FFT-based high-performance spherical harmonic transformation

CHRISTIAN GRUBER[1], PAVEL NOVÁK[2,3] AND JOSEF SEBERA[4]

1 GFZ German Research Centre for Geosciences, Section 1.2: Global Geomonitoring and Gravity Field, c/o DLR Oberpfaffenhofen, D-82230 Wessling, Germany (gruber@gfz-potsdam.de)

2 Research Institute of Geodesy, Topography and Cartography, 25066 Zdiby, Czech Republic (panovak@kma.zcu.cz)

3 University of West Bohemia, Univerzitní 22, 306 14 Plzeň, Czech Republic

4 Technical University in Prague, Thákurova 7/2077, 166 29 Praha 6, Czech Republic

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ABSTRACT

Spherical harmonic transformation is of practical interest in geodesy for transformation of globally distributed quantities such as gravity between space and frequency domains. The increasing spatial resolution of the latest and forthcoming gravitational models pose true computational challenges for classical algorithms since serious numerical instabilities arise during the computation of the respective base functions of the spherical harmonic expansion. A possible solution is the evaluation of the associated Legendre functions in the Fourier domain where numerical instabilities can be circumvented by an independent frequency-wise scaling of numerical coefficients into a numerically suitable double precision range. It is then rather straightforward to commit global fast data transformation into the Fourier domain and to evaluate subsequently spherical harmonic coefficients. For the inverse, the computation of respective Fourier coefficients from a given spherical harmonic model is performed as an inverse Fast Fourier Transform into globally distributed data points. The two-step formulation turns out to be stable even for very high resolutions as well as efficient when using state-of-the-art shared memory/multi-core architectures. In principle, any functional of the geopotential can be computed in this way. To give an example for the overall performance of the algorithm, we transformed an equiangular 1 arcmin grid of terrain elevation data corresponding to spherical harmonic degree and order 10800.

Keywords: 2-D Fourier expansion, geopotential, spherical harmonics, spectral transformation, shared memory/multi-thread computation, spherical harmonic analysis and synthesis

1. INTRODUCTION

During the last decade the need to model global geophysical processes with an unprecedented spatial resolution in the Earth sciences has generated a corresponding need for stable and efficient computational algorithms. A very important expansion used predominately in geodesy as well as in geophysics is the expansion of 3-D functions into spherical harmonic series. These series are based on the solution of the Laplace equation by the associated Legendre functions; however their applicability is limited by the stability of algorithms that are used to generate their values. Their stable evaluation can be achieved by either choosing extremely large floating point numbers with an extended mantissa, cf. *Wittwer et al. (2008)*, or by re-scaling numbers, that occur during runtime, into the numerical range of double precision numbers. Since current computers and compilers are usually optimized for these numbers, respective programs are widely compliant, efficient and precise. Therefore, we opt rather for introduction of external re-scaling factors of numerical parameters in case of under-/overflow than for committing necessary calculations in extended precision domain. The scaling factors can easily be stored as additional integer values and applied in case of under-/overflow during recursive computations (cf. *Gruber, 2011*).

In the following we show two different processing results. First, a closed-loop simulation using a synthetic global gravity field model is evaluated (Spherical Harmonic Synthesis - SHS) at different grid resolutions and again expanded (Spherical Harmonic Analysis - SHA) into spherical harmonic coefficients (see Fig. 1). Root mean square errors (*RMS*) based on differences of the model after the expansion are compared. Since

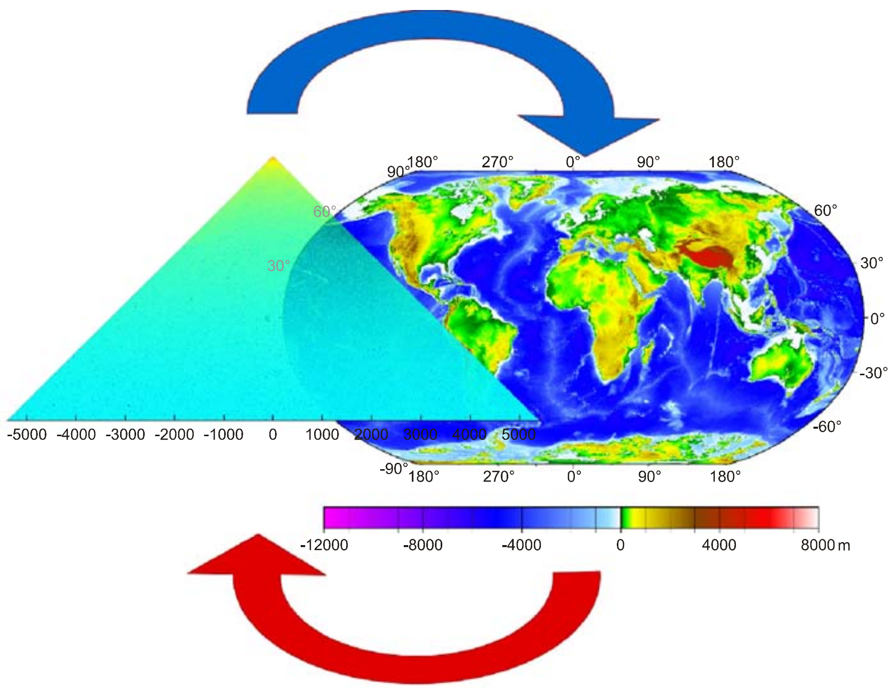

Fig. 1. Spherical harmonic analysis and spherical harmonic synthesis seen as global data grid → coefficient transformation. The image on the right was created with Generic Mapping Tools, see *Wessel and Smith (2010)*.

the process has basically been reversed, the results show the accuracy of its application but do not provide a confidence level about the evaluated grid points on the spherical grid. Thus, we compared our result with available reference solutions. This can be done until degree and order (D/O) 2700 with a software package for global SHS (HARMONIC SYNTH, see *Holmes and Pavlis, 2008*) or beyond D/O 2700 with SPHEREPACK (see *Adams and Swartztauber, 1997*). Finally, we compare these packages at a selected meridian with an alternative recursive computational method where the instability of the associated Legendre functions has entirely been eliminated (*Nesvadba, unpublished results*).

2. METHODOLOGY

The Fast Fourier Transform (FFT) can be used to expand a given regular function on the sphere into a spherical harmonic series. There are numerous algorithms that can be used for its realization, (cf. *Driscoll and Healy, 1994*; *Mohlenkamp, 1997*; *Wieczorek, 2009* and *Schwarztrauber, 1979*). However, they often leak transparency when transforming spherical harmonics into a direct 2-D Fourier series. Moreover, it is often overlooked that there exists a trigonometric series for each associated Legendre function, (see, e.g., *Hofsommer and Potters, 1960*; *Sneeuw and Bun, 1996*; *Gruber, 2008*). Due to the direct processing of the Fourier constants for the associated Legendre functions, spherical harmonics can be transformed into 2-D Fourier coefficients. Spherical harmonic series on the sphere are equivalent to exponential functions on the circle and they can be applied through SHA and SHS with the highest accuracy to data on the surface of a reference sphere. The data must be free of gaps and continuous in order to fulfil all requirements for properly posed problems.

Starting with the expansion of the gravitational potential in spherical harmonics (*Heiskanen and Moritz, 1967*)

$$V(\phi,\lambda,r)=\frac{\mu}{a_e}\sum_{l}^{\infty}\left(\frac{a_e}{r}\right)^{l+1}\sum_{m=-l}^{l}\hat{c}_{lm}\hat{Y}_{lm}(\phi,\lambda)\,, \tag{1}$$

where a_e is the reference radius (major semi-axis of the reference ellipsoid), r is the radius of the desired expansion, μ is the geocentric gravitational constant (product of the universal gravitational constant and the mass of the Earth). Complex base functions $\hat{Y}_{lm}$ are the normalized surface harmonics and $\hat{c}_{lm}$ are respective normalized spherical harmonic coefficients. Finally, the triplet (ϕ,λ,r) defines the position in terms of the geocentric radius r, spherical co-latitude ϕ and longitude λ.

The compact harmonic expression for the geopotential reads

$$V(\phi,\lambda,r)=\frac{\mu}{a_e}\sum_{l}^{\infty}\sum_{m=-l}^{l}\sum_{k=-l}^{l}\left(\frac{a_e}{r}\right)^{l+1}\exp\left[\mathrm{i}(k\phi+m\lambda)\right]\hat{q}_{lm}^{k}\,, \tag{2}$$

with newly introduced quantities

$$\hat{q}_{lm}^{k}=A_{lm}^{k}\hat{c}_{lm}\,,\quad k=-l,\,\ldots,\,l\ \text{step }2, \tag{3}$$

obtained from a Fourier expansion of the associated Legendre function

$$\bar{P}_{lm}(\sin\phi) = \sum_{k=-l}^{l} A_{lm}^{k} \exp(\mathrm{i}k\phi) \, . \tag{4}$$

Since the complex constants A_{lm}^{k} always take either an imaginary or real value (phase shift), the inverse Fourier transform can be evaluated by real coefficients a_{lm}^{k} more suitable for computations and storage (*Gruber, 2011*)

$$\bar{P}_{lm}(\sin\phi) = \mathrm{Re}\left[\sum_{k}\left(2-\delta_{k}^{0}\right)\exp(\mathrm{i}k\phi)\, a_{lm}^{k}\, \mathrm{i}^{(l-m)\bmod 2}\right], \quad k = (l \bmod 2)\ldots l,(2) \, . \tag{5}$$

The coefficients a_{lm}^{k} can be computed according to the following scheme if additional special attention is drawn to numerical instability

$$a_{l,m+1}^{k} = \begin{cases} \sqrt{j_m}\,\beta_l\, k\, a_{lm}^{k} \, , & m = 0 \, , \\ \left(\beta_{l-m}\, k\, a_{lm}^{k} + d_{lm}\, a_{l,m-1}^{k}\right) \Big/ e_{lm} \, , & l \ge m > 0 \, , \end{cases} \tag{6}$$

starting with $a_{l,0}^{k}$ for the Legendre polynomial determined directly. The stable reverse solution instead

$$a_{l,m-1}^{k} = \begin{cases} -2k\, a_{ll}^{k} \Big/ \sqrt{2l} \, , & 1 \le m = l \, , \\ \left(e_{lm} a_{l,m+1}^{k} - \beta_{l-m}\, k\, a_{lm}^{k} \Big/ d_{lm}\right) \Big/ \sqrt{j_{m-1}} \, , & 1 \le m < l \, , \end{cases} \tag{7}$$

where the sectorial ($m = l$) coefficient has to be known, can be used in combination with rescaling operations. Auxiliary values can be computed as follows (for more details, see *Gruber, 2011*)

$$\beta_{l-m} = \begin{cases} -1, & \text{for } (l-m) \text{ even} \, , \\ 1, & \text{for } (l-m) \text{ odd} \, , \end{cases}$$

$$j_m = 1 + \delta_m^0 \, ,$$

$$d_{lm} = \sqrt{(l+m)(l-m+1)} \, ,$$

$$e_{lm} = \sqrt{(l-m)(l+m+1)} \, .$$

The Legendre transformation in the spatial domain

$$\hat{f}(l,m) = \int_{0}^{\pi} \hat{f}(\phi,m)\, \bar{P}_{lm}(\sin\phi) \cos\phi \,\mathrm{d}\phi \, , \tag{8}$$

from Eq.(3) has been replaced by the multiplication of the corresponding coefficients in the spectral domain. This explains the good performance and processing speed of the method. As such, the forward computational steps are: (1) calculation of the associated Legendre functions in the Fourier base, (2) assembly of the spherical harmonic coefficients with the Fourier constants of the associated Legendre functions, and (3) a subsequent 2-D Fast Fourier Transformation.

Few modifications to Eq.(2) are necessary for its efficient evaluation. Introducing L as the maximum degree of expansion, we can transform Eq.(2) for positive orders ($0 \le m \le l$)

$$V(\phi,\lambda,r) = \frac{\mu}{a_e} \sum_{l}^{L} \sum_{m=0}^{L} \sum_{k=-l}^{l} \left(\frac{a_e}{r}\right)^{l+1} \left[\hat{q}_{lmk}^{\mathrm{Re}} \cos(k\phi + m\lambda) - \hat{q}_{lmk}^{\mathrm{Im}} \sin(k\phi + m\lambda)\right], \quad (9)$$

where $\hat{q}_{lmk}^{\mathrm{Re}}$ and $\hat{q}_{lmk}^{\mathrm{Im}}$ are real and complex components

$$\left.\begin{array}{l} \hat{q}_{lmk}^{\mathrm{Re}} \\ \hat{q}_{lmk}^{\mathrm{Im}} \end{array}\right\} = \left(2 - \delta_m^0\right) \hat{q}_{lmk}\,, \ \forall m \ge 0\,, \text{ with the Kronecker function } \delta_m^0\,. \quad (10)$$

The simplification of Eq.(9) is feasible for the real-valued function V. In the second step the summation over k will be set to positive values as well. One can put

$$V(\phi,\lambda,\bar{r}) = \sum_{m=0}^{L} \sum_{k=0}^{L} \mathrm{Re}\left[\hat{Q}_{m,+k} \mathrm{e}^{\mathrm{i}(k\phi+m\lambda)} + \hat{Q}_{m,-k} \mathrm{e}^{-\mathrm{i}(k\phi+m\lambda)}\right] \quad (11)$$

by using pro-/retrograde coefficients $\hat{Q}_{m,\pm k}$, thus concentrating all degrees $-l$ belonging to a certain order $-m$. It holds then for values k the following: $\left(+k \middle| 0 \le k \le L\right)$ as well as $\left(-k \middle| -L \le -k \le -1\right)$. For the expansion on the sphere of radius $\bar{r}$ we obtain the coefficients

$$\hat{Q}_{m,\pm k} = \frac{\mu}{a_e} \sum_{l}^{L} \left(\frac{a_e}{\bar{r}}\right)^{l+1} \left(2 - \delta_m^0\right) \hat{q}_{lm}^{k}\,, \qquad \forall m \ge 0\,. \quad (12)$$

The coefficients $Q_{m,\pm k}$ are often designated as ‘lumped coefficients’, since they combine signal amplitudes of all degrees belonging to a certain frequency. Goniometric decomposition of Eq.(11)

$$\begin{aligned} V(\phi,\lambda,\bar{r}) = \sum_{m=0}^{L} \sum_{k=0}^{L} & cc(m,k) \cos k\phi \cos m\lambda + ss(m,k) \sin k\phi \sin m\lambda \\ & + sc(m,k) \sin k\phi \cos m\lambda + cs(m,k) \cos k\phi \sin m\lambda \end{aligned} \quad (13)$$

with the coefficients

$$\begin{aligned} cc(m,k) &= +\hat{Q}_{m,+k}^{\mathrm{Re}} + \hat{Q}_{m,-k}^{\mathrm{Re}}\,, \quad ss(m,k) = -\hat{Q}_{m,+k}^{\mathrm{Re}} + \hat{Q}_{m,-k}^{\mathrm{Re}}\,, \\ sc(m,k) &= -\hat{Q}_{m,+k}^{\mathrm{Im}} + \hat{Q}_{m,-k}^{\mathrm{Im}}\,, \quad cs(m,k) = -\hat{Q}_{m,+k}^{\mathrm{Im}} - \hat{Q}_{m,-k}^{\mathrm{Im}}\,, \end{aligned} \quad (14)$$

can then be directly applied to the FFT operator.

The projection of 'lumped coefficients' or 2-D Fourier coefficients to spherical harmonic coefficients is an over-determined system, except for the zeroth order (see *Sneeuw and Bun, 1996*). The apparatus of linear algebra can be used to compute SH coefficients. The problem results in a block-diagonal normal equation system, since there are no correlations between orders m. Recalling the pro-/retrograde constants $\hat{Q}_{m,\pm k}$ from Eq.(12) given by

$$\hat{Q}_{m,\pm k} = \frac{cc \mp ss}{2} + \mathrm{i}\frac{sc \pm cs}{2} \tag{15}$$

for each order m, a system for linearly combined degrees can be solved for. The relation is given by

$$\left.\begin{matrix} \hat{q}_{m,\pm k}^{\mathrm{Re}} \\ \hat{q}_{m,\pm k}^{\mathrm{Im}} \end{matrix}\right\} = \sum_{l_{min}}^{L} \left[\lambda_l \frac{\mu}{a_e} \left(\frac{a_e}{\overline{r}} \right)^{l+1} \left(2 - \delta_m^0 \right) \right] A_{lm}^k \left\{ \begin{matrix} \overline{C}_{lm} \\ \overline{S}_{lm} \end{matrix} \right. . \tag{16}$$

The right-hand side is now the sequence $\hat{z}_m^k = \left\{ \hat{Q}_{m,-k}, \hat{Q}_{m,+k} \right\}$, where $\left(k \middle| 0 \le k \le L \right)$. The linear matrix to a certain order m is then determined by the Fourier constants of the Legendre functions, A_{lm}^k and takes the shape of a trapezoid. The coefficients are estimated by least squares, (cf. *Colombo, 1981*; *Wagner, 1983*; *Koop, 1993*; *Sneeuw, 2000*) where inclined grids have been used as a common practice in satellite geodesy,

$$\hat{\mathbf{r}}_{lm} = \left(\mathbf{A}_{lm}^k \mathbf{C}^{-1} \mathbf{A}_{lm}^k \right)^{-1} \mathbf{A}_{lm}^k \mathbf{C}^{-1} \hat{\mathbf{z}}_m^k \text{ , where } m \le l \le L, \tag{17}$$

with the a priori covariance matrix

$$\mathbf{C} = \begin{pmatrix} \sigma_{m,-L}^2 & & 0 \\ & \ddots & \\ 0 & & \sigma_{m,+L}^2 \end{pmatrix}. \tag{18}$$

The division of $\hat{r}_{lm}$ by the corresponding sensitivity coefficients from Eq.(16) completes the recovery of SH coefficients

$$\hat{c}_{lm} = \hat{r}_{lm} \left[\lambda_l \frac{\mu}{a_e} \left(\frac{a_e}{\overline{r}} \right)^{l+1} \left(2 - \delta_m^0 \right) \right]^{-1} . \tag{19}$$

Beside the absence of correlations between different orders m, only coefficients with degrees of the same parity are correlated. There is also no relation between real and imaginary quantities (*Lelgemann and Cui, 1999*), which reduces the effective system size for each order-wise recovery to a minimum range.

3. NUMERICAL TESTING OF THE PROPOSED ALGORITHM

Starting from the Earth Gravitational Model EGM08 (see *Pavlis et al., 2008*), a random method has been used to append additional synthetic geopotential coefficients up to D/O 5400 that is equivalent to the equiangular resolution 2 arcmin. A synthetic Earth gravitational model up to D/O 5400 was developed as its extension by re-scaling and recycling the SH coefficients by an algorithm of *Novák et al. (2001)* that produces a power spectrum similar to Kaula's power law and re-ordered in each degree to avoid a systematic signature.

Generally, the synthetic gravitational model consists of two parts. Spherical harmonic coefficients for D/O up to 2160/2190 were taken from EGM08. Remaining synthetic coefficients for D/O up to 5400 were generated from an artificially constructed sequence of pairs of real numbers taken from the EGM08 coefficients. Since this approach yields an unrealistic degree variance of the synthetic field, each pair of high-degree synthetic coefficients was multiplied by a simple scale factor to yield a more realistic degree variance. Scaling synthetic coefficients provided a convenient means by which the degree variance of the synthetic field would smoothly extend from EGM08 into the higher degrees providing at the same time a decaying degree variance similar to current expectations. Of course, no physical interpretation should be made regarding the synthetic gravitational model.

Using simulated gravity field parameters, a global equiangular data grid of 2 arcmin gravity disturbances has been generated by FFT and compared to the results of standard recursive computations in the spatial domain. An error in co-latitudes of $\simeq$20–30 arcdeg can be observed that is not outstanding due to the power spectral density of the spherical harmonic expansion but already reaches values up to 1 mGal. For the ultra-high resolutions, the FFT method outperforms any other calculation in time domain beyond D/O 2700.

In order to verify the performance and numerical stability of the developed software package, the experimental data were extended to a much higher resolution. The spherical harmonic expansion is not necessarily restricted to functions fulfilling the Laplace differential equation. The global topographic model ETOPO1 has been used as an example of such a function. The derived spherical harmonic model of D/O 10800 can be evaluated in different resolutions as illustrated in Fig. 2.

The software has been ported to a multi-core, shared memory implementation using OpenMP (2.5) standards. Bottle-necks, including namely matrix-matrix products, have been expanded explicitly to best suite the multi-thread approach. Further computer libraries were used including BLAS, LAPACK and FFTW3 routines. In order not to exceed the available RAM storage, larger grid and coefficient matrices had to be partitioned and swapped between RAM and permanent disks. Nevertheless, the run-time results in Table 1 - see also Fig. 3 - were achieved.

4. COMPARISON WITH OTHER METHODS

In order to test the FFT-based approach independently, the evaluation in space domain of Eq.(1) was adopted as well, whereas only the Greenwich meridian was considered for

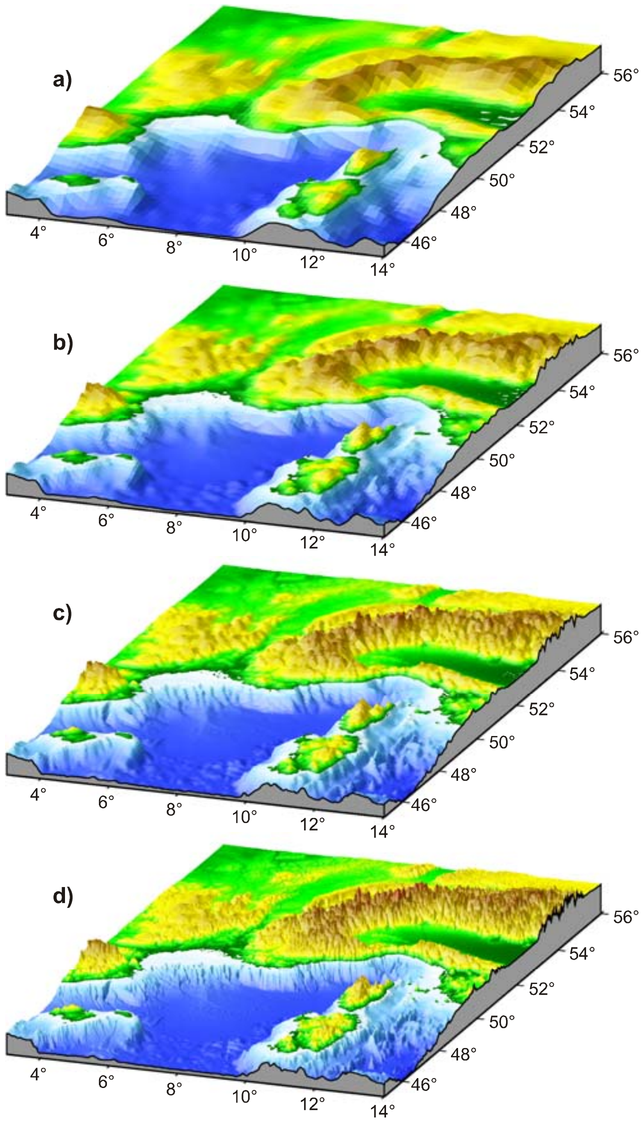

Fig. 2. Resolution refinement by use of spherical harmonics for the northern Mediterranean region. From **a)** to **d)** in degree and order 1080, 2160, 4320, 10800.

the high resolution harmonic synthesis of the gravity disturbance δg since the direct computing of Eq.(1) by means of summation is very time consuming. The associated Legendre functions of the first kind were for this purpose generated by a common recursive formula denoted as a standard column method (see *Holmes and Featherstone, 2002*),

Table 1. CPU time [hh:mm:ss] on Intel Xenon 2 × quad-core (up to 16 effective threads) architecture.

Degree	Time (SHS) [hh:mm:ss]	Scaling	Grid [pts/sec]	Time (SHA) [hh:mm:ss]	Scaling	Coefficients/sec
1080	00:00:06	4.5	389160	00:00:53	8.1	21246
2160	00:00:22	8.2	424342	00:12:08	9.5	5189
3240	00:00:58	10.6	362098	00:58:20	10.1	3003
4320	00:02:12	12.0	282829	03:11:00	9.3	1498
5400	00:04:58	12.5	195740	08:20:00	9.5	972
6480	00:06:50	13.0	204863	18:12:10	9.6	641
7560	00:10:38	13.3	179189	36:02:00	9.7	441
8640	00:18:57	13.9	131324	62:25:00	9.9	332
9720	00:22:49	13.7	138039	108:09:00	10.1	242
10800	00:41:30	14.4	93658	169:04:00	10.3	191

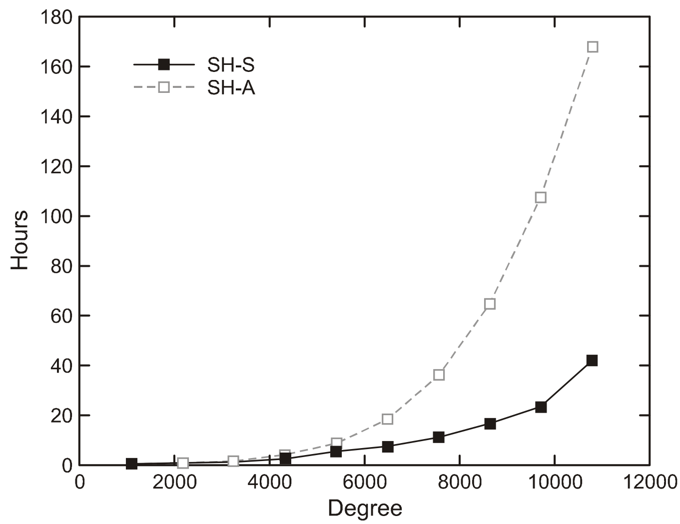

Fig. 3. CPU time estimates for SHS and SHA (multi-thread implementation, see Table 1 for details about scaling).

$$\bar{P}_{lm} = \alpha \cos\phi \bar{P}_{l-1,m} - \beta \sin\phi \bar{P}_{l-2,m} , \tag{20}$$

where

$$\alpha = \sqrt{\frac{(2n+1)(2n-1)}{(n+m)(n-m)}} , \tag{21}$$

$$\beta = \sqrt{\frac{(2n+1)(n+m-1)(m-m-1)}{(2n-3)(n-m)(n+m)}} . \tag{22}$$

The problem with this recurrence for high D/O computations is an underflow occurring when a seed (sectorial terms $\bar{P}_{ll}$) reaches the representation limit to store that value in the computer memory depending on single, double or extended precision. Using the same recursive relation relatively with regard to the mantissa (including sign) and the exponent such that the algorithm considers only relative numbers within one recursive step, one can produce associated Legendre functions almost without any D/O restrictions when neglecting rounding errors (*Nesvadba, unpublished results*). Rewriting Eq.(20) exponent-wise we get

$$M\left(\bar{P}_{lm}\right) = \alpha \cos\phi M\left(\bar{P}_{l-1,m}\right) - \beta \sin\phi M\left(\bar{P}_{l-2,m}\right) k\,, \tag{23}$$

where k is the exponent difference satisfying $k = 10^{E\left(\bar{P}_{l-2,m}\right) - E\left(\bar{P}_{l-1,m}\right)}$, M denotes the mantissa of a particular number and E its exponent. Once we have the Legendre functions split into two parts, all values in-between the limits of computation precision can be used in SHS and the rest (with very low magnitudes) can be set zero.

Differences between the refined FFT-based approach presented in this article and respectively SPHEREPACK, HARMONIC SYNTH and the standard column method with the significant exponent division are shown in Fig. 4. The upper left part shows SHS of δg up to D/O 3600. One notices that HARMONIC SYNTH built specially for EGM08

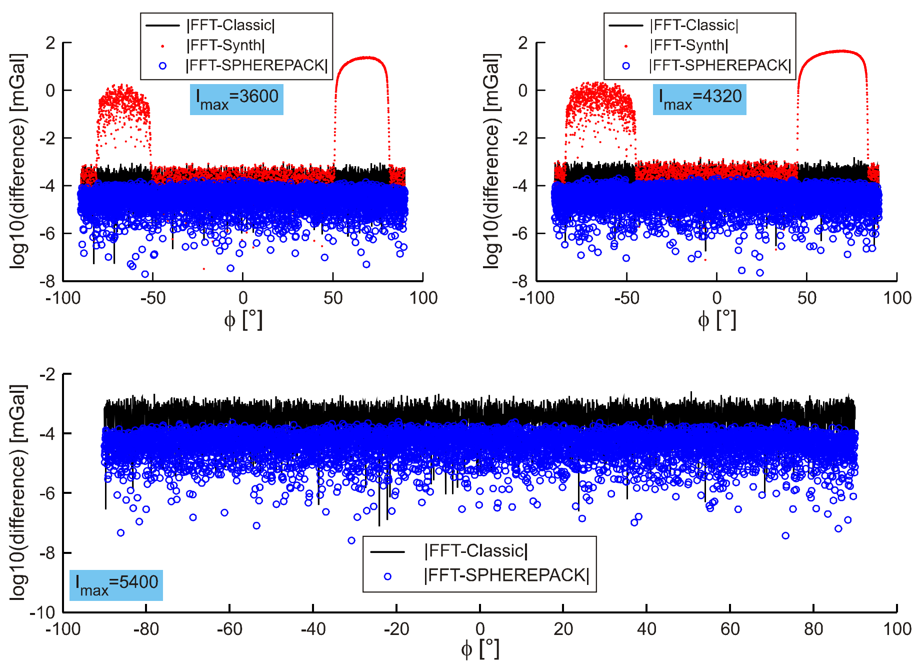

Fig. 4. Comparison of FFT-based approach and other solutions (1 arcmin equiangular sampling along the Greenwich meridian).

(D/O 2190) fails in some critical regions. These areas enlarged when we considered even higher resolution D/O 4320 as shown in the upper right part of Fig. 4. Comparing FFT, SPHEREPACK with the exponent-wise recurrence it can be concluded that we get a satisfactory agreement even up to D/O 5400 (lower part of Fig. 4) for all latitudes. However, the agreement between the refined FFT-based approach and the SPHEREPACK solution is at least one order of magnitude better than compared with our exponent-wise algorithm due to its implicit truncation.

5. CONCLUSIONS

The use of 2-D Fourier methods for the calculation of surface spherical harmonic synthesis as well as analysis of geophysical data is a true alternative to specialized program packages for spherical harmonic transformation of a scalar function on the sphere. When using common multi-processor architecture highly competitive run-times can be achieved. The stability of the algorithm, which is a critical issue in many alterative approaches, is maintained up to very high spatial resolutions. Our test demonstrated that the algorithm can be stable up to D/O 10800, which corresponds to an angular resolution of 1 arcmin.

The increasing amount and availability of global geodetic and geophysical data, the need for their processing and analysis in both spatial and spectral domains will see many applications of harmonic transformations in the future. The method described above can be used as general algorithm for spherical harmonic synthesis and analysis for D/O of the order of tens of thousands.

The development of the proposed method still continues with the intention to eventually develop a program capable of computing not only values of the respective scalar function itself but also values of its functionals (first- and second-order directional derivatives). This is very often required in geodesy where SH coefficients of the geopotential are given but values of its gradients are needed. Further improvements include the change of coordinates (spherical to one-parametric ellipsoidal) and evaluation of values in a general point outside the reference sphere.

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