OPTIMAL TOPOGRAPHIC - ISOSTATIC CRUST MODELS FOR GLOBAL GEOPOTENTIAL INTERPRETATION

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Abstract

The topographic-isostatic potential of the earth's crust can be computed easily using average crustal density parameters, a global isostatic model and a numerical dataset of mean continental and oceanic heights. In lack of the detailed data for density, crustal thickness and isostatic compensation, a least squares estimation is suggested to determine global horizontal variation of crustal parameters.

These variations can be determined using a minimum principle to yield a minimum variance high frequency residual geoid. The basic mathematical tool for the determination of such parameter variation functions is the Clebsch-Gordan product-sum conversion formula of spherical harmonics.

Computer programs were developed based on the above mentioned mathematical algorithm to determine optimal linear topographic-isostatic crust models (OLTM). Previous calculations detected significant global density variations inside the crust with respect to the simple Airy model of uniform crustal parameters. The result would perhaps show us a better insight into the global isostatic behaviour of the crust.

Keywords: topographic-isostatic model, lateral density variations, spherical harmonics, isostasy of the earth's crust.

1. Introduction

The behaviour of our earth's crust on a global scale is rather difficult to model. The gravitational potential caused by mass irregularities inside the crust can only be predicted using various crustal density models. On the other side the gravitational potential of the earth's crust is included in the total gravity potential, which is well-measured on a global scale.

The disturbing potential due to the density irregularities inside the earth's crust is termed shortly *topographic-isostatic* potential. It can only be evaluated through certain global topographic-isostatic models.

The importance of such models is at least twofold.

1) They can be used to reduce measured gravity signal so as to make residual gravity field as smooth as possible for *prediction* purposes.

2) Such models allow us to *remove the disturbing effect of the crust* and they produce a clearer overall insight into the effect of deeper mass irregularities.

The conventional simple Airy-Heiskanen isostatic model was first investigated RUMMEL et. al. (1988) developed a very efficient *FFT-based (Fast Fourier Transform)* - technique for the computation of this model's topographic-isostatic potential. In the first part of this report their method will be described and the results of our calculations with this model will be presented.

In the second part of this report the detailed study of so-called optimal linear *topographic-isostatic models (OLTM)* will follow. In these models a minimum criterion is

introduced to determine a topographic-isostatic model. This model physically is an optimum Airy-type model with *lateral variations* in density, crust thickness and isostasy. It gives the best possible agreement between topographic-isostatic potential and the earth's disturbing potential. Finally, some *results* and *conclusions* will be considered for simple and optimal Airy-type topographic-isostatic models.

2. Airy Topographic-Isostatic Model

The Airy model supposes that the light crust matter of density ρ_{cr} floats on the more heavy material of the upper mantle of density ρ_m. Each crust "column" is in an equilibrium state. This requires for ocean columns the anti-root thickness d^* for ocean depth h^*; and root thickness d for land elevations h to exist. *(Fig. 1).*
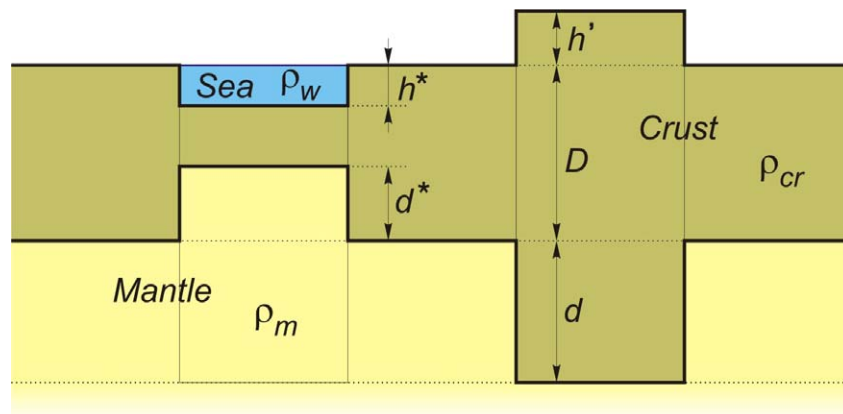

Fig. 1. Airy isostatic model

From the equilibrium equations

$$\text{root-thickness:} \quad d = \frac{\rho_{cr}}{\Delta\rho} h \, , \tag{1a}$$

$$\text{anti-root thickness:} \quad d^* = \frac{\rho_{cr} - \rho_w}{\Delta\rho} h^* \, , \tag{1b}$$

where $\Delta\rho = \rho_m - \rho_{cr}$ and ρ_w is the ocean water density.

If the factor

$$c_h = 1 \quad \text{if} \quad h > 0 \quad \text{and} \quad c_h = 1 - \frac{\rho_w}{\rho_{cr}} \quad \text{if} \quad h < 0$$

is introduced then the Eqs. (1a, 1b) can be unified in one equation

$$d = \frac{\rho_{cr}}{\Delta\rho} h = kh \tag{2}$$

where

$$h = c_h h' \ .$$

Here h is often termed as equivalent topographic height, and k is the compensation factor.

For a flat earth (i.e. plane approximation), the compensation factor k is constant and equal to

$$k = k_0 = \frac{\rho_{cr}}{\rho_m - \rho_{cr}} \ . \tag{3}$$

For a spherical earth k will be slightly modified and it can be computed from the mass balance principle of isostasy. It will become dependent on both h and D. (SÜNKEL, 1986):

$$\frac{kh'}{R - D} = \left\{ 1 - \left(1 - \frac{D}{R}\right)^{-3} k_0 c_h \left[\left(1 + \frac{h'}{R}\right)^3 - 1\right]\right\}^{\frac{1}{3}} \tag{4}$$

where R denotes mean earth radius (approximately 6371 km).

Even if this simple Airy model is not accepted as which reflects the real behaviour of the earth's crust, it will be quite useful to investigate it first as computationally simple and straightforward.

3. Spherical Harmonic Analysis of the Topographic-Isostatic Potential of the Simple Airy Model

The simple Airy topographic-isostatic potential, T^{Airy} is defined as the potential generated by mass irregularities with respect to an ideal homogeneous crust (with density ρ_{cr} and uniform thickness D lying on a homogeneous mantle with density σ_{cr}). If $\delta\rho$ denotes mass irregularities according to the Airy model the topographic-isostatic potential of the volume density distribution $\delta\rho$ will be

$$T^{Airy}(P) = G \iiint_V l^{-1}(P,Q) \delta\rho(Q) \, dv(Q) \, , \tag{5}$$

where   G   Newton's gravitational constant,
          $l(P, Q)$ spatial distance of P and Q,
          dv volume element.

$T^{Airy}(P)$ is harmonic outside a sphere and its spherical harmonic expansion is surely convergent outside the sphere enclosing total mass of the earth. Outside of this sphere the following series expansion is valid for l^{-1}:

$$l^{-1}(P,Q) = \sum_{n=0}^{\infty} \frac{r^n(Q)}{r^{n+1}(P)} P_n(\cos\psi_{PQ}) \tag{6}$$

where r magnitude of radius vector,

         ψ_{PQ} angular distance of P and Q,

         P_n Legendre polynomial of degree n.

If $\overline{U}_{nm}$, $\overline{V}_{nm}$ denote fully normalized spherical harmonics of degree n and order m, their definition is

$$\begin{Bmatrix} \overline{U}_{nm}(P) \\ \overline{V}_{nm}(P) \end{Bmatrix} = \sqrt{2^{1-\delta_{m0}}(2n+1)\frac{(n-m)!}{(n+m)!}} \, \overline{P}_{nm}(\cos\Theta_P) \begin{Bmatrix} \cos m\lambda_P \\ \sin m\lambda_P \end{Bmatrix} , \tag{7}$$

where Θ_P polar distance,

         λ_P longitude,

         δ_{ij} Kronecker's delta,

        $n = 0, 1, 2, ...; \quad m = 0, 1, ..., n.$

   In the above expression the $P_{nm}(t)$ associated Legendre functions of degree n and order m are defined by the following equation:

$$P_{nm}(t) = \frac{1}{2^n n!}(1-t^2)^{m/2} \frac{d^{n+m}}{dt^{n+m}}(t^2-1)^n . \tag{8}$$

The $P_n(\cos\psi_{PQ})$ function can be decomposed into the sum

$$P_n(\cos\psi_{PQ}) = \frac{1}{2n+1} \sum_{m=0}^{n} \left[\overline{U}_{nm}(P)\,\overline{U}_{nm}(Q) + \overline{V}_{nm}(P)\,\overline{V}_{nm}(Q) \right] . \tag{9}$$

Inserting the expression (9) into the integral (5) will yield the following 3D spherical harmonic representation of the topographic-isostatic potential of the Airy model:

$$T^{Airy}(P) = \frac{GM}{r_P} \sum_{n=1}^{\infty} \left(\frac{R}{r_P}\right)^n \sum_{m=0}^{n} \left(\overline{C}_{nm}^{Airy} \cos m\lambda_P + \overline{S}_{nm}^{Airy} \sin m\lambda_P \right) \overline{P}_{nm}(\cos\Theta_P) , \tag{10}$$

where M total mass of the earth,

         $\overline{P}$ normalized Legendre function, defined as

$$\overline{P}_{nm}(t) = \sqrt{2^{1-\delta_{m0}}(2n+1)\frac{(n-m)!}{(n+m)!}} \, P_{nm}(t) , \tag{11}$$

and $\overline{C}_{nm}^{Airy}$, $\overline{S}_{nm}^{Airy}$ are normalized spherical harmonic coefficients of the topographic-isostatic potential of the simple Airy model with uniform crustal parameters. The summation in Eq. (10) begins at $n = 1$ because there is no mass surplus or deficit in this compensation model.

4. Computation of the Spherical Harmonic Coefficients of the Simple Airy Topographic-Isostatic Potential

In the following discussion we summarize the formulae necessary for the computation. The detailed derivation and discussion of the above formulae can be found in the papers of SÜNKEL (1986) and RUMMEL et al. (1988).

Firstly we split up the topographic-isostatic potential into the following two parts:

$$T^{Airy} = T^{(t)} + T^{(c)} \quad,$$

where $T^{(t)}$ denotes disturbing potential of topographic and $T^{(c)}$ disturbing potential of isostatic masses. The spherical harmonic coefficients of $T^{(t)}$ are then

$$\begin{Bmatrix} \overline{C}_{nm}^{(t)} \\ \overline{S}_{nm}^{(t)} \end{Bmatrix} = \frac{3\rho_{cr}}{\overline{\rho}} \frac{1}{(2n+1)(n+3)} \frac{1}{4\pi} \iint_{\sigma} c_h \left[\left(1 + \frac{h_Q}{R}\right)^{n+3} - 1 \right] \begin{Bmatrix} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{Bmatrix} d\sigma(Q) \;, \qquad (12)$$

where $\quad \overline{\sigma} = \dfrac{3M}{4\pi R^3} \quad$ mean earth density $(5514\, kg\, m^{-3})$,

$\displaystyle \iint_{\sigma} .... d\sigma \qquad$ denotes integration over the unit sphere.

The spherical harmonic coefficients of $T^{(c)}$ for the simple Airy model will be expressed by the integral expression

$$\begin{Bmatrix} \overline{C}_{nm}^{(c)} \\ \overline{S}_{nm}^{(c)} \end{Bmatrix} = \frac{3\rho_{cr}}{\overline{\rho}} \frac{1}{(2n+1)(n+3)} \left(1 - \frac{D}{R}\right)^{n+3} k_0^{-1} \frac{1}{4\pi} \iint_{\sigma} c_h \left[\left(1 + \frac{kh}{R-D}\right)^{n+3} - 1 \right] \begin{Bmatrix} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{Bmatrix} d\sigma(Q) \;.$$

$$(13)$$

When a second order approximation is accepted for the computation of the spherical harmonic coefficients of T^{Airy},

$$\begin{Bmatrix} \overline{C}_{nm}^{Airy} \\ \overline{S}_{nm}^{Airy} \end{Bmatrix} = \begin{Bmatrix} \overline{C}_{nm}^{(t)} \\ \overline{S}_{nm}^{(t)} \end{Bmatrix} + \begin{Bmatrix} \overline{C}_{nm}^{(c)} \\ \overline{S}_{nm}^{(c)} \end{Bmatrix} \;, \qquad (14)$$

one gets the second order approximation formula for the computation of spherical harmonic coefficients of the simple Airy model's topographic-isostatic potential. The result is

$$\begin{Bmatrix} \overline{C}_{nm}^{Airy} \\ \overline{S}_{nm}^{Airy} \end{Bmatrix} = \frac{3}{2n+1} \frac{\rho_{cr}}{\overline{\rho}} \left[\begin{array}{l} \left[1 - \left(\dfrac{R-D}{R}\right)^n\right] \dfrac{1}{4\pi} \iint_{\sigma} \dfrac{h_Q}{R} \begin{Bmatrix} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{Bmatrix} d\sigma(Q) + \\[2em] \dfrac{n+2}{2} \left[1 - \dfrac{\rho_{cr}}{\Delta\rho}\left(\dfrac{R-D}{R}\right)^{n-3}\right] \dfrac{1}{4\pi} \iint_{\sigma} \left(\dfrac{h_Q}{R}\right)^2 \begin{Bmatrix} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{Bmatrix} d\sigma(Q) \end{array} \right] \;, \qquad (15)$$

5

The numerical FFT-based technique developed by COLOMBO (1981) is an extremely efficient tool for the fast computation of integrals of the type

$$\frac{1}{4\pi} \iint_{\sigma} f(Q)\, d\sigma(Q)$$

on the sphere. The expression (15) is well-suited for the application of O.Colombo's method, and its application to the computation of Airy topographic-isostatic potential is well established (see RUMMEL et al., 1988).

Let us introduce the following 2D (surface) spherical harmonic coefficients of the equivalent topography:

$$\left\{ \begin{array}{c} hc_{nm} \\ hs_{nm} \end{array} \right\} = \frac{1}{4\pi} \iint_{\sigma} \frac{h(Q)}{R} \left\{ \begin{array}{c} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{array} \right\} d\sigma(Q) \qquad (16a)$$

$$\left\{ \begin{array}{c} h2c_{nm} \\ h2s_{nm} \end{array} \right\} = \frac{1}{4\pi} \iint_{\sigma} \frac{h(Q)^2}{R} \left\{ \begin{array}{c} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{array} \right\} d\sigma(Q) \qquad (16b)$$

These integrals can be evaluated by the efficient FFT method and thus the coefficients (15) may be obtained by the following equation:

$$\left\{ \begin{array}{c} \overline{C}_{nm}^{Airy} \\ \overline{S}_{nm}^{Airy} \end{array} \right\} = \frac{3}{(2n+1)} \frac{\rho_{cr}}{\overline{\rho}} \left[\left[1 - \left(\frac{R-D}{R} \right)^n \right] \left\{ \begin{array}{c} hc_{nm} \\ hs_{nm} \end{array} \right\} + \frac{n+2}{2} \left[1 - \frac{\rho_{cr}}{\Delta\rho} \left(\frac{R-D}{R} \right)^{n-3} \right] \left\{ \begin{array}{c} h2c_{nm} \\ h2s_{nm} \end{array} \right\} \right]$$

$$n = 0, 1, \ldots \qquad m = 0, 1, \ldots, n \quad . \qquad (17)$$

Now the practical computation of the potential coefficients of isostatically reduced topographic potential of the simple Airy model is straightforward.

5. Computations with the Simple Airy Topographic-Isostatic Model

The computer programs HARMIN and SSYNTH listed in the report of COLOMBO (1981) were adapted to Microsoft FORTRAN and also the Mixed-Radix FFT algorithm of SINGLETON (1969). These programs were used to compute the hc_{nm}, hs_{nm}, $h2c_{nm}$, $h2s_{nm}$ coefficients from 1° x 1° mean topographic height dataset (64,800 mean height for the entire earth). This dataset was kindly provided by H.SÜNKEL on a magnetic tape to us in 1986. These 2D spherical harmonic coefficients in Eq. (16) were then used to determine the 3D spherical harmonic coefficients of topographic-isostatic potential complete up to degree and order 180. The topographic-isostatic geoid computed with the uniform $D = 30km$ crust thickness can be seen on *Fig. 2*.

The following statistical quantities were then computed to see the agreement between topographic-isostatic potential of the simple Airy model and the gravity potential represented by the RAPP (1981) model. If we define the differences of spherical harmonic coefficients

$\overline{C}_{nm}$, $\overline{S}_{nm}$ of the observed gravity potential and $\overline{C}_{nm}^{Airy}$, $\overline{S}_{nm}^{Airy}$ coefficients of the simple Airy model topographic-isostatic potential

$$\Delta C_{nm} = \overline{C}_{nm} - \overline{C}_{nm}^{Airy}$$
$$\Delta S_{nm} = \overline{S}_{nm} - \overline{S}_{nm}^{Airy}$$

(18a, b)

then the first statistical quantity one may define is the root mean square (rms) *undulation difference* δN between degrees n_1 and n_2:

$$\delta N = \left[R^2 \sum_{n=n_1}^{n_2} \sum_{m-0}^{n} (\Delta \overline{C}_{nm}^2 + \Delta \overline{S}_{nm}^2) \right]^{\frac{1}{2}} .$$

(19)

The next quantity is the *rms* anomaly difference between degrees n_1 and n_2:

$$\delta g = \left[\gamma^2 \sum_{n=n_1}^{n_2} (n-1)^2 \sum_{m-0}^{n} (\Delta \overline{C}_{nm}^2 + \Delta \overline{S}_{nm}^2) \right]^{\frac{1}{2}} .$$

(20)

Let us denote by $\sigma_n^2(T)$ the signal variance

$$\sigma_n^2(T) = \sum_{m-0}^{n} (\Delta \overline{C}_{nm}^2 + \Delta \overline{S}_{nm}^2)$$

(21)

of the observed gravity potential T, the correlation coefficient by degree, c_n is another measure of potential coefficient fit,

$$c_n = \frac{\sum_{m-0}^{n} (\overline{C}_{nm} \overline{C}_{nm}^{Airy} + \overline{S}_{nm} \overline{S}_{nm}^{Airy})}{\sigma_n(T) \sigma_n(T^{Airy})} .$$

(22)

Finally the average correlation coefficient between degrees n_1 and n_2 is

$$\overline{c} = \frac{1}{n_2 - n_1 + 1} \sum_{n=n_1}^{n_2} c_n$$

(23)

Table 1 shows the value of above statistical quantity for D = 30 km compensation depth.

The fit between the two potential coefficient sets is rather bad even in the higher degree range when the greater part of the gravity signal is expected to be yielded by the topographic-isostatic mass irregularities. This comparison clearly shows that this simple Airy model

cannot be expected to reflect the very behaviour of the earth's crust on a global scale, even if it is physically more tenable than the Pratt model.

We agree with the following conclusion of the authors of RUMMEL et al. (1988): `Since the isostatic behaviour of the earth is dependent on a number of factors, and considering that such behaviour varies substantially from area to area, global models cannot be expected to reflect the full picture.'

Even the simple Airy model depends on a number of factors, e. g. crust and mantle density, crust thickness, etc. which may vary from area to area, so it seems reasonable to allow the changes of these factors. This will lead us to the study of Airy type global isostatic models with *horizontally varying crustal parameters*.

6. Lateral Variations of Crustal Parameters

When the compensation is complete, the following approximation is valid for the topographic-isostatic potential (see SÜNKEL, 1986):

$$T^{Airy}(P) = 2\pi G D \rho_{cr} c_h h \tag{24}$$

This approximation can be derived from the Eqs. (10) and (17) by retaining only the linear term in h in the Eq. (17). Let us allow now the ρ_{cr}, D parameters to be horizontally variable, i. e.

$$\rho_{cr}(P) = \overline{\rho}_{cr} + \Delta\rho_{cr}(P) \tag{25}$$

$$D(P) = \overline{D} + \Delta D(P) \tag{26}$$

where $\overline{\rho}_{cr}$ average crust density (2670 $kg\ m^{-3}$),

$\overline{D}$ average crust thickness (e.g. 30 km),

then the ΔT^{Airy} potential change will be linearly dependent on $h(P)$:

$$\Delta T^{Airy}(P) = 2\pi G \left[\Delta\rho_{cr}(P) + \Delta D(P)\right] c_h\ h(P). \tag{27}$$

To be more rigorous if we introduce horizontal changes of crustal parameters, the following changes will result in the topographic-isostatic potential coefficients in Eq. (17), if we restrict ourselves to the first-order term only:

$$\begin{Bmatrix} \Delta\overline{C}_{nm} \\ \Delta\overline{S}_{nm} \end{Bmatrix} = \frac{3}{(2n+1)} \frac{\rho_{cr}}{\overline{\rho}} \left[1 - \left(\frac{R-D}{R}\right)^n\right] \begin{Bmatrix} \Delta h\,c_{nm} \\ \Delta h\,s_{nm} \end{Bmatrix}, \tag{28}$$

where the 2D spherical harmonic coefficients $\Delta h\,c_{nm}$, $\Delta h\,s_{nm}$ are defined by the following equation:

$$\begin{Bmatrix} \Delta h\,c_{nm} \\ \Delta h\,s_{nm} \end{Bmatrix} = \frac{1}{4\pi} \iint\limits_{\sigma} \left(\frac{h(Q)}{R}\right) \delta_1(Q) \begin{Bmatrix} \overline{U}_{nmn}(Q) \\ \overline{V}_{nmn}(Q) \end{Bmatrix} d\sigma(Q)\ . \tag{29}$$

Here we used the abbreviation $\delta_1(Q)$ for the following *parameter function*

$$\delta_1(P) = \frac{\Delta\rho_{cr}(P)}{\overline{\rho}_{cr}} + \frac{\Delta D(P)}{\overline{D}} \ , \tag{30}$$

which describes the total effect of horizontal variations in *crustal density* and *crust thickness*. It clearly shows that if linear approximation is used it is impossible to separate the effects of crust density and thickness onto the topographic-isostatic potential.

The effect of compensation disturbances will be examined next. In the spherical Airy model when the compensation is complete, the root-antiroot thickness can be computed from the equation (see RUMMEL et al., 1988)

$$t(P) = \frac{\rho_{cr}}{\Delta\rho} \frac{R^2}{(R-D)^2} h(P) \ . \tag{31}$$

When an area is isostatically over-, or undercompensated, the above condition is not valid. Instead we may write the following equation

$$t(P) = \frac{\rho_{cr}}{\Delta\rho} \frac{R^2}{(R-D)^2} [1 + f(P)]h(P) \ , \tag{32}$$

where the (smoothly varying) $f(P)$ function expresses deviations of compensation with respect to the Airy model. The root-antiroot surface will remain linearly dependent on the surface topography, but now the mass balance criterion is not satisfied. If the $f(P)$ parameter function is negative/positive, the area now becomes under/overcompensated according to the traditional Airy hypothesis.

If we keep again only the first-order term in Eq. (17), the coefficient change due to the imperfect compensation will be

$$\left\{ \begin{array}{c} \Delta\overline{C}_{nm}^{comp} \\ \Delta\overline{S}_{nm}^{comp} \end{array} \right\} = \frac{3}{(2n+1)} \frac{\rho_{cr}}{\overline{\rho}} \left[\left[1 - \left(\frac{R-D}{R} \right)^n \right] \left\{ \begin{array}{c} f\,c_{nm} \\ f\,s_{nm} \end{array} \right\} - \left\{ \begin{array}{c} f\,c_{nm} \\ f\,s_{nm} \end{array} \right\} \right] \tag{33}$$

In this equation the $f\,c_{nm}$, $f\,s_{nm}$ coefficients are

$$\left\{ \begin{array}{c} f\,c_{nm} \\ f\,s_{nm} \end{array} \right\} = \frac{1}{4\pi} \iint\limits_{\sigma} \left(\frac{h(Q)}{R} \right) f(Q) \left\{ \begin{array}{c} \overline{U}_{nmn}(Q) \\ \overline{V}_{nmn}(Q) \end{array} \right\} d\sigma(Q) \ , \tag{34}$$

Table 1
Average correlation coefficients between Rapp 1981 model and simple Airy model

Degree range	$2-180$	$15-180$	$30-180$	$90-180$
$\overline{c}$	0.486	0.504	0.496	0.436

Let us introduce now the following parameter function

$$\delta(P) = \delta_1(P) + f(P) = \frac{\Delta\underline{\sigma}_{cr}(P)}{\underline{\sigma}_{cr}} + \frac{\Delta\overline{D}(P)}{\overline{D}} + f(P) \ , \qquad (35)$$

and the following 2D spherical harmonic coefficients of the product function $[h(P)/R]\delta(P)$

$$\begin{Bmatrix} h\delta c_{nm} \\ h\delta s_{nm} \end{Bmatrix} = \frac{1}{4\pi} \int\!\!\int_{\sigma} \left(\frac{h(Q)}{R}\right) \delta(Q) \begin{Bmatrix} \overline{U}_{nm}(Q) \\ \overline{V}_{nm}(Q) \end{Bmatrix} d\sigma(Q) \ , \qquad (36)$$

then the change in the topographic-isostatic coefficients will be

$$\begin{Bmatrix} \Delta\overline{C}_{nm} \\ \Delta\overline{S}_{nm} \end{Bmatrix} = \frac{3}{(2n+1)} \frac{\overline{\rho}_{cr}}{\overline{\rho}} \left[\left[1 - \left(\frac{R-D}{R}\right)^n\right] \begin{Bmatrix} h\delta c_{nm} \\ h\delta s_{nm} \end{Bmatrix} - \begin{Bmatrix} fc_{nm} \\ fs_{nm} \end{Bmatrix} \right] . \qquad (37)$$

The first term in this equation represents a double layer potential similarly to the linear term in the Eq. (17). In the Eq. (33) the relative magnitude of the first to the second term is

$$1 - \left(\frac{R-D}{R}\right)^n \ ,$$

which ratio is tabulated for the compensation depths D=30 and 60 km for various degrees *n* in Table 2.

Table 2
Relative magnitude of the double layer term in Eq. (37)

n	2	30	60	90	150	180
D = 30 km	0.009	0.132	0.247	0.346	0.507	0.572
D = 60 km	0.019	0.247	0.433	0.573	0.758	0.818

This comparison clearly shows that for the degree range 2 - 180 both terms should be used in Eq. (33) for the computation.

The expression (30) shows that in linear approximation in (*h/R*), the effects of crustal density and crust thickness anomalies cannot be separated, i.e. only their sum, $\delta_1(P)$ can be determined.

Now the following three combinations exist for the determination of horizontal parameter variations in the crust.

Model 1. Determine the function $\delta_1(P)$ only (i.e. crust density and thickness are variable, but perfect compensation is assumed everywhere according to the Airy hypothesis).

Model 2. Determine the function $f(P)$ only (i.e. laterally variable imperfect compensation, but constant crust density and thickness).

Model 3. Determine both functions $\delta_1(P)$ and $f(P)$ (i.e. neither crust density/thickness nor compensation is treated as fixed).

Mathematically *models 1* and *2* are equally simple but the results will certainly be distorted by the effects of changes in certain neglected parameters (for *model 1* compensation, for *model 2* crust density/thickness). The *model 3* seems to be the more realistic although it requires mathematically the determination of two parameter functions simultaneously.

7. Optimum Criterion for Topographic-Isostatic Crust Models

The gravity potential of the Earth includes the topographic-isostatic potential of the real crust of the Earth. This potential is included in the gravity potential in such a way that the shorter the wavelength of the gravity potential terms in the spherical harmonic expansion, the higher the contribution of the topographic-isostatic potential is to it. This fact is due to the rather shallow source depth of the topographic-isostatic potential. Simply saying the crust should become the most important density source of the gravity potential as the frequency increases. This also means that the shorter the wavelength, the smaller the disturbing effect of other masses is.

If the topographic-isostatic potential is modeled, our model has to reflect the gravity potential well at short wavelengths. This criterion can be used to judge between such models. From this point of view, the above criterion may be used to select a best or optimal model. This optimality criterion will be investigated next.

Let

$$\sigma^2(\Delta T) = \sum_{m=0}^{n}\left[\left(\overline{C}_{nm} - \overline{C}_{nm}^{\,model}\right)^2 + \left(\overline{S}_{nm} - \overline{S}_{nm}^{\,model}\right)^2\right] \tag{38}$$

denote the signal variances of the residual $\Delta T = T - T^{model}$ gravity potential field, where T is the earth's, and T^{model} is our `best' topographic-isostatic model's anomalous potential. The *optimum* criterion

$$\sum_{n=n_1}^{n_2}\beta_n\sigma_n^2(T) = minimum \;, \tag{39}$$

with the *de-smoothing factor*, β_n expresses a minimum condition for the residual anomalous potential field in the degree range $n_1 - n_2$. This way the high frequency part of the residual field will be minimized and it yields a topographic-isostatic model which approximates best the short wavelength anomalous potential field.

The *de-smoothing factor* β_n amplifies the higher frequency residual anomalous potential field components, and it can be determined in various ways. In the following discussion we present a purely theoretical approach to determine β_n.

Let us assume that the density inhomogeneities are uncorrelated, i.e. they have an ideal `white noise' distribution inside the earth. Their covariance function is then

$$\text{cov}[\Delta\rho(P), \Delta\rho(Q)] = C\delta(P,Q) , \tag{40}$$

where $\delta(P,Q)$ now denotes the 3D Dirac delta `function'. From covariance propagation through the integral

$$T(P) = G \iiint\limits_{sphere\ R} l^{-1}(P,Q)\,\Delta\rho(Q)\,dR(Q) \tag{41}$$

one may derive the covariance function of T arising from the density distribution inside the spherical shell between radii R_1 and R_2,

$$\text{cov}[T(P), T(Q)] = 4\pi G^2 CR \sum_{n=0}^{\infty} \frac{1}{(2n+1)(2n+3)} \left[\left(\frac{R_2}{R}\right)^{2n+3} - \left(\frac{R_1}{R}\right)^{2n+3} \right] P_n(\cos\psi_{P_1 Q_1}) \tag{42}$$

where points P_1, Q_1 lie on the earth's surface and P, Q are inside the spherical shell. If we compare this expression to the

$$\text{cov}[T(P_1), T(Q_1)] = \sum_{n=0}^{\infty} \sigma_n^2(T) P_n(\cos\psi_{P_1 Q_1}) \tag{43}$$

covariance function of anomalous potential T, we get the theoretical signal variances of T for the spherical shell as

$$\sigma_n^2(T) = \frac{4\pi G^2 CR}{(2n+1)(2n+3)} \left[\left(\frac{R_2}{R}\right)^{2n+3} - \left(\frac{R_1}{R}\right)^{2n+3} \right] \tag{44}$$

Let now D_{max} denote the maximum depth of crustal density anomalies. The $\sigma_n^2(T)_{D_{max}} / \sigma_n^2(T)$ ratio then theoretically should increase as the following de-smoothing function

$$\beta_n = 1 - \left(\frac{R - D_{max}}{R}\right)^{2n+3} \tag{45}$$

Values of this function β_n are tabulated for $D_{max} = 70km$ in *Table 3*.

Table 3
Theoretical de-smoothing function for maximum crustal depth 70 km

n	2	30	60	90	150	180
$D_{max} = 70km$	0.074	0.501	0.743	0.868	0.965	0.982

The function β_n shows the increasing theoretical signal variance of the gravity anomalous potential generated by the crust relative to the total signal variance of the anomalous potential.

8. Optimal Linear Topographic Model Determination

The determination of an optimal linear topographic-isostatic model requires mathematically the determination of one (two) optimal parameter function(s) δ_1 and/or f, defined on the surface of the earth. For the sake of simplicity the determination of only one parameter function δ_1 will be discussed in detail next. The computation of more than one parameter function will be quite straightforward then.

In the following discussion let $\delta(\Theta, \lambda)$ denote the following parameter function

$$\delta(\Theta, \lambda) = \frac{\Delta \rho_{cr}(\Theta, \lambda)}{\overline{\rho}_{cr}} + \frac{\Delta D(\Theta, \lambda)}{\overline{D}} \tag{46}$$

where Θ, λ polar distance and longitude,

   ρ_{cr} mean crust density,

   D mean crust thickness.

This equation corresponds to Eq. (30) and *Model 1* in Sec. 6.

The spherical harmonic coefficients $\overline{C}_{nm}^{model}$, $\overline{S}_{nm}^{model}$ of the optimal model will then be computed from the formulae below, which are analogous to the expressions (28) and (29).

$$\left\{\begin{matrix} \overline{C}_{nm}^{model} \\ \overline{S}_{nm}^{model} \end{matrix}\right\} = t_n \left\{\begin{matrix} h\delta c_{nm} \\ h\delta s_{nm} \end{matrix}\right\} + \left\{\begin{matrix} \overline{C}_{nm}^{Airy} \\ \overline{S}_{nm}^{Airy} \end{matrix}\right\} . \tag{47}$$

Here $\overline{C}_{nm}^{Airy}$, $\overline{S}_{nm}^{Airy}$ are determined by the expression (15),

$$t_n = \frac{3}{(2n+1)} \frac{\overline{\rho}_{cr}}{\overline{\rho}} \left[1 - \left(\frac{R - \overline{D}}{R} \right)^n \right], \tag{48}$$

and the 2D spherical harmonic coefficients in Eq. (47) are

$$\left\{\begin{matrix} h\delta c_{nm} \\ h\delta s_{nm} \end{matrix}\right\} = \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \left(\frac{h(\Theta, \lambda)}{R} \right) \delta(\Theta, \lambda) \left\{\begin{matrix} \overline{U}_{nm}(\Theta, \lambda) \\ \overline{V}_{nm}(\Theta, \lambda) \end{matrix}\right\} \sin\Theta \, d\Theta \, d\lambda . \tag{49}$$

These are the surface spherical harmonic coefficients of the *product function* $(h/R)\delta$. In the following we shall see how they may be represented by the 2D spherical harmonic coefficients of its component functions.

Let the functions h and δ be represented mathematically by the following 2D spherical harmonic series and coefficients:

$$h(\Theta,\lambda) = R \sum_{l=0}^{\infty} \sum_{k=0}^{l} \left[hc_{lk} \overline{U}_{lk}(\Theta,\lambda) + hs_{lk} \overline{V}_{lk}(\Theta,\lambda) \right], \tag{50}$$

$$\delta(\Theta,\lambda) = \sum_{i=0}^{\infty} \sum_{j=0}^{l} \left[oc_{ij} \overline{U}_{ij}(\Theta,\lambda) + os_{ij} \overline{V}_{ij}(\Theta,\lambda) \right], \tag{51}$$

$$\begin{Bmatrix} hc_{lk} \\ hs_{lk} \end{Bmatrix} = \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \left(\frac{h(\Theta,\lambda)}{R} \right) \begin{Bmatrix} \overline{U}_{lk}(\Theta,\lambda) \\ \overline{V}_{lk}(\Theta,\lambda) \end{Bmatrix} \sin\Theta \, d\Theta \, d\lambda, \tag{52}$$

$$\begin{Bmatrix} oc_{ij} \\ os_{ij} \end{Bmatrix} = \frac{1}{4\pi} \int_0^\pi \int_0^{2\pi} \delta(\Theta,\lambda) \begin{Bmatrix} \overline{U}_{ij}(\Theta,\lambda) \\ \overline{V}_{ij}(\Theta,\lambda) \end{Bmatrix} \sin\Theta \, d\Theta \, d\lambda. \tag{53}$$

In analogy to the theory of ordinary Fourier series, where to a convolution of two functions in the space domain there corresponds a simple product in the frequency domain and vice versa; now to a product of two functions on the sphere there corresponds a `convolution' in the discrete `frequency' domain between the 2D spherical harmonic coefficients. The mathematical tool needed for such a computation is the *product-sum conversion formula of spherical harmonics* (see Appendix A).

In an abbreviated form the following relationship holds for the determination of $h\delta c_{nm}$, $h\delta s_{nm}$ coefficients:

$$\begin{Bmatrix} h\delta c_{nm} \\ h\delta s_{nm} \end{Bmatrix} = \sum_{i=0}^{\infty} \sum_{j=0}^{i} \left[\begin{Bmatrix} a_{cc}(n,m,i,j) \\ a_{sc}(n,m,i,j) \end{Bmatrix} oc_{ij} + \begin{Bmatrix} a_{cs}(n,m,i,j) \\ a_{ss}(n,m,i,j) \end{Bmatrix} os_{ij} \right] \tag{54}$$

The a_{cc}, a_{sc}, a_{cs}, a_{ss} coefficients can be determined from the hc_{ik}, hs_{ik} 2D spherical harmonic coefficients and the Clebsch-Gordan coefficients. The definition and a practical computation method of Clebsch-Gordan coefficients can be found in Appendices B and C. Detailed derivation of the expression (54) can be found in Appendix A and thus the following equations will be obtained for the a_{cc}, a_{sc}, a_{cs}, a_{ss} coefficients:

$$
\begin{Bmatrix} a_{cc} \\ a_{sc} \\ a_{cs} \\ a_{ss} \end{Bmatrix} = \sum_l \sqrt{\frac{(2i+1)(2l+1)}{2(2n+1)}} C(i,l,n;\,0,0,0) \frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{j0})}} \quad \times
$$

$$
\times \left(
C(i,l,n;\,j,m-j,m)
\begin{bmatrix}
\sqrt{(1+\delta_{m-j,0})} \begin{Bmatrix} hc_{l,m-j} \\ hs_{l,m-j} \\ -hs_{l,m-j} \\ hc_{l,m-j} \end{Bmatrix}, & \text{if } m \geq j, \\[2em]
\text{but} \quad (-1)^{j-m}\sqrt{(1+\delta_{j-m,0})} \begin{Bmatrix} hc_{l,j-m} \\ -hs_{l,j-m} \\ hs_{l,j-m} \\ hc_{l,j-m} \end{Bmatrix}, & \text{if } m \leq j
\end{bmatrix}
\right.
$$

$$
\left.
+ C(i,l,n;\,-j,m+j,m)\,(-1)^{j}\,\sqrt{(1+\delta_{j+m,0})} \begin{Bmatrix} hc_{l,m-j} \\ hs_{l,m-j} \\ -hs_{l,m-j} \\ hc_{l,m-j} \end{Bmatrix}
\right) \qquad (55)
$$

In this equation the summation according to the index l must be done for all the values of l where the $C(i,l,n;\,j,k,m)$ Clebsch-Gordan coeflicients in this expression do not vanish. The δ_{ij} symbol here denotes the *Kronecker delta*.

Now we introduce the matrix elements

$$
\begin{Bmatrix} A_{cc}(q;r) \\ A_{sc}(q;r) \\ A_{cs}(q;r) \\ A_{ss}(q;r) \end{Bmatrix} = t_n \begin{Bmatrix} a_{cc}(n,m;\ i,j) \\ a_{sc}(n,m;\ i,j) \\ a_{cs}(n,m;\ i,j) \\ a_{ss}(n,m;\ i,j) \end{Bmatrix} \qquad (56)
$$

of the matrices A_{cc}, A_{sc}, A_{cs}, A_{ss} arranged according to the single indices $q = n(n+1)/2 + m+1$ and $r = i(i+1)/2 + j+1$ and similarly the column vectors **oc**, **os**, $\mathbf{C}^{\text{model}}$, $\mathbf{S}^{\text{model}}$, $\mathbf{C}^{\text{Airy}}$, $\mathbf{S}^{\text{Airy}}$ arranged according to the single indices r and q, respectively. With this notation the Eqs. (47) and (54) will result finally in the following linear system of equations:

$$
\begin{bmatrix} \mathbf{C}^{\text{model}} \\ \dots \\ \mathbf{S}^{\text{model}} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_{cc} & \dots & \mathbf{A}_{cs} \\ \dots & \dots & \dots \\ \mathbf{A}_{sc} & \dots & \mathbf{A}_{ss} \end{bmatrix} \begin{bmatrix} \mathbf{oc} \\ \dots \\ \mathbf{os} \end{bmatrix} + \begin{bmatrix} \mathbf{C}^{\text{Airy}} \\ \dots \\ \mathbf{S}^{\text{Airyl}} \end{bmatrix} \qquad (57)
$$

The optimal parameter vector $[\mathbf{oc}, \mathbf{os}]^T$ may now be estimated (up to a certain maximum degree and order $i_{max} = K$) to make the variance of the high frequency residual field *minimum* according to the condition (39). This is mathematically a well-known least squares estimation procedure for the optimal parameter vector.

This way the optimum parameter function $\delta(\Theta, \lambda)$ through its 2D spherical harmonic coefficients will be determined. The computation of the spherical harmonic coefficients of topographic-isostatic potential of our optimal linear model (OLTM) from the linear system (57) is quite simple.

9. Numerical Results

Computer programs and subroutines were developed in *MS FORTRAN* to determine optimal linear topographic-isostatic models. Subroutine *NORMCP* computes the arrays of the linear system and the normal equations. Subroutine *GAUSS* solves the normal equations and main program *CRUSTPAR* determines the optimal model coefficients. Some statistical quantities are also computed to judge the fit between our model and the Earth's anomalous potential.

For our previous calculations the spherical harmonic coefficients of the anomalous potential of the earth were the RAPP (1981) coefficients limited up to degree and order 90. The $1^0 \times 1^0$ average height dataset of H. SÜNKEL was used to produce 2D spherical harmonic coefficients of the equivalent topography up to the same degree and order 90.
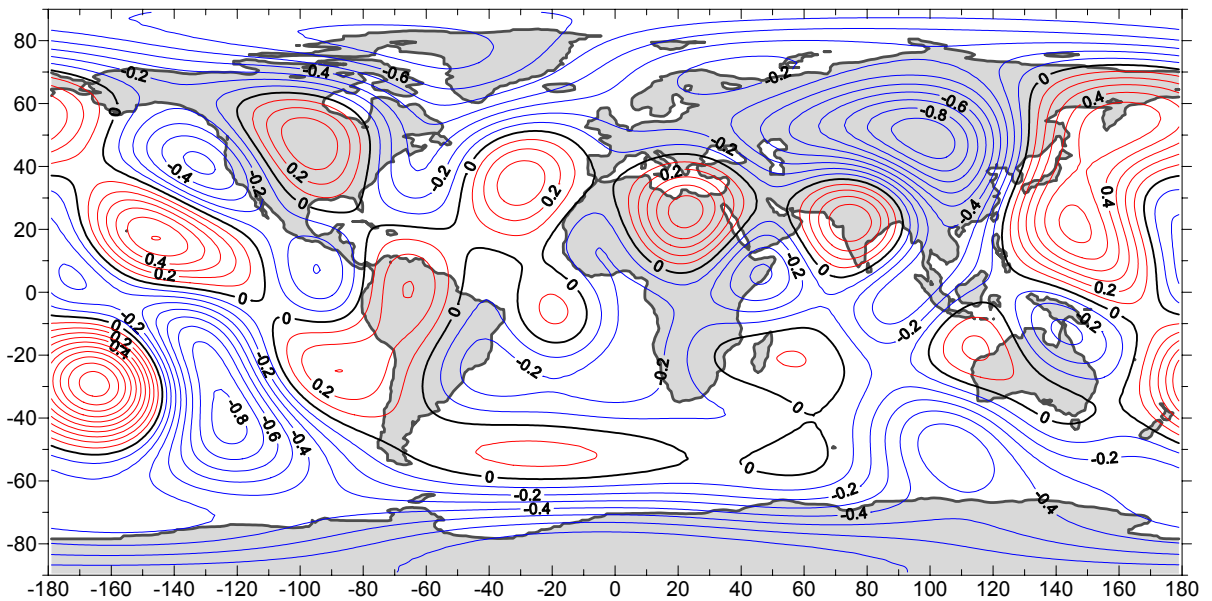

Fig. 2. Optimal crustal parameter function up to spherical harmonic degree *K*=8

Optimal linear topographic-isostatic models were computed up to $K = i_{max} = 8$ and 12. The OLTM was as described by *Model 1*. The optimality criterion was as described by Eq. (39) and for the β_n de-smoothing function $D_{max} = 70\,km$ was used in *Eq.* (45). The average crust parameters were $\overline{\rho}_{cr} = 2670\,kg\,m^{-3}$, $D = 30\,km$ and $\Delta\rho = 600\,kg\,m^{-3}$. The second

order approximation of T^{Airy} was used in *Eq.* (15) and the fit interval was chosen to be in the spherical harmonic degree range $n = 60 - 90$.

Computed optimal parameter functions for $K = 8$ and 12 can be seen in the *Figs. 2* and *3*. The topographic-isostatic geoid differences for $K = 12$ are shown in *Fig. 4*. Correlation spectra for the simple and OLTM models are shown in *Fig. 5*.
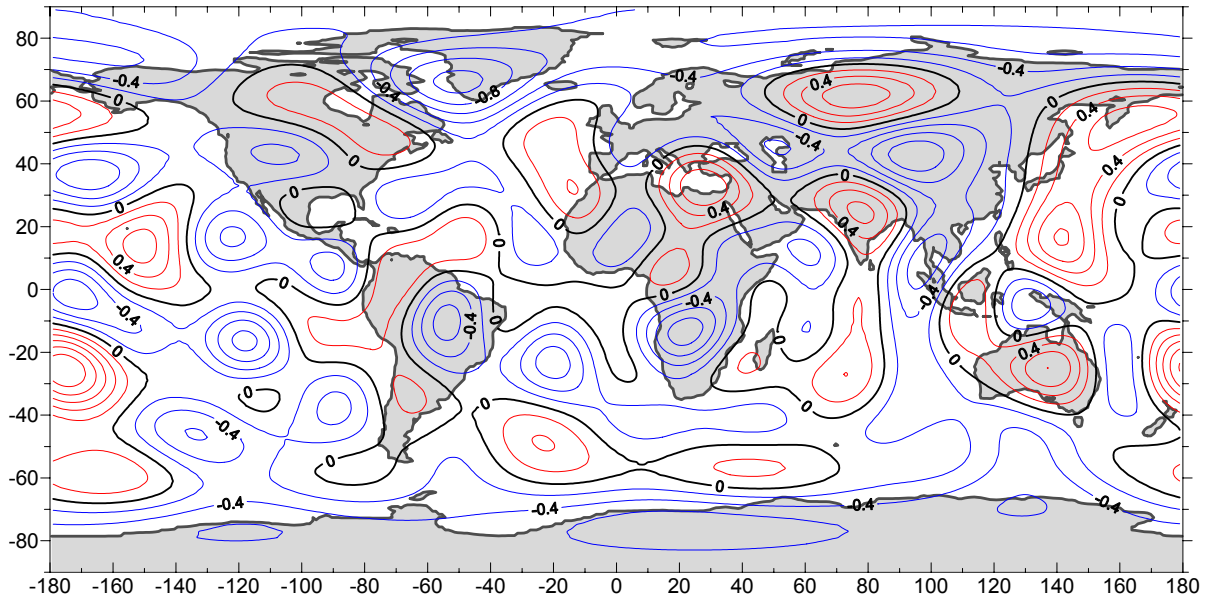

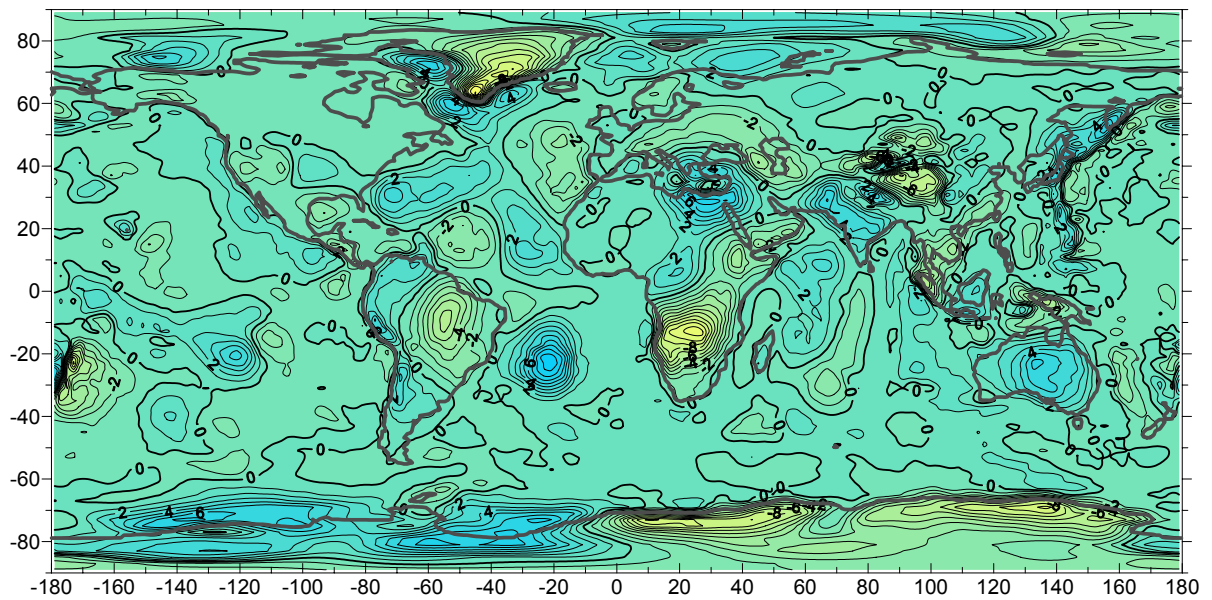*Fig. 3.* Optimal crustal parameter function up to spherical harmonic degree *K*=12

Fig. 4. Optimal topographic-isostatic vs. Airy model geoid height differences for *K*=12 model
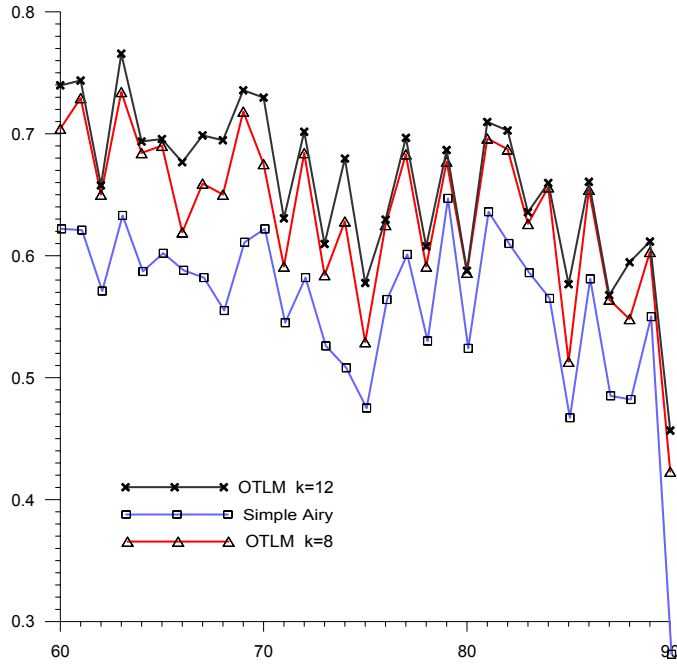
Fig. 5. Geopotential vs. OLTM model correlation spectra for the fit range 60 - 90

Table 4 shows the average correlation coefficients (22) in various degree ranges for Airy versus OLTM models.

Table 4
Average correlation coefficients of various topographic-isostatic models

Degree range	15 - 90	30 - 90	60 - 90
Simple Airy	0.576	0.583	0.559
OLTM $K = 8$	0.617	0.631	0.634
OLTM $K = 12$	0.623	0.643	0.659

These previous results were derived from the simple *Model 1* and in the relatively low degree range 60 - 90. Further investigations are planned to derive OLTM for the higher degree range up to $n = 180$ and with higher resolution of the parameter function (higher $K = i_{max}$. Calculations are also needed with *Model 2* and *3*, and with other minimum principles. The effect of smoothing of root-antiroot surface according to the physically more realistic Vening-Meinesz model we would like to investigate as well.

10. Conclusions

Our previous results show that a clear improvement of global topographic-isostatic models, compared to the simple Airy model can be achieved by allowing horizontal change of the crustal parameters. Our results also show that *significant departures must occur on a global scale* due to crust density and thickness change *with respect to the Airy model of uniform crust parameters*. These departures vary from area to area and they show the complex behaviour of the crust. Large negative values resulted for areas of significant ice coverage,

because no *ice thicknesses* were included in the topographic height dataset. Negative values are mostly correlated with large mountain zones and ocean bottom areas. Positive values are associated with ocean trenches and old continental massifs. These results suggest the *nonlinearity* of compensation, i.e. there is no strict linear relation (1) between topographic heights and root thicknesses.

Of course it is hard to interpret these previous results of *Model 1* physically, but it is expected that the physically more relevant *Model 3* with higher resolution will be a more adequate tool to support some *global mechanism* of isostatic compensation. We think that in the lack of accurate global geophysical data, the anomalous potential field still remains a very important source of information to support or reject any global mechanism of isostatic compensation.

Finally it should be mentioned that the whole procedure is rather independent of the choice of the original topographic-isostatic model. It can be used with various topographic-isostatic models as well. The only assumption is that the model change should be in linear relation with topographic heights.

Appendix A
The Spherical Harmonic Product-Sum Conversion Formula

Complex spherical harmonics

Let us introduce the following complex spherical harmonics (ROSE, 1957):

$$Y_{nm}(\Theta, \lambda) = e^{im\lambda} \overline{P}_n^m(\cos\Theta) \ , \qquad \begin{matrix} n = 0, 1, ... \\ m = -n, ..., -1, 0, 1, ..., n \end{matrix} \tag{A1}$$

where i denotes imaginary unit and $\overline{P}_n^m \cos(\Theta)$ is defined by the following equation:

$$\overline{P}_n^m \cos(\Theta) = (-1)^m \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos\Theta)$$
$$n = 0, 1, ...$$
$$m = -n, ..., 0, ..., n \tag{A2}$$

Here the $P_n^m(t)$ functions are defined through the expression

$$P_n^m(t) = \frac{1}{2^n n!} \left(1 - t^2\right)^{m/2} \frac{d^{n+m}}{dt^{n+m}} \left(t^2 - 1\right)^n \ , \qquad \begin{matrix} n = 0, 1, ... \\ m = -n, ..., 0, ..., n \end{matrix} \tag{A3}$$

The defining *Eq.* (A2) is a useful extension of the associated Legendre Functions for the negative *m* values. If such definition is used, the following symmetry relations

$$\overline{P}_n^{-m}(\cos\Theta) = (-1)^m \overline{P}_n^m(\cos\Theta) \tag{A4}$$

and

$$Y_{nm}^*(\Theta, \lambda) = Y_{nm}(\Theta, -\lambda) = (-1)^m Y_{n,-m}(\Theta, \lambda) \tag{A5}$$

will hold for the associated Legendre functions and complex spherical harmonics. Here the sign * denotes complex conjugate.

Orthogonality relations

Th orthogonality relation of complex spherical harmonics (A1) is

$$\int\limits_{0}^{2\pi}\int\limits_{0}^{\pi} Y_{nm}^{*}(\Theta,\lambda)\, Y_{n'm'}(\Theta,\lambda)\, \sin\Theta\; d\Theta\; d\lambda = \delta_{nn'}\delta_{mm'} \quad . \tag{A6}$$

Triple product integral (see ROSE, 1957)

$$\iint\limits_{\sigma} Y_{nm}^{*}(P)\, Y_{n_1 m_1}(P)\, Y_{n_2 m_2}(P)\, \mathrm{d}\sigma(P) = $$

$$\sqrt{\frac{(2n_1+1)(n_2-m)!}{4\pi(n+m)!}}\; C(n_1,n_2,n,0,0,0)\, C(n_1,n_2,n;m_1,m_2,m) \tag{A7}$$

where $C(n_1,n_2,n,m_1,m_2,m)$ denotes the Clebs-Gordan coefficients (see Appendix B). Now we are able to derive the

Complex spherical harmonic product-sum conversion formula

for the complex coefficients.

Let the functions $a(\Theta,\lambda)$ and $b(\Theta,\lambda)$ be expanded into the following 2D spherical harmonic series

$$a(\Theta,\lambda) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} A_{nm} Y_{nm}(\Theta,\lambda) \tag{A8}$$

$$b(\Theta,\lambda) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} B_{nm} Y_{nm}(\Theta,\lambda) \tag{A9}$$

with the complex A_{nm}, B_{nm} coefficients. Now the question is how to determine the complex Z_{nm} spherical harmonic coefficients of the product function

$$z(\Theta,\lambda) = a(\Theta,\lambda)\, b(\Theta,\lambda) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Z_{nm}\, Y_{nm}(\Theta,\lambda) \quad . \tag{A10}$$

Now if we substitute the expressions (A8) and (A9) into the left side of Eq. (A10) and perform index change, the result is the equation

$$\sum_{n_3=0}^{\infty}\sum_{m_3=-n_3}^{n_3} Z_{n_3 m_3} Y_{n_3 m_3}(\Theta,\lambda) = \sum_{n_1=0}^{\infty}\sum_{m_1=-n_1}^{n_1}\sum_{n_2=0}^{\infty}\sum_{m_2=-n_2}^{n_2} B_{n_1 m_1} A_{n_2 m_2} Y_{n_1 m_1}(\Theta,\lambda) Y_{n_2 m_2}(\Theta,\lambda) \ . \quad \text{(A11)}$$

Let us multiply both sides of this equation by the function $Y_{nm}^{*}(\Theta,\lambda)$ and then integrate it onto the surface of the unit sphere σ termwise. Then if we apply the relations (A6) and (A7), the terms on the left side will not vanish only if $n_3 = n$ and $m_3 = m$. Thus finally we get the following equation for complex Z_{nm} coefficients:

$$Z_{nm} = \sum_{n_1=0}^{\infty}\sum_{m_1=-n_1}^{n_1}\sum_{n_2=0}^{\infty}\sum_{m_2=-n_2}^{n_2} \sqrt{\frac{(2n_1+1)(2n_2+1)}{4\pi(2n+1)}} \, C(n_1, n_2, n; 0, 0, 0)$$
$$\times \ C(n_1, n_2, n; m_1, m_2, m) \, A_{n_2 m_2} B_{n_1 m_1} \qquad\qquad \text{(A12)}$$

From the properties of the Clebsch-Gordan coefficients (see Appendix B) it is clear that the $C(n_1, n_2, n, m_1, m_2, m)$ coefficients will not vanish only if $m = m - m_1$. The sum with respect to n_2 should be extended over the integers

$$|n - n_1| \le n_2 \le n + n_1$$

where

$$n_1 + n_2 + n = 2k = even \ .$$

With these restrictions for indices in the *Eq.* (A12), it will assume the following form:

$$Z_{nm} = \sum_{n_1=0}^{n_1}\sum_{m_1=-n_1}^{\infty}\sum_{n_2} \sqrt{\frac{(2n_1+1)(2n_2+1)}{4\pi(2n+1)}} \, C(n_1, n_2, n; 0, 0, 0)$$
$$\times \ C(n_1, n_2, n; m_1, m-m_1, m) \, A_{n_2 m_2} B_{n_1 m_1} \qquad\qquad \text{. (A13)}$$

Real spherical harmonics

When we would like to use real 2D spherical harmonic series with conventional real spherical harmonics (7), the following relations will hold between real and complex coefficients:

$$\sqrt{8\pi(1+\delta_{m0})}\begin{Bmatrix} C_{nm} \\ -iS_{nm} \end{Bmatrix} = \left[(-1)^m Z_{nm} \begin{Bmatrix} + \\ - \end{Bmatrix} Z_{n,-m} \right] \qquad m \ge 0 \qquad \text{(A14)}$$

$$\sqrt{8\pi(1+\delta_{m_2 0})}\begin{Bmatrix} G_{n_2 m_2} \\ -iH_{n_2 m_2} \end{Bmatrix} = \left[(-1)^{m_2} A_{n_2 m_2} \begin{Bmatrix} + \\ - \end{Bmatrix} A_{n_2,-m_2} \right] \qquad m_2 \ge 0 \qquad \text{(A15)}$$

$$\sqrt{8\pi(1+\delta_{m_1 0})}\begin{Bmatrix} E_{n_2 m_2} \\ -iF_{n_2 m_2} \end{Bmatrix} = \left[(-1)^{m_1} A_{n_1 m_1} \begin{Bmatrix} + \\ - \end{Bmatrix} A_{n_1,-m_1} \right] \qquad m_1 \ge 0 \qquad \text{(A16)}$$

Now let us substitute Z_{nm} and $Z_{n,-m}$ from (A13) into the right side of (A14). If the summation with respect to m_1 now runs on positive values only, we get the following equation

$$\sqrt{8\pi(1+\delta_{m0})}\begin{Bmatrix} C_{nm} \\ -iS_{nm} \end{Bmatrix} = \sum_{n_1=0}^{\infty}\sum_{n_2}\sqrt{\frac{(2n_1+1)(2n_2+1)}{4\pi(2n+1)}}\,C(n_1,n_2,n;0,0,0)\ \times$$

$$\times \sum_{m_1=0}^{n_1}\frac{1}{1+\delta_{m_10}}\begin{bmatrix} C(n_1,n_2,n;m_1,m-m_1,m)\left[(-1)^m A_{n_2,m-m_1}B_{n_1m_1}\begin{Bmatrix}+\\-\end{Bmatrix}A_{n_2,-(m-m_1)}B_{n_1,=m_1}\right]+ \\ +C(n_1,n_2,n;-m_1,m+m_1,m)\left[(-1)^m A_{n_2,m-m_1}B_{n_1,-m_1}\begin{Bmatrix}+\\-\end{Bmatrix}A_{n_2,-(m+m_1)}B_{n_1m_1}\right]\end{bmatrix}$$

Finally we introduce real coefficients instead of the complex coefficients A and B from the *Eqs.* (A15) and (A16) and we get the following real equation pair for C_{nm} and S_{nm}:

$$\begin{Bmatrix} C_{nm} \\ S_{nm} \end{Bmatrix} = \sum_{n_1=0}^{\infty}\sum_{n_2}\sqrt{\frac{(2n_1+1)(2n_2+1)}{4\pi(2n+1)}}\,C(n_1,n_2,n,0,0,0)\ \times$$

$$\times \left\{ \begin{aligned} &\sum_{m_1=m+1}^{n_1}\frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{m_10})}}\times \\ &\times\begin{bmatrix} (-1)^{m_1-m}C(n_1,n_2,n;m_1,m-m_1,m)\times \\ \times\sqrt{1+\delta_{m=m_1,0}}\left[\begin{Bmatrix} C_{n_2,m_1-m} \\ -H_{n_2,m_1-m} \end{Bmatrix}E_{n_1m_1}+\begin{Bmatrix} H_{n_2,m_1-m} \\ G_{n_2,m_1-m} \end{Bmatrix}F_{n_1m_1}\right]+ \\ +(-1)^{m_1}C(n_1,n_2,n;-m_1,m+m_1,m)\times \\ \times\sqrt{1+\delta_{m_1+m,0}}\left[\begin{Bmatrix} G_{n_2,m_1+m} \\ H_{n_2,m_1+m} \end{Bmatrix}E_{n_1m_1}+\begin{Bmatrix} H_{n_2,m_1+m} \\ -G_{n_2,m_1+m} \end{Bmatrix}F_{n_1m_1}\right] \end{bmatrix} + \\ &+\sum_{m_1=0}^{m}\frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{m_10})}}\times \\ &\times\begin{bmatrix} C(n_1,n_2,n;m_1,m-m_1,m)\times \\ \times\sqrt{1+\delta_{m=m_1,0}}\left[\begin{Bmatrix} G_{n_2,m-m_1} \\ H_{n_2,m-m_1} \end{Bmatrix}E_{n_1m_1}+\begin{Bmatrix} H_{n_2,m-m_1} \\ G_{n_2,m-m_1} \end{Bmatrix}F_{n_1m_1}\right]+ \\ +(-1)^{m_1}C(n_1,n_2,n;-m_1,m+m_1,m)\times \\ \times\sqrt{1+\delta_{m_1+m,0}}\left[\begin{Bmatrix} G_{n_2,m_1+m} \\ H_{n_2,m_1+m} \end{Bmatrix}E_{n_1m_1}+\begin{Bmatrix} H_{n_2,m_1+m} \\ -G_{n_2,m_1+m} \end{Bmatrix}F_{n_1m_1}\right] \end{bmatrix} \end{aligned} \right\}. \qquad (A17)$$

Now if the following notations

$$\begin{Bmatrix} C_{nm} \\ S_{nm} \end{Bmatrix} = \sum_{n_1=0}^{\infty} \sum_{m_1=0}^{n_1} \left[\begin{Bmatrix} a_{cc}(n,m,n_1,m_1) \\ a_{sc}(n,m,n,m) \end{Bmatrix} E_{n_1 m_1} + \begin{Bmatrix} a_{cs}(n,m,n_1,m_1) \\ a_{ss}(n,m,n,m) \end{Bmatrix} F_{n_1 m_1} \right] \tag{A18}$$

and

$$Q(n_1,n_2,n) = \sqrt{\frac{(2n_1+1)(2n_2+1)}{2(2n+1)}} \, C(n_1,n_2,n,0,0,0) \tag{A19}$$

are introduced, then the a_{cc}, a_{sc}, a_{cs}, a_{ss} coefficients will be defined through the following equations:

$$a_{cc} = \sum_{n_2} \frac{Q(n_1,n_2,n)}{\sqrt{(1+\delta_{m0})(1+\delta_{m_1 0})}} \left[\sqrt{1+\delta_{m=m_1,0}} \begin{cases} G_{n_2,m-m_1}, & \text{if } m_1 \le m \\ (-1)^{m_1-m} G_{n_2,m_1-m}, & \text{if } m_1 \ge m \end{cases} + \\ + \sqrt{1+\delta_{m=m_1,0}} (-1)^{m_1} G_{n_2,m+m_1} \right], \tag{A20a}$$

$$a_{sc} = \sum_{n_2} \frac{Q(n_1,n_2,n)}{\sqrt{(1+\delta_{m0})(1+\delta_{m_1 0})}} \left[\sqrt{1+\delta_{m=m_1,0}} \begin{cases} H_{n_2,m-m_1}, & \text{if } m_1 \le m \\ (-1)^{m_1-m+1} H_{n_2,m_1-m}, & \text{if } m_1 \ge m \end{cases} + \\ + \sqrt{1+\delta_{m+m_1,0}} (-1)^{m_1} H_{n_2,m+m_1} \right], \tag{A20b}$$

$$a_{cs} = \sum_{n_2} \frac{Q(n_1,n_2,n)}{\sqrt{(1+\delta_{m0})(1+\delta_{m_1 0})}} \left[\sqrt{1+\delta_{m=m_1,0}} \begin{cases} -H_{n_2,m-m_1}, & \text{if } m_1 \le m \\ (-1)^{m_1-m} H_{n_2,m_1-m}, & \text{if } m_1 \ge m \end{cases} + \\ + \sqrt{1+\delta_{m+m_1,0}} (-1)^{m_1} H_{n_2,m+m_1} \right], \tag{A20c}$$

$$a_{ss} = \sum_{n_2} \frac{Q(n_1,n_2,n)}{\sqrt{(1+\delta_{m0})(1+\delta_{m_1 0})}} \left[\sqrt{1+\delta_{m=m_1,0}} \begin{cases} G_{n_2,m-m_1}, & \text{if } m_1 \le m \\ (-1)^{m_1-m} G_{n_2,m_1-m}, & \text{if } m_1 \ge m \end{cases} + \\ + \sqrt{1+\delta_{m+m_1,0}} (-1)^{m_1+1} G_{n_2,m+m_1} \right], \tag{A20d}$$

If we perform the index change

$$i = n_1 \ , \quad j = m_1 \ , \quad l = n_2 \ , \quad k = m_2$$

in the *Eqs*. (A18), (A19) and (A20a-d), the *Eq*. (55) will be yielded.

The program *NORMCP* uses formulae (A18-20) for the computation. The cornmutativity of the product (A10) was tested numerically, and the maximum errors were of order 10^{-14} using 8-byte reals.

Appendix B
The Clebsch-Gordan Coefficients

The definition of the Clebsch-Gordan coefficients (see ROSE, 1957 and WIGNER, 1959) is

$$C(n_1, n_2, n_3; m_1, m_2, m_3) = \delta_{m_3, m_1+m_2} \times$$

$$\sqrt{(2n_3+1) \frac{(n_3+n_1-n_2)!\,(n_3-n_1+n_2)!\,(n_1+n_2-n_3)!\,(+n_1-n_2)!\,(n_3+m_3)!\,(n_3-m_3)!}{(n_1+n_2+n_3+1)!\,(n_1-m_1)!\,(n_1+m_1)!\,(n_2-m_2)!\,(n_2+m_2)!}} \,, \quad \text{(B1)}$$

$$\times \sum_k \frac{(-1)^{k-n_2+m_2}}{k!} \frac{(n_3+n_2+m_1-k)!\,(n_1-m_1+k)!}{(n_3-n_1+n_2-k)!\,(n_3+m_3-k)!\,(k+n_1-n_2-m_3)!}$$

where the index k assumes all integer values for which none of the factorials is negative.

The Clebsch-Gordan coefficients are non-vanishing only if the following three conditions are satisfied.

1.) $|m_1| \le n_1$, $|m_2| \le n_2$, $|m_3| \le n_3$; (n_1, n_2, n_3 are non-negative integers)

2.) m_3 is the algebraic sum of m_1 and m_2: $m_3 = m_1 + m_2$

3.) n_3 is the `vectorial sum' of n_1 and n_2; i.e. a triangle can be formed by the vectors of lengths n_1, n_2, n_3, respectively. This triangle condition, $\Delta(n_1, n_2, n_3)$ is satisfied if $|n_1 - n_2| \le n_3 \le n_1 + n_2$.

Properties of the Clebsch-Gordan coefficients

$$C(n_1, n_2, n_1+n_2; n_1, n_2, n_1+n_2) = 1$$
$$C(n_1, n_2, n_1+n_2; 0, 0, 0) = 0, \qquad \text{except if} \quad n_1+n_2+n_3 = \text{even} \quad \textit{(parity coefficient)}$$
$$C(n_1, 0, n_3; m_1, 0, m_3) = \delta_{n_1, n_3} \delta_{m_1, m_3}$$

symmetry relations:

$$C(n_1, n_2, n_3; m_1, m_2, m_3) = (-1)^{n_1+n_2+n_3} C(n_1, n_2, n_3; -m_1, -m_2, -m_3) =$$
$$= (-1)^{n_1+n_2+n_3} C(n_2, n_1, n_3; m_2, m_1, m_3)$$

Detailed other formulae for the computation of Clebsch-Gordan coefficients for special index values can be found in the paper of PEC (1983), in Appendix A1.

Appendix C
Practical Computation of Clebsch-Gordan Coefficients

The aim of the following discussion is to present suitable recursion formulae for the computation of Clebsch-Gordan coefficients instead of the direct formula (B1), which is well-suited only for the computation of several, but not all coefficients. The recursive method described here can be easily adapted for computers.

Parity Clebsch-Gordan coefficient

It is straightforward to derive a recursive computation method for the $Q(n_1, n_2, n)$ coefficient, which is in connection with the parity/ClebschGordan coefficient through the equation (A19).

The following closed expression can be found for the parity ClebschGordan coefficient (see ROSE, 1957):

$$C(n_1, n_2, n) = \frac{(-1)^{k-n} k!}{(k - n_1)! (k - n_2)! (k - n)!} \sqrt{\frac{(2k - 2n_1)! (2k - 2n_2)! (2k - 2n)!}{(2k + 1)!}} \quad , \qquad \text{(C1)}$$

where

$$k = \frac{1}{2}(n_1 + n_2 + n)) \quad .$$

From this expression the following recursion scheme can easily be derived:

1. initial value:

$$Q(0, n, n) = \frac{1}{\sqrt{2}} \qquad\qquad \text{(C2)}$$

2. recursion with respect to n_1:

$$Q(n_1 + 1, n_1 + n + 1, n) = \sqrt{\frac{(2n_1 + 3)(n_1 + n + 1)}{(n_1 + 1)(2n_1 + 2n + 1)}} \, Q(n_1, n_1 + n, n) \quad , \qquad \text{(C3)}$$

3. recursive computation with respect to n_2 according to the index

$$p = \frac{1}{2}(n_1 - n_2 + n)) \quad , \qquad p = 0, 1, 2, ..., \min(n_n, n) :$$

$$Q(n_1, p + 1, n) = -\sqrt{\frac{(2p + 1)(n - p)(n_1 - p)(2n + 2n_1 - 2p + 1)(2n + 2n_1 - 4p - 3)}{(p + 1)(2n - 2p - 1)(2n_1 - 2p - 1)(n + n_1 - p)(2n + 2n_1 - 4p + 1)}} \, Q(n_1, p, n)$$

$$\text{(C4)}$$

where the initial value $Q(n_1, 0, n) = Q(n_1, n_1 + n, n)$ was computed from (C3).

Recursive computation of Clebsch-Gordan coefficients

In the foregoing discussion we used the special values of these coefficients as described in the paper of PEC (1983) and recursive formulae were as found in M. ROSE (1957).

By the term row we denote all non-vanishing coefficients where the indices n, n_1, m, m_1 are fixed but n_2 is variable. The term column refers to all those non-vanishing coefficients for which n, n_1, n_2, m are fixed but m_1 is variable.

Now the general scheme for the computation is briefly the following.

1.) Compute four initial values to start the computation of two rows at a time

2.) Compute two complete rows at a time to be the initial value for 3).

3.) Compute all the columns for which the coefficients exist.

4.) Repeat 1.) - 3.) for all possible n, m, n_1 values.

We define the following two different cases for the recursion:

$$\text{Case A:} \quad \text{when} \quad m < n_1,$$
$$\text{Case B:} \quad \text{when} \quad m \geq n_1.$$

l.) Initial value computation

Case A

$$C(0, n, n; 0, 0, 0) = 1 \tag{C5}$$

$$C(m+1, n+m+1, n; m+1, 0, m+1) = \sqrt{\frac{n-m}{2(2n+2m+3)}}\, C(m, n+m, n; m+1, 0, m+1)$$
$$m = 0, 1, ..., n-1 \tag{C6}$$

Four initial values for two rows for $n_1 \neq 0$, $n_1 = m, m+1, ...,$ etc. are

value 1:

$$C(n_1, n_1+n+1, n; m, 0, m) =$$
$$= -\sqrt{\frac{(n_1+1)(2n_1+1)(n+n_1+1)}{(2n+2n_1+3)(n_1+m_1+1)(n_1-m+1)}}\, C(n_1, n_1+n, n; m, 0, m) \tag{C7}$$

with initial values (C6),

value 2:

$$C(n_1, n_1+n, n; m=1, 1, m) = -\sqrt{\frac{(n_1+m)(n+n_1+1)}{(n+n_1)(n_1-m+1)}}\, C(n_1, n_1+n, n; m, 0, m) \tag{C8}$$

can be computed from (C7),

value 3:

$$C(n_1, n_1+n-1, n; m, 0, m) = m\sqrt{\frac{(2n+2n_1+1)}{nn_1}}\, C(n_1, n_1+n, n; m, 0, m) \tag{C9}$$

can be computed from (C7), and finally

value 4:

$$C(n_1, n_1 + n - 1, n; m - 1, 1, m) =$$

$$= \left[n(m-1) + n_1 m\right]\sqrt{\frac{(2n + 2n_1 + 1)}{n_1 n \, (n + n_1 + 1)(n + n_1 - 1)}} C(n_1, n_1 + n, n; m - 1, 1, m) \quad \text{(C10)}$$

can be obtained by the coefficient (C8).

Case B

$$C(0, n, n; 0, m, m) = 1 \quad \text{(C11)}$$

Four initial values for two rows for successive n_1 values are

value 1:

$$C(n_1 + 1, n_1 + n - 1, n; n_1 + 1, m - n_1 - 1, m) =$$

$$= \sqrt{\frac{(n - m + 2n_1 + 1)(n - m + 2n_1 + 2)}{(2n + 2n_1 + 2)(2n + 2n_1 + 3)}} C(n_1 + 1, n_1 + n + 1, n; n_1 + 1, m - n_1 - 1, m)$$

$$n_1 = 0, 1, ..., m - 1 \quad \text{(C12)}$$

then compute from (C12) the following

value 2:

$$C(n_1, n_1 + n, n; n_1 - 1, m - n_1 + 1, m) =$$

$$= -\sqrt{\frac{2n_1(n + m + 1)}{n - m + 2n_1}} \, C(n_1, n_1 + n, n; n_1, m - n_1, m) \quad \text{(C13)}$$

and

value 3:

$$C(n_1, n_1 + n - 1, n; n_1, m - n_1, m) =$$

$$= \sqrt{\frac{n_1(n + m)(2n + 2n_1 + 1)}{n(n - m + 2n_1)}} \, C(n_1, n_1 + n, n; n_1, m - n_1, m) \quad \text{(C14)}$$

Finally, then from (C13) compute the following for $n_1 > 0$,

value 4:

$$C(n_1, n_1 + n - 1, n; n_1 - 1, m - n_1 + 1, m) =$$

$$= \left[n(n_1 - 1) + n_1 m\right]\sqrt{\frac{(2n + 2n_1 + 1)}{n_1 n \, (n + m + 1)(n - m + 2n_1 - 1)}} \, C(n_1, n_1 + n, n; n_1 - 1, m - n_1 + 1, m)$$

$$\text{(C15)}$$

2.) Recursive computation of two complete rows for Case A or B

General formula (see ROSE, 1957)

$$C(n_1, n_2 - 1, n; m_1, m - m_1, m) =$$

$$= \frac{1}{W(n_2)} \left[\sqrt{\frac{2n_2 + 1}{2n_2 - 1}} \, V(n_2) \, C(n_1, n_2, n; m_1, m - m_1, m) - \right. \\ \left. - \sqrt{\frac{2n_2 + 3}{2n_2 - 1}} \, W(n_2 + 1) \, C(n_1, n_2 + 1, n; m_1, m - m_1, m) \right] \quad \text{(C16)}$$

where we'have used the following abbreviations:

$$V(n_2) = m_1 + (m - m_1) \frac{n_1(n_1 + 1) - (n(n + 1) + n_2(n_2 + 1))}{2n_2(n_2 + 1)}$$

and

$$W(n_2) = \sqrt{\frac{\left[n_2^2 - (m - m_1)^2\right](n_2 - n_1 + n)(n_2 + n_1 - n)(n_1 + n + n_2 + 1)(n_1 + n - n_2 + 1)}{4n_2^2(2n_2 - 1)(2n_2 + 1)}}$$

Initial values for recursion with respect to n_2 are obtained through the expressions (C7 - C10) or (C12 - C15) to start the computation of *two rows* at a time.

3.) Compute all the columns

This type of computation requires the following general recursion formulae with respect to the integer m_2:

for increasing m_1:

$$C(n_1, n_2, n; m_1 + 1, m - m_1 - 1, m) =$$

$$= \frac{1}{N(m_1)} \left[M(m_1) \, C(n_1, n_2, n; m_1, m - m_1, m) - \\ - N(m_1 - 1) \, C(n_1, n_2, n; m_1 - 1, m - m_1 + 1, m) \right] \quad \text{(C17a)}$$

for decreasing m_1:

$$C(n_1, n_2, n; m_1 - 1, m - m_1 + 1, m) =$$

$$= \frac{1}{N(m_1 - 1)} \left[M(m_1) \, C(n_1, n_2, n; m_1, m - m_1, m) - \\ - N(m_1) \, C(n_1, n_2, n; m_1 + 1, m - m_1 - 1, m) \right] \quad \text{(C17b)}$$

where

$$M(m_1) = n(n + 1) - n_1(n_1 + 1) - n_2(n_2 + 1) - 2m_1(m - m_1)$$

and

$$N(m_1) = \sqrt{(n_1 - m_1)(n_1 + m_1 + 1)(n_2 - m + m_1 + 1)(n_2 + m - m_1)}\ .$$

The initial values for this recursion are those two rows, which were previously computed from the equation (C16).

The FORTRAN subroutine NORMCP utilizes the above sketched procedure to compute all the necessary Clebsch-Gordan coefficients. This algorithm was tested numerically using the direct formula (B1).

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