defined by means of comparing respective spherical density functions of two successive volumetric mass layers. Since it is assumed that these layers have radially-changing densities, this definition does not refer to a density contrast directly at the interface between these two layers, but it describes the radial density changes through two successive layers. We could also define the density contrast directly at the interface. The spherical density-contrast functions then comprise a radial density change within the overlying layer \( q \) while an additional term is applied to describe a radial density change within the underlying layer \( q+1 \). In this case, the density contrast at the interface is defined as:

\[ \Delta \rho_{q+1,q} (L_q, \Omega) = \rho_{q+1} (U_{q+1}, \Omega) - \rho_q (U_q, \Omega) - q \beta (\Omega) \sum_{i=1}^{I_q} q \alpha_i (\Omega) (r - R)^i \quad q = 1, 2, ..., Q - 1. \quad (16) \]

Alternatively, we can also treat the lateral and radial density changes separately. The density contrast at the interface is then defined according to Eq. (2) by taking into account lateral density variations while radial density changes within the overlying and underlying layers \( q \) and \( q + 1 \) are defined individually by the radial-density terms \( \delta \rho_q \) and \( \delta \rho_{q+1} \). The radial density terms \( \{ \delta \rho_q : q = 1, 2, ..., Q \} \) read:

\[ \delta \rho_q = q \beta (\Omega) \sum_{i=1}^{I_q} q \alpha_i (\Omega) (r - R)^i \quad q = 1, 2, ..., Q. \quad (17) \]

The spherical density-contrast functions (in Eq. 13) then become:

\[ q_{+1,q} (\Delta \rho L)_n^{(k+i)} = q_{+1,q} (\Delta \rho L)_n^{(k)} + q_{+1} \delta \rho_n^{(k+i)} - q \delta \rho_{qn}^{(k+i)}, \quad (18) \]

where the coefficients \( q_{+1,q} (\Delta \rho L)_n^{(k)} \) read:
\[ q+1,q \left( \Delta \rho L \right)^{(k)}_{n} = \frac{2n+1}{4\pi} \int_{\Phi} q+1,q \Delta \rho \left( L_{q}^{i}, \Omega \right) L_{q}^{i} \left( \Omega \right) P_{n} \left( \cos \psi \right) \, d\Omega' = \]
\[ = \sum_{m=-n}^{n} q+1,q \left( \Delta \rho L \right)^{(k)}_{n,m} Y_{n,m} \left( \Omega \right). \]  

As seen in Eqs. (5) and (19), these definitions are identical.

The spherical radial-density functions of two successive volumetric mass layers \( q \) and \( q + 1 \) in Eq. (18) are given by:

\[ q \delta \rho^{(k+i)}_{n} = \frac{2n+1}{4\pi} \int_{\Phi} q \beta \left( \Omega' \right) q \alpha_{i} \left( \Omega' \right) L_{q}^{k+i} \left( \Omega' \right) P_{n} \left( \cos \psi \right) \, d\Omega' = \]
\[ = \sum_{m=-n}^{n} q \delta \rho^{(k+i)}_{n,m} Y_{n,m} \left( \Omega \right) \quad i = 1, 2, ..., I_{q}, \]  

and

\[ q+1 \delta \rho^{(k+i)}_{n} = \frac{2n+1}{4\pi} \int_{\Phi} q+1 \beta \left( \Omega' \right) q+1 \alpha_{i} \left( \Omega' \right) L_{q}^{k+i} \left( \Omega' \right) P_{n} \left( \cos \psi \right) \, d\Omega' = \]
\[ = \sum_{m=-n}^{n} q+1 \delta \rho^{(k+i)}_{n,m} Y_{n,m} \left( \Omega \right) \quad i = 1, 2, ..., I_{q+1}. \]  

### 3.3. 3-D Earth’s density structure

We now apply the spherical density functions defined in Eqs. (11) and (12) to describe the 3-D Earth’s density structure. Hence:

\[ \sum_{q=1}^{Q} \left[ q \left( \rho U \right)^{(i)}_{n} - q \left( \rho L \right)^{(i)}_{n} \right] = \]
\[ = \sum_{q=1}^{Q} \left[ q \left( \rho U \right)_{n} - q \left( \rho L \right)_{n} \right] + \sum_{q=1}^{Q} \sum_{i=1}^{I_{q}} \left[ q \left( \rho U \right)^{(i)}_{n} - q \left( \rho L \right)^{(i)}_{n} \right] = \]
\[ = \frac{2n+1}{4\pi} \sum_{q=1}^{Q} \int_{\Phi} \rho_{q} \left( U_{q}, \Omega' \right) U_{q} \left( \Omega' \right) P_{n} \left( \cos \psi \right) \, d\Omega' - \]

78
We further rearrange the 3-D Earth’s density model in Eq. (22) into a form which utilizes the spherical density-contrast functions (Eq. 19) and the spherical radial-density functions (Eqs. 20 and 21). We then write:

\[
\sum_{q=1}^{Q} \left[ q (\rho U)_{n}^{(i)} - q (\rho L)_{n}^{(i)} \right] =
\]  

\[
= \frac{2n+1}{4\pi} \int_{\Phi} q \rho (U_{q}, \Omega') L_{q}(\Omega') P_{n}(\cos \psi) \, d\Omega' + 
\]

\[
+ \frac{2n+1}{4\pi} \sum_{q=1}^{I_{q}} \sum_{i=1}^{l_{q}} \int_{\Phi} q \beta (\Omega') q \alpha_{i}(\Omega') U_{q}^{i}(\Omega') P_{n}(\cos \psi) \, d\Omega' - 
\]

\[
- \frac{2n+1}{4\pi} \sum_{q=1}^{I_{q}} \sum_{i=1}^{l_{q}} \int_{\Phi} q \beta (\Omega') q \alpha_{i}(\Omega') L_{q}^{i}(\Omega') P_{n}(\cos \psi) \, d\Omega'. 
\]

(22)

We further rearrange the 3-D Earth’s density model in Eq. (22) into a form which utilizes the spherical density-contrast functions (Eq. 19) and the spherical radial-density functions (Eqs. 20 and 21). We then write:

\[
\sum_{q=1}^{Q} \left[ q (\rho U)_{n}^{(i)} - q (\rho L)_{n}^{(i)} \right] =
\]  

\[
= \frac{2n+1}{4\pi} \int_{\Phi} q \rho (U_{q}, \Omega') U_{1}^{(i)}(\Omega') P_{n}(\cos \psi) \, d\Omega' + 
\]

\[
+ \frac{2n+1}{4\pi} \sum_{i=1}^{l_{1}} \int_{\Phi} q \beta (\Omega') q \alpha_{1}(\Omega') U_{1}^{1}(\Omega') P_{n}(\cos \psi) \, d\Omega' + 
\]

\[
+ \frac{2n+1}{4\pi} \sum_{q=1}^{Q-1} \int_{\Phi} q+1 \rho \Delta \rho (L_{q}, \Omega') L_{q}(\Omega') P_{n}(\cos \psi) \, d\Omega' + 
\]

\[
+ \frac{2n+1}{4\pi} \sum_{q=1}^{Q-1} \int_{\Phi} q+1 \rho \Delta \rho (L_{q}, \Omega') L_{q}(\Omega') P_{n}(\cos \psi) \, d\Omega' - 
\]

\[
- \frac{2n+1}{4\pi} \sum_{q=1}^{I_{q}} \sum_{i=1}^{l_{q}} \int_{\Phi} q \beta (\Omega') q \alpha_{i}(\Omega') L_{q}^{i}(\Omega') P_{n}(\cos \psi) \, d\Omega' - 
\]

\[
- \frac{2n+1}{4\pi} \sum_{q=1}^{I_{q}} \sum_{i=1}^{l_{q}} \int_{\Phi} q \beta (\Omega') q \alpha_{i}(\Omega') L_{q}^{i}(\Omega') P_{n}(\cos \psi) \, d\Omega' - 
\]

\[
- \frac{2n+1}{4\pi} \int_{\Phi} q \rho (U_{Q}, \Omega') L_{Q}(\Omega') P_{n}(\cos \psi) \, d\Omega' - 
\]

\[
- \frac{2n+1}{4\pi} \int_{\Phi} q \rho (U_{Q}, \Omega') L_{Q}(\Omega') P_{n}(\cos \psi) \, d\Omega'. 
\]

(23)
Substituting from Eqs. (19–21) to Eq. (22), we arrive at:

\[
\sum_{q=1}^{Q} \left[ q(\rho U)_{n}^{(i)} - q(\rho L)_{n}^{(i)} \right] = \sum_{i=0}^{I_{1}} \sum_{m=-n}^{n} (\rho U)_{n,m}^{(i)} Y_{n,m}(\Omega) - \\
- \sum_{i=0}^{I_{Q}} \sum_{m=-n}^{n} q(\rho L)_{n,m}^{(i)} Y_{n,m}(\Omega) + \sum_{q=1}^{Q-1} \sum_{m=-n}^{n} \sum_{q+1,q}(\Delta \rho L)_{n,m} Y_{n,m}(\Omega) + \\
+ \sum_{q=1}^{Q-1} \sum_{i=1}^{I_{q}} \sum_{m=-n}^{n} \left( q+1 \delta \rho_{n,m}^{(i)} - q \delta \rho_{n,m}^{(i)} \right) Y_{n,m}(\Omega). \tag{24}
\]

The 3-D Earth’s density model in Eq. (24) is described in terms of the upper-bound density coefficients \( (\rho U)_{n,m}^{(i)} \) of the first volumetric layer \( q = 1 \), the lower-bound density coefficients \( (\rho L)_{n,m}^{(i)} \) of the last volumetric layer \( q = Q \), the density-contrast coefficients \( (\Delta \rho L)_{n,m}^{(i)} \) and the differences of the radial-density coefficients \( (\Delta \rho)_{n,m}^{(i)} \) of two successive volumetric mass layers \( q + 1 \) and \( q \).

If we disregard radial density changes, the expressions in Eq. (24) and (9) become identical. Moreover, considering only a uniform density distribution within each volumetric mass layer, the Earth’s density model in Eq. (9) is further simplified to a following form:

\[
\sum_{q=1}^{Q} \left[ q(\rho U) - q(\rho L) \right] = \rho_{1} \sum_{m=-n}^{n} U_{n,m} Y_{n,m}(\Omega) - \\
- \rho_{Q} \sum_{m=-n}^{n} L_{n,m} Y_{n,m}(\Omega) + \sum_{q=1}^{Q-1} \sum_{m=-n}^{n} \sum_{q+1,q} \Delta \rho L_{n,m} Y_{n,m}(\Omega), \tag{25}
\]

where \( \{ \rho_{q} : q = 1, 2, ..., Q \} \) are the constant density values of volumetric mass layers, and \( \{ q+1,q \Delta \rho = \rho_{q+1} - \rho_{q} : q = 1, 2, ..., Q - 1 \} \) are the constant values of respective density contrasts. The spherical upper- and lower-bound functions \( q U_{n} \) and \( q L_{n} \) in Eq. (25) comprise only the geometric information. Hence, we have:

\[
q U_{n} = \frac{2n+1}{4\pi} \int_{\Phi} U_{q}(\Omega') P_{n}(\cos \psi) \ d\Omega' = \sum_{m=-n}^{n} q U_{n,m} Y_{n,m}(\Omega), \tag{26}
\]
and
\[ qL_n = \frac{2n+1}{4\pi} \int_{\Phi} L_q(\Omega') P_n(\cos \psi') \, d\Omega' = \sum_{m=-n}^{n} qL_{n,m}Y_{n,m}(\Omega). \tag{27} \]

Furthermore, for a uniform density of a spherically symmetric layers (such as PREM), we obtain the 1-D Earth’s density model in the following simple form:
\[ \sum_{q=1}^{Q} [q(\rho U)_n - q(\rho L)_n] = \rho_1 U_1 - \rho_1 L_1 + \sum_{q=1}^{Q-1} \rho \Delta L_q, \tag{28} \]
where \( \{U_q = \text{const}, \quad L_q = \text{const} : q = 1, 2, ..., Q\} \) are constant values of the upper and lower bounds. For the density model of the whole Earth, \( L_1 = 0 \).

4. Applications in gravimetric forward modeling

The coefficients \( \{q(\rho L)_{n,m}^{(k+i)}, q(\rho U)_{n,m}^{(k+i)} : k = 1, 2, ..., i = 0, 1, ..., I_q; q = 1, 2, ..., Q\} \) defined in Eq. (11) and (12) can be applied in the gravimetric forward modeling. According to the method developed by Tenzer et al. (2012a, 2012b) the gravitational potential \( V \) and attraction \( g \approx -\partial V/\partial r \) at a point \( (r, \Omega) \), for \( r \geq R \), are computed using the following expressions:
\[ V(r, \Omega) = \frac{GM}{R} \sum_{q=1}^{Q} \sum_{n=0}^{\bar{n}} \left( \frac{R}{r} \right)^{n+1} \sum_{m=-n}^{n} qV_{n,m}Y_{n,m}(\Omega), \tag{29} \]
and
\[ g(r, \Omega) = \frac{GM}{R^2} \sum_{q=1}^{Q} \sum_{n=0}^{\bar{n}} \left( \frac{R}{r} \right)^{n+2} (n+1) \sum_{m=-n}^{n} qV_{n,m}Y_{n,m}(\Omega), \tag{30} \]
where \( \bar{\rho}^{\text{Earth}} = 5500 \, \text{kg m}^{-3} \) is the Earth’s mean density, \( \bar{n} \) is a maximum degree of spherical harmonics, and the potential coefficients \( \{qV_{n,m} : q = 1, 2, ..., Q\} \) read:
\[
q V_{n,m} = \frac{3}{2n + 1} \frac{1}{\bar{\rho}_{\text{Earth}}} \sum_{i=0}^{I_q} \left( qF_{n,m}^{(i)} - qF_{n,m}^{(i)} \right). 
\]  

(31)

The numerical coefficients \( \{ qF_{n,m}^{(i)} : i = 0, 1, ..., I_q; q = 1, 2, ..., Q \} \) in Eq. (31) are given by:

\[
qF_{n,m}^{(i)} = \sum_{k=1}^{n+2} \frac{(n + 2)}{(k - 1)} (-1)^{k-1} \frac{q(\rho U)^{(k+i)}}{R^k}, 
\]

(32)

and

\[
qF_{n,m}^{(i)} = \sum_{k=1}^{n+2} \frac{(n + 2)}{(k - 1)} (-1)^{k-1} \frac{q(\rho L)^{(k+i)}}{R^k}, 
\]

(33)

As seen in Eqs. (29–33), the gravitational field quantities are computed from the spherical density coefficients \( q(\rho U)^{(k+i)} \) and \( q(\rho L)^{(k+i)} \) of volumetric mass layers. Alternatively, this computation can be done using the spherical density-contrast coefficients. With reference to a conversion between the spherical density and density-contrast functions in Eq. (24), the expression for computing the gravitational potential in Eq. (29) is introduced in the following form:

\[
V(r, \Omega) = \frac{GM}{R^2} \sum_{n=0}^{\bar{n}} \left( \frac{R}{r} \right)^{n+1} \sum_{m=-n}^{n} \left[ \hat{1}_V^{\rho U} - Q V^{\rho L} + \hat{Q} V^{\rho L} \right] Y_{n,m}(\Omega). 
\]

(34)

Similarly, the gravitational attraction in Eq. (30) becomes:

\[
g(r, \Omega) = \frac{GM}{R^2} \sum_{n=0}^{\bar{n}} \left( \frac{R}{r} \right)^{n+2} \left( n + 1 \right) \sum_{m=-n}^{n} \left[ \hat{1}_V^{\rho U} - Q V^{\rho L} + \hat{Q} V^{\rho L} \right] Y_{n,m}(\Omega). 
\]

(35)

The potential coefficients \( \hat{1}_V^{\rho U}, Q V^{\rho L} \) and \( \{ q+1,q V^{\rho L} : q = 1, 2, ..., Q - 1 \} \) in Eqs. (34) and (35) are defined by:
\[ V_{n,m}^{\rho U} = \frac{3}{2n + 1} \rho_{\text{Earth}} \sum_{i=0}^{l_1} \frac{1}{\rho_{\text{Earth}}} \sum_{i=0}^{l_2} Q F l_{n,m}^{(i)} \]  

\[ Q V_{n,m}^{\rho L} = \frac{3}{2n + 1} \rho_{\text{Earth}} \sum_{i=0}^{l_2} Q F l_{n,m}^{(i)} \]  

\[ q+1,q V_{n,m}^{\Delta \rho L} = \frac{3}{2n + 1} \rho_{\text{Earth}} \sum_{i=0}^{l_2} q+1,q F \Delta \rho l_{n,m}^{(i)} \]  

and

\[ q+1,q V_{n,m}^{\delta \rho} = \frac{3}{2n + 1} \rho_{\text{Earth}} \sum_{i=0}^{l_2} (q+1,q F \delta \rho l_{n,m}^{(i)} - q F \delta \rho l_{n,m}^{(i)}) \]  

The coefficients \( F u_{n,m}^{(i)} \) (for \( q = 1 \)) and \( F l_{n,m}^{(i)} \) (for \( q = Q \)) are computed according to the expression given in Eqs. (32) and (33). The coefficients \( \{q+1,q F \Delta \rho l_{n,m}^{(i)} : q = 1, 2, ..., Q - 1\} \) in Eq. (38) are given by:

\[ q+1,q F \Delta \rho l_{n,m}^{(i)} = \sum_{k=1}^{n+2} \frac{n+2}{k} \frac{(-1)^{k-1}}{k} q+1,q (\Delta \rho L)^{(k)}_{n,m} R^k. \]  

Finally, the coefficients \( \{q F \delta \rho l_{n,m}^{(i)} : q = 1, 2, ..., Q - 1\} \) are generated using the following expression:

\[ q F \delta \rho l_{n,m}^{(i)} = \sum_{k=1}^{n+2} \frac{n+2}{k} \frac{(-1)^{k-1}}{k} q F \delta \rho l_{n,m}^{(k+i)} R^k. \]  

5. Discussion

The expressions for the gravimetric forward modeling presented in Eqs. (34–41) utilize for types of the spherical coefficients. The coefficients \( F u_{n,m}^{(i)} \) and \( F l_{n,m}^{(i)} \) define the density distribution at the uppermost and lowermost surfaces which enclose the whole volumetric body for which the gravitational effect is evaluated. If the inner structure does not comprise any density contrasts or changes in radial density distribution, these two...
types of coefficients uniquely describe the density within whole investigated volumetric mass body similarly to that used for a particular volumetric mass layer. For more complex density structures, consisting of volumetric mass layers with a lateral density distribution, the gravitational effect is evaluated from the expressions which include also the coefficients \(\{q+1, q F \Delta \rho l_{n,m} : q = 1, 2, ..., Q - 1\}\) (see Eq. 40). These coefficients define the lateral density contrasts of all interfaces within the investigated volumetric mass body. In the most generalized case, the complex density structures are described by 3-D density models of volumetric mass layers. The gravitational effect is then computed using the expressions which comprise also the radial-density coefficients \(\{q F\delta \rho^{(i)}_{n,m} : q = 1, 2, ..., Q - 1\}\) (see Eq. 41). These coefficients describe radial density changes within every individual volumetric mass layers. Obviously, depending on the density structure approximated by a particular volumetric mass layer the density parameters of these layers might differ significantly.

To give particular examples, we assume that the Earth’s structure is divided into several layers which closely resemble major geological structures. This is particularly illustrative for the upper lithosphere structure. As mentioned before, the gravitational effect of atmosphere is typically neglected in geophysical studies while it might be considered in more accurate geodetic applications for the gravimetric geoid determination. In this case, the density distribution of the atmosphere can be defined using the standard model of the static atmosphere (ISO 2533:1975). Several different atmospheric density models were developed and applied in the gravimetric forward modeling. Among them we can mention studies by Sjöberg (1993, 1998, 2006), Sjöberg and Nahavandchi (1999, 2000), Nahavandchi (2004), Novák and Grafarend (2006) and Tenzer et al. (2006, 2009b).

The Earth’s crustal structure is typically divided into density components of polar ice sheets including mountain glaciers, continental water bodies (lakes), ocean seawater, marine and continental sediments and bedrock (i.e., the consolidated crystalline crust). These density structures have very distinctive density distributions which can be represented by specific density models. Moreover, density interfaces between these crustal structures are typically well pronounced and represent maxima of density contrasts, particularly between ice (and lakes) and underlying sediments or bedrock layers. The fresh water can be very accurately approximated by a uniform
density model. Similarly also the ice density can accurately be approximated by a constant density of the consolidated glacial ice of 917 kg m\(^{-3}\) \cite{Cutnell1995}, because the layers of snow and firn ice are much thinner \cite{van2008}. The actual seawater density distribution can be approximated by a depth-dependent density model \cite{Tenzer2012b}. This empirical density model was developed by \textit{Gladkikh and Tenzer} \cite{Gladkikh2011} based on the analysis of oceanographic data of the World Ocean Atlas 2009 \cite{Johnson2009} and the World Ocean Circulation Experiment 2004 \cite{Gouretski2004}.

Similarly, the increasing sediment density with depth due to compaction and further lithification could be described by applying a depth-dependent density model. \textit{Artemjev et al.} \cite{Artemjev1994}, for instance, applied a depth-dependent sediment density model in the gravimetric study of the sub-crustal density inhomogeneities of the Northern Eurasia. They used several different depth-dependent density models for approximating the sediment structure of major continental sedimentary basins in the Northern Eurasia obtained based on the published results of drilling and seismic studies. \textit{Hamilton} \cite{Hamilton1976} investigated how the density and porosity of deep-sea sediments vary with depth and established the depth-dependent density models of four types of sediments, namely calcareous and siliceous oozes, pelagic clay and terrigenous sediments. \textit{Cowie and Karner} \cite{Cowie1990} established an exponential function of porosity to describe the depth-dependent density change due to compaction based on the analysis of the regional sediment data from the North Sea and the Rhine Graben. \textit{Tenzer and Gladkikh} \cite{Tenzer2014} derived the 3-D density model of marine sediments (as a function of ocean and sediment depths) based on the analysis of global samples of marine sediments recorded in the NOAA’s National Geophysical Data Center (NGDC). These records were prepared from core data collected during the Deep Sea Drilling Project.

Large density variations and complex geological structures of the Earth’s lithosphere were confirmed from drilling profiles and seismic studies. The most pronounced feature is the difference between typically heavier oceanic lithosphere compared to continental crustal structures. The average density of 2670 kg m\(^{-3}\) is typically attributed to the upper continental crust in geological and gravity surveys, geophysical explorations, gravimetric geoid modeling, compilation of regional gravity maps, and other applications. Al-
though this density value is widely used, its origin remains unclear. *Woollard (1966)* suggested that this density was used for the first time by *Hayford and Bowie (1912)*. In reviewing several studies seeking a representative mean density from various rock type formations, *Hinze (2003)* argued that this value was used earlier by *Hayford (1909)* for the gravity reduction. *Hayford (1909)* referred to *Harkness (1891)* who averaged five published values of surface rock density. The value of *Harkness (1891)* of 2670 kg m\(^{-3}\) was confirmed later, for instance, by *Gibb (1968)* who estimated the mean density of the surface rocks in a significant portion of the Canadian Precambrian shield from over 2000 individual measurements. *Woollard (1962)* examined more than 1000 rock samples and estimated that the mean basement (crystalline) rock density is about 2740 kg m\(^{-3}\). *Subrahmanyam and Verma (1981)* determined that crystalline rocks in low-grade metamorphic terranes in India have the mean density of 2750 kg m\(^{-3}\), while 2850 kg m\(^{-3}\) in high-grade metamorphic terranes.

The oceanic lithosphere density is mainly controlled by thermal cooling due to mantle convection. The formation process of the oceanic lithosphere at the mid-ocean ridges, further spreading and subduction underneath the oceanic or continental lithosphere along the oceanic subduction zones is directly linked with the thickness and density changes of the oceanic lithosphere. The conductive cooling, which converts hot asthenosphere into lithospheric mantle at the mid-ocean ridges, causes the oceanic lithosphere to become increasingly thick and dense with age. At the early stage up to a few tens of millions of years the oceanic lithosphere is less dense than the asthenosphere. Its density then increases causing its subduction and re-assimilation into the asthenosphere. The ocean-floor spreading hypothesis was proposed by *Hess (1962)* and its mechanism was explained later by the mantle convection theory of *Walter (1971)*. The currently most complete data of the oceanic lithosphere age were derived from marine magnetic surveys (e.g. *Müller et al., 2008*). The principle of dating the ocean lithosphere is based on the comparison of marine magnetic anomalies with the events of magnetic reversals measured on land (e.g. *Vine and Matthews, 1963*). These data show that the oldest ocean floor is about 180 Myr (corresponding the late Jurassic geological period), while parts of the continental lithosphere are billions of years old. These data were validated using the age dating of ocean-floor rock samples.
The current knowledge of the density distribution within the asthenosphere, including the core-mantle boundary zone, is still very limited due to the fact that there is no direct link between the seismic velocity and density while gravimetric inversion solutions applied for a recovery of density structures are non-unique (i.e. infinitely many density configurations can be attributed to the observed gravity field). In practical applications, therefore, the density structure within the whole mantle and core is typically approximated by using only a spherically-symmetric density model such as PREM (Dziewonski and Anderson, 1981). Note that despite Simmons et al. (2010) derived a 3-D density structure within the whole mantle, these data were not yet released publically. Alternatively, in gravimetric methods the deep mantle density heterogeneities are often treated by means of subtracting the long-wavelength part of the gravitational spectrum.

6. Summary and concluding remarks

Two types of models describing the Earth’s density structure were developed and presented. Dividing the Earth’s interior into particular volumetric mass layers, the actual density distribution within each individual layer was approximated by the laterally-distributed radial density variation model. In the spectral domain, this density distribution was defined in terms of the spherical density functions of the upper- and lower-bounds of volumetric mass layer. An alternative description of the Earth’s density model was then given by means of the density contrast interfaces. In this case, the spherical density-contrast functions were applied to define the lateral density contrast between two successive layers while additional radial-density terms were applied to define the radial density changes within these layers. The Earth’s density structure is then described by sets of coefficients for each volumetric mass layer or density interface. These coefficients are generated from discrete data by applying methods for a spherical harmonic analysis of the Earth’s density structure.

The expressions for gravimetric forward modeling of the Earth’s density structures were further derived in terms of the spherical density and density-contrast coefficients. These coefficients can be used to evaluate the gravitational effect of a particular mass density structure within the Earth’s
interior based on applying the spherical harmonic synthesis (e.g. Tsoulis 2004a, 2004b; Tenzer et al. 2009, 2012a, 2012b, and reference herein). The expressions for the spherical harmonic synthesis derived in this study are fully compatible with the spectral representation of the Earth’s gravity models by means of Stokes’ coefficients (cf. Heiskanen and Moritz, 1967).

The description of the Earth’s inner density structure in terms of the spherical density coefficients is typically used for computing the global gravity corrections due to known density structures. One example can be given by the computation of the refined Bouguer gravity anomalies/disturbances. In this case, the topographic coefficients are used to evaluate the topographic correction. The description of the Earth’s density structure in terms of the spherical density-contrast coefficients is, on the other hand, more convenient in using inverse methods for a gravimetric interpretation of density contrast interfaces. Such methods are used, for instance, in predicting the ocean-floor topography from satellite-altimetry measurements. Since large parts of marine areas have not yet been covered by sounding reflection surveys (i.e. the multi-beam echo sounders), marine gravity data are primarily used to determine bathymetric depths. Another possible application is a mapping of the sediment basement topography using gravity observations, because seismic data are often absent.

References


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90


