On the Numerical Problems of Spherical Harmonics: Numerical and Algebraic Methods Avoiding Instabilities of the Associated Legendre's Functions

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Summary
Spherical harmonics are widely used to describe the structure of the Earth's gravity field. When detailed features of the Earth's gravity field are required one may be confronted with numerical problems of spherical harmonics. These problems can be treated by numerical and algebraic methods. Extending the range of real numbers on computer is preferred in numerical methods. This can be achieved by choosing a proper standard floating point arithmetic format or by extended-range arithmetic and arbitrary precision libraries. In algebraic methods the range of the magnitudes of the spherical harmonics is reduced by algebraic manipulations. Based on the algebraic methods normalized and scaled equivalents of the spherical harmonics can be derived.
In the present contribution numerical and algebraic methods avoiding the numerical problems of the spherical harmonics are discussed. Limits of the numerical and algebraic methods are studied in a numerical experiment. It is shown that current computer facilities and simple algebraic manipulations allow evaluation of the spherical harmonic expansions above degree and order 20000.

Zusammenfassung
In vielen Anwendungen ist es gebräuchlich, das Erdschwerefeld in eine Kugelfunktionsreihe zu entwickeln. Sobald jedoch hochfrequente Strukturen dargestellt werden sollen, kann es zu numerischen Instabilitäten bei der Berechnung der Kugelfunktionen kommen. Zur Bewältigung dieser Probleme stehen sowohl numerische als auch mathematische Methoden zur Verfügung. Auf numerischer Seite wird üblicherweise versucht, die Bandbreite der darstellbaren reellen Zahlen zu erhöhen. Hierzu wählt man entweder ein entsprechendes Standardformat für die Darstellung von Fließkommazahlen, oder man verwendet eine spezielle Bibliothek für Darstellungen mit beliebiger Genauigkeit. Im Rahmen der mathematischen Methoden wird versucht, den Wertebereich der Kugelfunktionen auf algebraische Weise einzuschränken, indem normierte bzw. skalierte Varianten der ursprünglichen Funktionen verwendet werden.
Im vorliegenden Beitrag werden bestehende numerische und mathematische Methoden zur Vermeidung numerischer Instabilitäten bei der Berechnung von Kugelfunktionen diskutiert. Die jeweiligen Beschränkungen werden anhand numerischer Experimente dargelegt. Damit lässt sich zeigen, dass derzeit verfügbare rechentechnische Methoden und einfache mathematische Manipulationen eine stabile Berechnung der Kugelfunktionsentwicklungen bis über Grad und Ordnung 20000 hinaus ermöglichen.

Keywords: Programming language C, Floating point arithmetic

1 Introduction

Scientific disciplines dealing with computational problems have been affected by the progress of personal computers. With proper hardware and software facilities, formerly scientific tasks can now be solved routinely. Moreover, improvement and development of new computational methods is directly stimulated. In spite of the advantages emerging from the exploitation of personal computers, limitations have to be considered. These are mainly introduced by the finite computer representation of real numbers according to floating point arithmetic (FPA). Therefore attention should be paid to the stability of the computational algorithms in order to avoid unexpected errors occurring from underflow or overflow problems.

Spherical harmonic expansions (SHEs) are of particular interest in many theoretical and practical applications. One is confronted with this relatively simple mathematical tool in a variety of problems and at different spatial scales. For example, spherical harmonics are employed to study particles in quantum chemistry, geomagnetic field, and cosmic electromagnetic radiation of the universe. In addition spherical harmonics are important when image recognition in computer graphics is performed. In geodesy, SHEs are widely used in the determination of the Earth's gravity field. Products of geopotential coefficients defining physical properties of the Earth and mathematically defined spherical harmonics are simply added up to a maximum degree of the expansion. In this way, the gravitational potential and its functionals can be approximated. However, when a more detailed description of the gravity field is required higher degree terms of the SHEs have to be taken into account. In this case, one is confronted with numerical problems which originate due to the colatitude dependent part of the spherical harmonics, i. e. the associated Legendre's functions of the first kind (ALFs). Depending on the spherical colatitude, degree and order of the SHEs magnitudes of the ALFs can reach several hundreds or even thousands of orders of magnitude.

Generally numerical problems of the spherical harmonics can be treated by two distinct methods. Choice of an extended computer representation of real numbers is preferred in the first method. In this way spherical harmonics should be represented on computer for all of their magnitudes. Modern representation of real numbers given by FPA standard can be followed in which single, double and quadruple formats are specified. Alternatively extended-range arithmetic or arbitrary precision libraries can be used. In the second method the magnitude range of the spherical harmonics is reduced by algebraic manipulations. This mathematical approach is important when bounds of the most precise FPA format are overrun. Spherical harmonics are multiplied by proper factors according to their degree, order and spherical colatitude. Based on the mathematical principles normalized and scaled equivalents of the spherical harmonics can be introduced.

In the present contribution numerical and algebraic methods to avoid numerical problems with spherical harmonics are demonstrated. In section 2, SHE of the gravitational potential is given and the origin of the numerical problems of the spherical harmonics is identified. FPA standards and representation of real numbers on computers are described in section 3. Numerical methods avoiding numerical problems of the spherical harmonics are discussed as well. In section 4 algebraic methods based on normalizing and scaling the spherical harmonics are introduced. Numerical experiments in which limits of the numerical and algebraic methods have been validated can be found in section 5. In the conclusions the significance of the present contribution and important facts are mentioned.

2 Definition of the problem

The gravitational potential representing a fundamental scalar quantity of the Earth's gravity field can be expanded in a series of spherical harmonics. In the same manner its functionals, such as geoid heights, gravity anomalies, gravity disturbances, deflections of the vertical and gravitational tensor components, can be expressed. Due to this versatility SHEs are widely used in geodetic applications. Recently the International Centre for Global Earth Models (ICGEM, http://icgem.gfz-potsdam.de/ICGEM) has been established by the International Association of Geodesy which directly stimulates even broader usage of the SHEs.

Derivation of the gravitational potential in the series of spherical harmonics can be found in classical textbooks (Vaníček and Krakiwsky 1982, Hofmann-Wellenhof and Moritz 2005). It is not our purpose to recapitulate this derivation. Rather the definition of individual variables and parameters of the final formula is given in this section. This section is also considered as a starting point from which the origin of the numerical problems of the spherical harmonics will be identified. From the mathematical point of view the final formula for the gravitational potential in the series of the spherical harmonics represents a double summation over degree n and order m of the following form (Hofmann-Wellenhof and Moritz 2005, Eq. 2-78)

$$V\left(r,\theta,\lambda\right) = \frac{GM}{a}\sum_{n=0}^{N_{\max}}\left(\frac{a}{r}\right)^{n+1}\sum_{m=0}^{n}\left[C_{n,m}\,R_{n,m}\left(\theta,\lambda\right)+S_{n,m}\,T_{n,m}\left(\theta,\lambda\right)\right]. \quad (1)$$

In Eq. (1), (r,θ,λ) is the triplet of the spherical coordinates (geocentric radius, spherical colatitude and spherical longitude), GM is the product of the Newtonian gravitational constant and the Earth's mass including oceans and atmosphere, a represents the semi-major axis of a reference ellipsoid, $C_{n,m}$, $S_{n,m}$ are the dimensionless geopotential coefficients and $R_{n,m}(\theta,\lambda)$, $T_{n,m}(\theta,\lambda)$ are the surface spherical harmonics. An important parameter in Eq. (1) is the maximum degree of the SHE, $N_{\max}$. Its value determines the maximum spatial resolution of the Earth's gravity field by $R\pi/N_{\max}$ where R is the radius of the Earth.

Computation of the gravitational potential at an arbitrary point defined by spherical coordinates (an evaluation point) is possible when all variables and parameters in Eq. (1) are known. Geopotential coefficients define physical properties of the Earth and their values are constant regardless of the position of an evaluation point. The set of geopotential coefficients up to degree and order $N_{\max}$ represents a global gravity model (GGM) including GM and a. A single GGM is a text file which contains numbers arranged by degree and order. Several GGMs are publicly available at the ICGEM webpage. In contrast to the geopotential coefficients, the spherical harmonics are mathematically defined and depend on the position of an evaluation point. Standard definition of the surface spherical harmonics is based on the separation into the spherical colatitude and longitude dependent parts when (Hofmann-Wellenhof and Moritz 2005, Eq. 1-50)

$$R_{n,m}\left(\theta,\lambda\right) = P_{n,m}\left(\theta\right)\cos m\lambda, \quad (2)$$

$$T_{n,m}\left(\theta,\lambda\right) = P_{n,m}\left(\theta\right)\sin m\lambda. \quad (3)$$

In Eqs. (2) and (3), the new functions $P_{n,m}(\theta)$ stand for the ALFs for which differential and integral definitions have been introduced (Ferrers 1877, Hobson 1965, Abramowitz and Stegun 1972, Hofmann-Wellenhof and Moritz 2005). Recursive formulae when the actual ALF is computed from the previous ones are especially convenient for the SHEs. Several recursion schemes have been proposed (Hobson 1965, Belikov 1991, Holmes and Featherstone 2002a, Holmes 2003). In this study we consider only one recursion scheme defined by the following set of Eqs. (Abramowitz and Stegun 1972)

$$P_{0,0}(\theta) = 1,\ P_{1,1}(\theta) = u = \sin\theta, \tag{4}$$

$$P_{m,m}(\theta) = (2m-1)\,u\,P_{m-1,m-1}(\theta), \forall\, m > 1\,, \tag{5}$$

$$P_{n,m}(\theta) = \begin{cases} \dfrac{2n-1}{n-m} t\, P_{n-1,m}(\theta), \forall\, n = m+1, \\ \dfrac{2n-1}{n-m} t\, P_{n-1,m}(\theta) - \dfrac{n+m-1}{n-m} P_{n-2,m}(\theta), \forall\, n > m+1\,. \end{cases} \tag{6}$$

where $t = \cos\theta$. Evaluation of the ALFs is initiated by the start values in Eq. (4). When $m > 1$ sectorial (i.e. $n = m$) ALFs are evaluated by Eq. (5) based on the previous sectorial ALF. Sectorial ALFs are computed in the direction of the diagonal, see Fig. 1. Zonal (i.e. $n = 0$) and tesseral (i.e. $n \neq m \wedge n \neq 0$) ALFs are generated by Eq. (6). These require sectorial ALFs of the same order when $n = m + 1$, otherwise previous two ALFs of the same order have to be given. Evidently zonal and tesseral ALFs of the same order are computed in the direction of a row in Fig. 1. Spherical harmonics are therefore completely defined by Eqs. (2)–(6). Now all parameters and variables in Eq. (1) are given.

In Eqs. (4)–(6), numerical problems of the spherical harmonics have been indirectly introduced. A simple analysis of Eq. (5) shows that $P_{m,m}(u = 1) = (2m-1)!!$ for evaluation points in the equatorial plane. It is well known that the evaluation of factorials is connected with numerical problems because of their large range of magnitudes. A similar behavior can be observed in the case

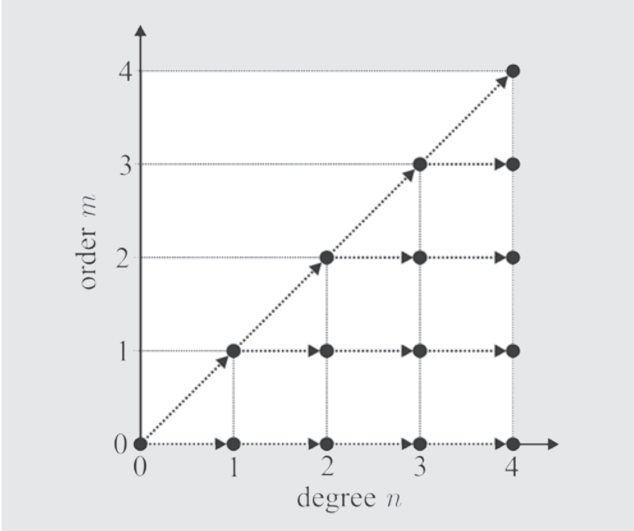

Fig. 1: Diagram for the computation of the ALFs by recursive formulae

of the ALFs, see Fig. 2. For a maximum degree of the SHE $N_{max} = 100$ ALFs cover almost 200 orders of magnitude. ALFs become larger with increasing degree and order for each spherical colatitude. It is also evident that the range of magnitude is increasing towards the equatorial plane even though there are only slight differences for colatitudes between 60° and 90°. At the equator itself the sectorial ALFs are predominant. Otherwise a special pattern is visible at the equator caused by the fact that most tesseral ALFs are equal to zero when the logarithm is not defined. On the other hand sectorial and tesseral ALFs are equal to zero at the poles. In the sequel the above

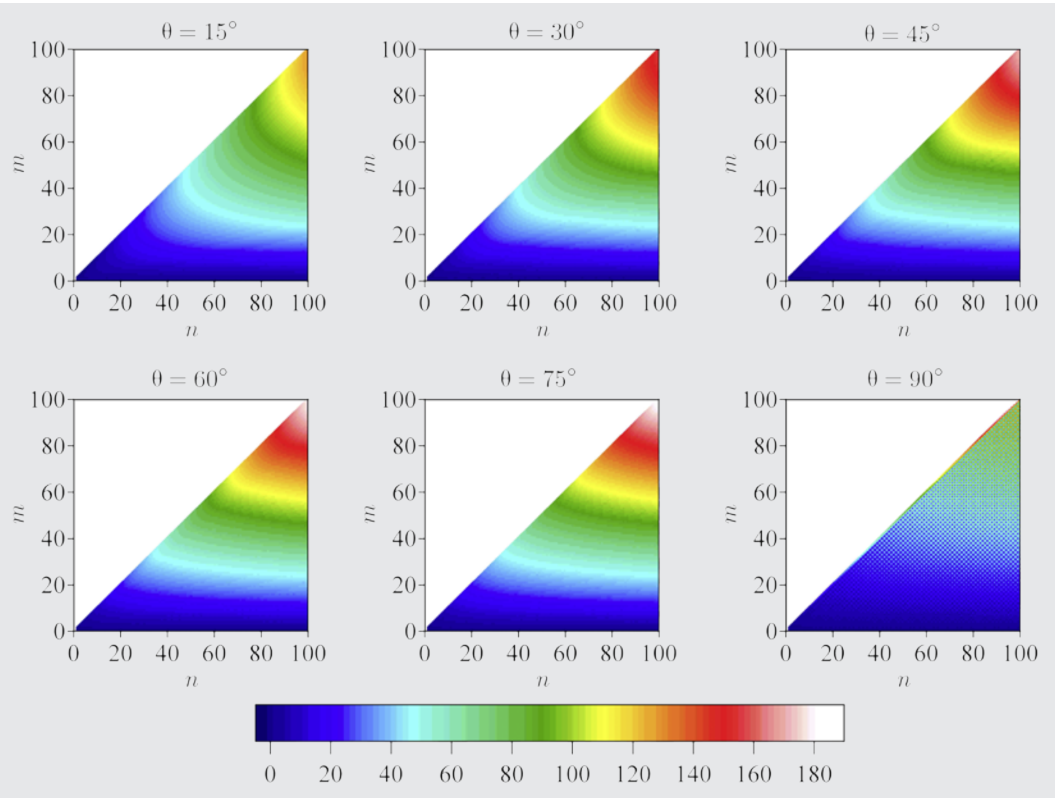

Fig. 2: Graphical representation of $\log_{10}|P_{n,m}(\theta)|$. Selected spherical colatitudes are depicted in each panel. Magnitude is indicated by color scale.

mentioned facts will be considered as numerical problems of the spherical harmonics. In geodesy numerical problems of the spherical harmonics have been treated according to requirements. Especially when a significant refinement of the maximum spatial resolution of the Earth's gravity field has been expected this question has arisen as well.

3 Numerical methods avoiding numerical problems of the spherical harmonics

The topic of a proper representation of real numbers in a computer arrived with the first computational problems. Among several possibilities for the representation of real numbers, FPA based computation became standard practice since mid 1950s. During the subsequent two decades each computer manufacturer designated its own FPA. This caused inconsistent results when a program was executed on different machines. In order to retain the portability of software, unification of the FPA proposals was required. Under the patronage of the Institute for Electrical and Electronics Engineers (IEEE) the first binary FPA standard (IEEE Computer Society 1985) was introduced. Later on radix-independent FPA standard (IEEE Computer Society 1987) was provided in order to support decimal floating point machines. A deep revision of the former standards lead to an up-to-date standard formulation (IEEE Computer Society 2008) based upon recent developments in computer science.

Generally FPA is based on exponential notation in which a real number x is expressed as (Overton 2001)

$$x = \pm S \times B^{E}, 1 \leq S < B - 1, \tag{7}$$

where S represents the significant (also called mantissa), B stands for the base and E is the exponent. A computer word representing a real number has the form of a bit sequence which can be divided into the sign, significant and exponent fields. One bit is required for the sign because only two values (positive or negative) are expected. The extent of the significant and exponent fields differs depending on the FPA format. In (IEEE Computer Society 2008) three binary and two decimal FPA basic formats are specified. However, we experience incomplete implementation of the decimal FPA basic formats in available mathematical libraries. Thus only binary FPA basic formats (single, double and quadruple) will be considered. Their important characteristics such as total number of bits, number of bits for the significant and exponent fields, range of the exponential values and of real numbers are summarized in Tab. 1. It is evident that the current FPA standard allows the magnitudes of real numbers to vary from several tens of orders in the single format up to several thousands of orders in the quadruple format. However, limitations of the FPA formats have to be kept in mind. Below the smallest number only zero is considered and the underflow problem occurs. Above the largest number NaN (Not a Number) or $\pm\infty$ exceptions lead to the overflow problem. A FPA format is defined not only by the range but also by the precision. Precision of FPA formats can be expressed in terms of the machine epsilon (representing a gap between one and the next floating point number) or by the number of significant digits. Machine epsilon and number of significant digits for single, double and quadruple binary FPA basic formats are summarized in Tab. 2. Individual FPA formats are often resolved in this context, therefore one is confronted with the terms single, double and quadruple precision.

Full capability of the FPA standard requires its implementation. Processor manufacturers are responsible

Tab. 2: Precision of binary FPA basic formats (approximate evaluation of the machine epsilon in decimal format is considered).

FPA format	Machine epsilon	Significant digits
Single	2^{-23} (10^{-7})	7
Double	2^{-52} (10^{-16})	16
Quadruple	2^{-112} (10^{-34})	34

Tab. 1: Binary FPA basic formats and their characteristics (E_{min} and E_{max} stand for the minimum and maximum values of the exponent; approximate evaluation of the smallest and largest numbers in decimal format is listed).

FPA format	Total number of bits	Exponent bits	Significant bits	E_{min}/E_{max}	smallest/largest numbers
Single	32	8	23	−126 / 127	$\pm 2^{-126}/\pm 2^{127}$ ($\pm 10^{-38}/\pm 10^{38}$)
Double	64	11	52	−1022 / 1023	$\pm 2^{-1022}/\pm 2^{1023}$ ($\pm 10^{-308}/\pm 10^{308}$)
Quadruple	128	15	112	−16382 / 16383	$\pm 2^{-16382}/\pm 2^{16383}$ ($\pm 10^{-4932}/\pm 10^{4932}$)

for hardware implementation. Simple mathematical operations on real numbers such as addition, subtraction, multiplication and division are performed directly by a processor. This allows considerable saving of computational time. Software developers involve FPA standard in compilers and mathematical libraries enabling software portability. However, implementation of FPA standard represents a complex problem which may take several years. Therefore more flexible extended-range arithmetic and arbitrary precision libraries have been developed, using the same principles as described for FPA standard. The extended-range arithmetic library is a collection of mathematical functions and routines for programming with a separate storage location for the exponent of a real number. An arbitrary precision library may be defined in a similar way. However, varying range of real numbers is achieved by direct choice of the total number of bits by which a real number is represented and mathematical operations are performed. Due to this flexible representation of real numbers hardware implementation of the extended-range arithmetic and arbitrary precision libraries in processors cannot be expected causing considerable growth of computational time.

Numerical methods to avoid numerical problems with spherical harmonics are based on the choice of a more suitable FPA format defined by standardized, extended-range arithmetic or by arbitrary precision libraries. Geodetic contributions addressing numerical problems of spherical harmonics have preferred standardized FPA formats. It is also logical that the FPA format with the highest total number of bits has been selected in geodetic applications. For example in the 1980s, shortly before the first FPA standard, limitations of the single format were discussed by Tscherning and Poder (1982) and Melvin (1985). A decade later standardized double format deserved attention for the same reason (Wenzel 1998, Holmes and Featherstone 2002a, b, Holmes 2003). Quadruple format is specified in the current FPA standard with consequent applications in recent studies (Petrovskaya and Vershkov 2008, Fantino and Casotto 2009). The quadruple format safely covers actual demands in the determination of the Earth's gravity field using SHEs. Extended-range arithmetic has also been applied to avoid numerical problems of spherical harmonics (Lozier and Smith 1981, Smith et al. 1981, Olver and Smith 1983, Nesvatba 2008). By this approach SHEs may be evaluated up to an arbitrary degree and order at the price of much higher computational time (Wittwer et al. 2008). On the other hand, the possibilities of arbitrary precision libraries (Brendt 1978, http://www.mpfr.org) have never been extensively studied in the context of the numerical problems of the spherical harmonics.

4 Algebraic methods avoiding numerical problems of spherical harmonics

Instead of relying on an extended range of real numbers in numerical methods, attenuation factors of the spherical harmonics are sought in algebraic methods. Two algebraic approaches to avoid numerical problems of the spherical harmonics are selected. Normalized and scaled equivalents of the spherical harmonics are defined and compared with those defined in section 2. Notions related to the FPA introduced in section 3 are used routinely. The expression "unnormalized spherical harmonics" refers to those defined by Eqs. (2) and (3).

4.1 Gravitational potential in a series of normalized spherical harmonics

Overflow problems may occur for unnormalized spherical harmonics of higher degrees and orders. Existence of a number dependent on degree and order by which the unnormalized spherical harmonics are multiplied in order to attenuate the range of their magnitudes may be intuitively supposed. Indeed such a number can be found applying the norm operator well known from functional analysis. Let us introduce the normalized spherical harmonics $\bar{R}_{n,m}(\theta,\lambda)$ and $\bar{T}_{n,m}(\theta,\lambda)$. Suppose that the average of any squared normalized spherical harmonic over a unit sphere σ is unity, i. e. (Hofmann-Wellenhof and Moritz 2005, Eq. 1-92)

$$\frac{1}{4\pi}\iint_{\sigma}\left[\bar{R}_{n,m}\left(\theta,\lambda\right)\right]^{2}\mathrm{d}\sigma=\frac{1}{4\pi}\iint_{\sigma}\left[\bar{T}_{n,m}\left(\theta,\lambda\right)\right]^{2}\mathrm{d}\sigma=1\,, \tag{8}$$

and in compliance with Eqs. (2) and (3) the normalized spherical harmonics can be defined as follows (ibid., Eq. 1-95)

$$\bar{R}_{n,m}\left(\theta,\lambda\right)=\bar{P}_{n,m}\left(\theta\right)\cos m\lambda\,, \tag{9}$$

$$\bar{T}_{n,m}\left(\theta,\lambda\right)=\bar{P}_{n,m}\left(\theta\right)\sin m\lambda\,, \tag{10}$$

where

$$\bar{P}_{n,m}(\theta)=P_{n,m}(\theta)\sqrt{\left(2n+1\right)\frac{2}{1+\delta_{m,0}}\frac{\left(n-m\right)!}{\left(n+m\right)!}}\,. \tag{11}$$

From Eq. (11), the square root term represents the desired number dependent on degree and order (thereafter denominated as normalization factor), therefore the assumption of its existence has been proved. In Eq. (11), $\bar{P}_{n,m}(\theta)$ are the normalized ALFs and $\delta_{m,0}$ represents Kronecker's delta symbol. Also the transition between the unnormalized and normalized spherical harmonics is provided by this equation.

In order to avoid numerical problems of the unnormalized spherical harmonics, normalization factors have to be taken into account in recursive formulae for the ALFs. Considering normalization factors in Eqs. (4)–(6), recursive formulae for the normalized ALFs are obtained in the following form (e.g., Colombo 1981)

$$\bar{P}_{0,0}(\theta) = 1,\ \bar{P}_{1,1}(\theta) = \sqrt{3}\,u\,, \tag{12}$$

$$\bar{P}_{m,m}(\theta) = \sqrt{\frac{2m+1}{2m}}\,u\,\bar{P}_{m-1,m-1}(\theta), \forall\, m > 1\,, \tag{13}$$

$$\bar{P}_{n,m}(\theta) = \sqrt{\frac{(2n-1)(2n+1)}{(n-m)(n+m)}}\,t\,\bar{P}_{n-1,m}(\theta) - \sqrt{\frac{(2n+1)(n+m-1)(n-m-1)}{(n-m)(n+m)(2n-3)}}\,\bar{P}_{n-2,m}(\theta), \forall\, n > m\,. \tag{14}$$

Finally the gravitational potential in the series of the normalized spherical harmonics is expressed as

$$V(r,\theta,\lambda) = \frac{GM}{a}\sum_{n=0}^{N_{\max}}\left(\frac{a}{r}\right)^{n+1}\sum_{m=0}^{n}\left[\bar{C}_{n,m}\,\bar{R}_{n,m}(\theta,\lambda) + \bar{S}_{n,m}\,\bar{T}_{n,m}(\theta,\lambda)\right]. \tag{15}$$

Comparing Eqs. (1) and (15), it can be seen that the SHE has slightly changed. Normalized spherical harmonics involve normalization factors for all degrees and orders. In order to preserve Eq. (1) valid, geopotential coefficients have to be divided by these factors. Therefore in Eq. (15), the so called normalized geopotential coefficients have been introduced by the symbols $\bar{C}_{n,m}$ and $\bar{S}_{n,m}$.

The normalization factors reduce numerical problems. In Fig. 3, the logarithm of the normalized spherical harmonics is illustrated for the selected spherical colatitudes. It is immediately evident that the magnitudes cover only a few tens of orders for colatitudes between 45° and 90°. The range of their magnitudes is increasing towards the poles. Directly at the poles only zeros for sectorial and tesseral normalized ALFs can be found when the logarithm is not defined. In comparison with Fig. 2 we observe completely different patterns. The logarithm of the normalized ALFs reaches negative values indicating very small numbers close to zero. Introduction of the normalization factor turns the overflow problem into its underflow counterpart. While the range of magnitudes of unnormalized ALFs increases towards the equatorial plane, the range of magnitudes of normalized ALFs increases towards the poles. The unnormalized ALFs in Fig. 2 reach almost 200 orders of magnitudes for the maximum degree of the SHE $N_{\max} = 100$. A similar range of magnitudes for the normalized ALFs occurs at the maximum degree of the SHE $N_{\max} = 360$. Therefore we may obtain more detailed features of the Earth's gravity field. Indeed, while unnormalized spherical harmonics allowed SHEs approximately up to $N_{\max} = 30$ (Rapp 1997), their normalization provided SHEs up to degree and order 360 (Lemoine et al. 1998). Probably for this reason normalized spherical harmonics became convention in the determination of the Earth gravity field. We also note that state-of-the-art GGMs are composed of purely normalized geopotential coefficients.

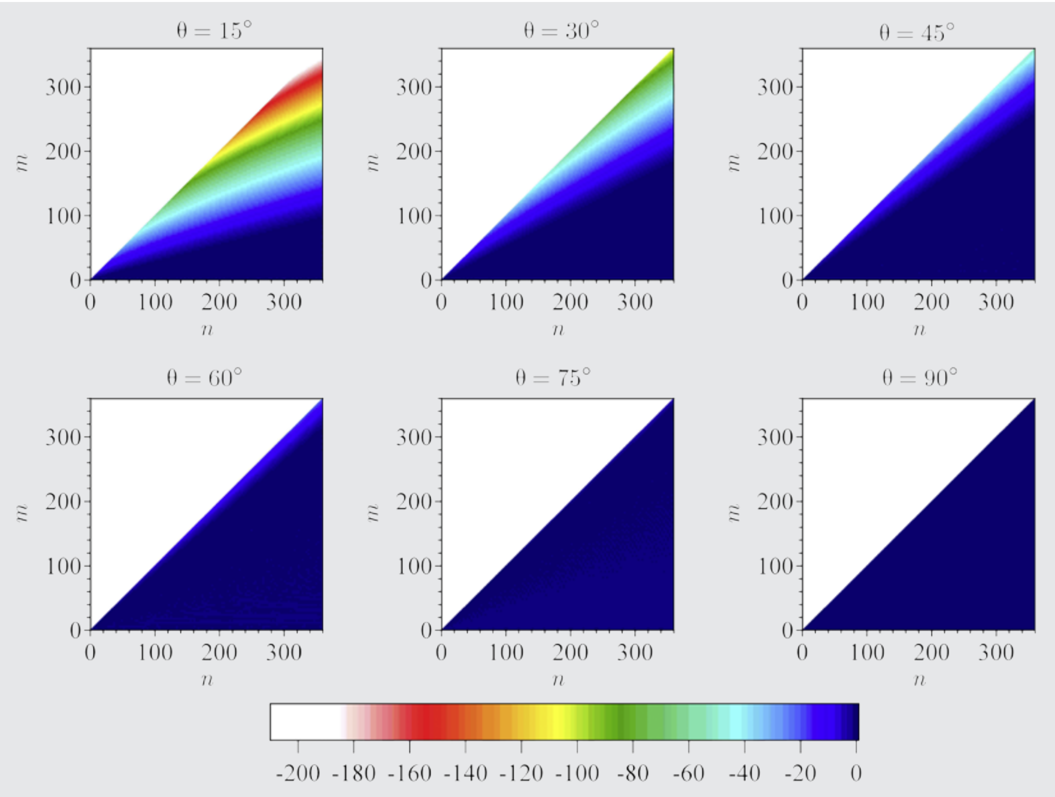

Fig. 3: Graphical representation of $\log_{10}\left|\bar{P}_{n,m}(\theta)\right|$. Selected spherical colatitudes are depicted in each panel. Magnitude is indicated by color scale.

4.2 Gravitational potential in a series of scaled spherical harmonics

The values of the normalized spherical harmonics tend to zero. Towards the poles the values become smaller and underflow problems may occur for a certain degree and order. The origin of this behaviour is hidden in Eq. (13), by which sectorial ALFs are generated. Recursive computation in this equation requires evaluation of u^m which tends to zero especially when $u \to 0$ ($\theta \to 0°$). It is therefore natural to multiply the recursive formulae (12)–(14) by an inverse of u^m in order to avoid possible underflow problems. We thus obtain the scaled ALFs which can be evaluated by the following recursive formulae (Holmes and Featherstone 2002a, Holmes 2003)

$$\frac{\bar{P}_{0,0}(\theta)}{u^0} = 1, \quad \frac{\bar{P}_{1,1}(\theta)}{u^1} = \sqrt{3}, \tag{16}$$

$$\frac{\bar{P}_{m,m}(\theta)}{u^m} = \sqrt{\frac{(2m+1)}{2m}}\,\frac{\bar{P}_{m-1,m-1}(\theta)}{u^{m-1}}, \forall\, m > 1, \tag{17}$$

$$\frac{\bar{P}_{n,m}(\theta)}{u^m} = \sqrt{\frac{(2n-1)(2n+1)}{(n-m)(n+m)}}\,t\,\frac{\bar{P}_{n-1,m}(\theta)}{u^m} - \sqrt{\frac{(2n+1)(n+m-1)(n-m-1)}{(n-m)(n+m)(2n-3)}}\,\frac{\bar{P}_{n-2,m}(\theta)}{u^m}, \forall\, n > m. \tag{18}$$

Correspondingly scaled spherical harmonics are introduced in the form

$$\bar{\bar{R}}_{n,m}(\theta,\lambda) = \frac{\bar{P}_{n,m}(\theta)}{u^m}\cos m\lambda, \tag{19}$$

$$\bar{\bar{T}}_{n,m}(\theta,\lambda) = \frac{\bar{P}_{n,m}(\theta)}{u^m}\sin m\lambda. \tag{20}$$

We note that the expression of the gravitational potential by a series of scaled spherical harmonics is not straightforward. For normalized spherical harmonics the normalization factor depends on degree and order. The presence of its inverse in the normalized geopotential coefficients $\bar{C}_{n,m}$ and $\bar{S}_{n,m}$ preserves the validity of Eq. (1). However, the additional factor $1/u^m$ introduced by the scaled spherical harmonics in Eqs. (19) and (20), depends also on the position of an evaluation point. If we multiply the normalized geopotential coefficients by u^m, we preserve the validity of Eq. (1). But the normalized geopotential coefficients become dependent on the position, which is not reasonable. Fortunately position independent normalized geopotential coefficients and the validity of Eq. (1) can be accomplished by an algorithm which is known as Horner's scheme (see, e.g., Harris and Stöcker 1998). According to Horner's scheme the following expression for the gravitational potential in the series of scaled spherical harmonics can be found

$$\begin{aligned} V(r,\theta,\lambda) &= \frac{GM}{a}\sum_{m=0}^{N_{\max}} V_m(r,\theta,\lambda) \\ &= \frac{GM}{a} V_0(r,\theta,\lambda) \\ &+ \frac{GM}{a} u\left\{V_1(r,\theta,\lambda) + u\left[V_2(r,\theta,\lambda) + \ldots + u\left(V_{N_{\max}}(r,\theta,\lambda)\right)\right]\right\}, \end{aligned} \tag{21}$$

where

$$V_m(r,\theta,\lambda) = \sum_{n=m}^{N_{\max}} \left(\frac{a}{r}\right)^{n+1} \left[\bar{C}_{n,m}\bar{\bar{R}}_{n,m}(\theta,\lambda) + \bar{S}_{n,m}\bar{\bar{T}}_{n,m}(\theta,\lambda)\right]. \tag{22}$$

In Eq. (22), partial sums of order m are computed for the gravitational potential using the scaled spherical harmonics and normalized geopotential coefficients. Consequently rescaling is performed in Eq. (21) by which the resulting value of the gravitational potential is evaluated.

We now consider numerical aspects of the scaled spherical harmonics. The graphical representation of the scaled ALFs in Fig. 4 reveals an increasing range of magnitudes towards the poles. At the poles, the scaled spherical harmonics reach their highest range of magnitudes with increasing degree and order. We note from Fig. 4 that scaled ALFs are not exactly equal to zero at the equator. Assuming the maximum degree of the SHE $N_{\max} = 1000$ more than 200 orders of magnitudes can be observed. For the normalized spherical harmonics in Fig. 3 comparable amount of orders has been reached at $N_{\max} = 360$. Evidently further improvement of numerical problems has been achieved by the scaled spherical harmonics. From the numerical point of view, by introducing the scaled spherical harmonics the underflow problem has been reversed again to an overflow problem.

Originally, the concept of scaled spherical harmonics was introduced by Tschering and Poder (1982) and independently by Libbrecht (1985). However, it did not attract special attention until ultra high SHEs ($N_{\max} > 2000$) were required. This concept has been revisited by Holmes and Featherstone (2002a, b) and Holmes (2003) and lead to first ultra high SHEs provided by synthetic Earth gravity models up to $N_{\max} = 2160$ (Haagmans 2000, Novák et al. 2001). Recently a significant improvement in the resolution of the Earth gravity field has been achieved by the EGM2008 (Pavlis et al. 2008). Normalized geopotential coefficients of this model are available up to $N_{\max} = 2190$ corresponding to the maximum spatial resolution $5' \times 5'$.

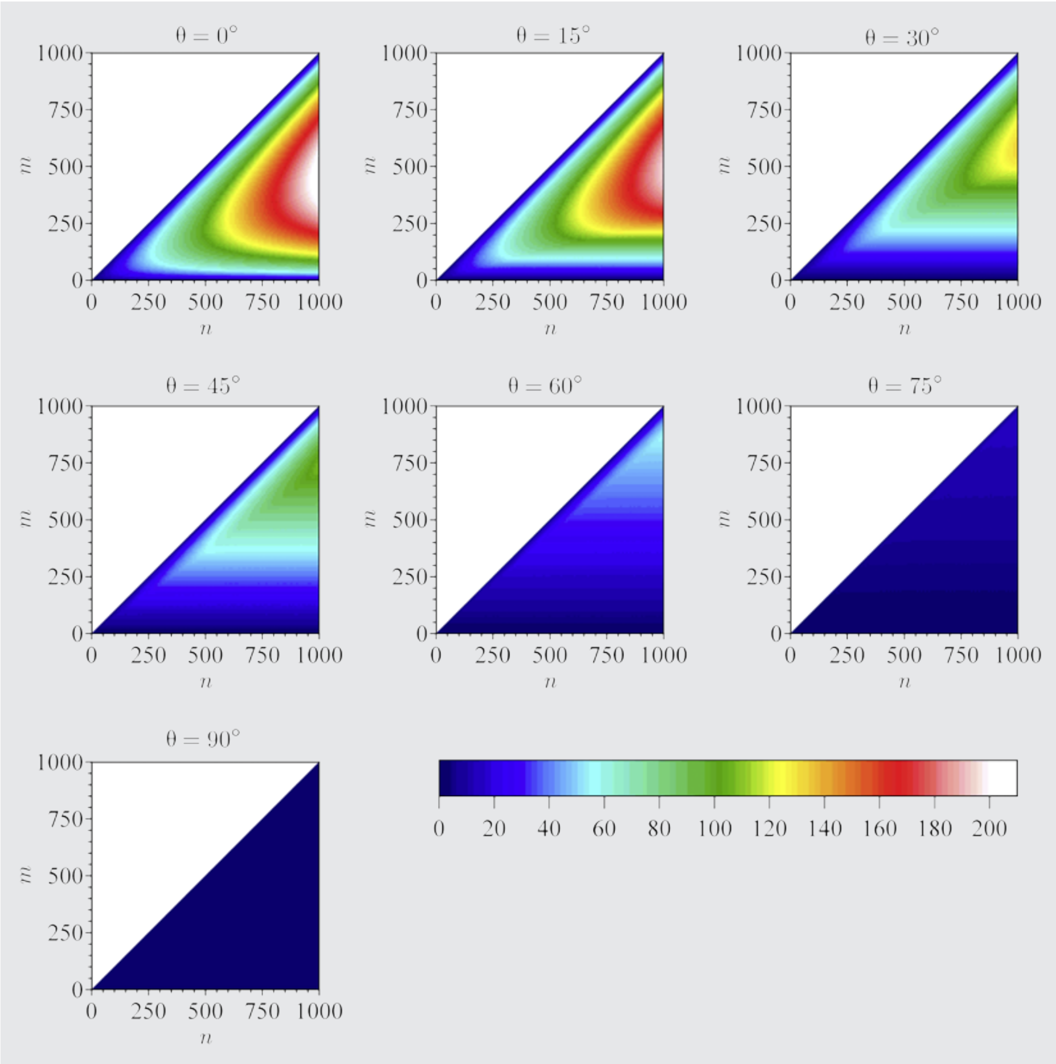

Fig. 4: Graphical representation of $\log_{10}\left|\frac{\overline{P}_{n,m}(\theta)}{u^m}\right|$. Selected spherical colatitudes are depicted in each panel. Magnitude is indicated by color scale.

5 Numerical experiment

It remains to be decided if these methods introduce limits in terms of the maximum spatial resolution of the Earth's gravity field. We need to determine the maximum possible degree of the spherical harmonics for which overflow or underflow problems occur. This may be done by a detailed analysis of the recursive formulae for the ALFs. We have decided to do it in a computational way because this strategy allows independent validation of an implementation of the current FPA standard.

For the purpose of the numerical experiment three independent source codes have been written in programming language C (Kernighan and Ritchie 1988). In each source code different types of ALFs (i.e. unnormalized, normalized and scaled) have been considered according to the recursive formulae defined. Computation of the three types of the ALFs has been performed up to degree and order 100000 in the range of spherical colatitudes $\theta \in \langle 0.1°, 90° \rangle$. During the computation, occurrence of overflow or underflow problems has been checked by macros of the mathematical library provided by programming language C. We tested unnormalized and scaled ALFs for occurrence of overflow, and the normalized ALFs for occurrence of underflow. When these problems appear, the minimum of the actual degree and order of the ALFs has been considered as the maximum possible degree for the given spherical colatitude. The same procedure has been followed in single, double and quadruple formats. The numerical experiments were made on a computer with x86 architecture in a Linux operating system. Source codes have been compiled by publicly available GNU Compiler Collection in version 4.4.3 (http://gcc.gnu.org). We note that according to our first plan binary and decimal FPA basic formats defined in (IEEE Computer Society 2008) have been considered in the numerical experiment. However, our experience has shown incomplete software implementation for decimal FPA basic formats. Definition of variables as decimal types in programming language C has not been recognized after compilation of the source codes. In addition macros testing overflow or underflow problems have not been provided in mathematical library. For these reasons only binary FPA basic formats have been considered in the numerical experiment.

All results of the numerical computations are summarized in Fig. 5 and in Tab. 3. In Fig. 5, the occurrence of overflow or underflow problems for corresponding types of the ALFs and FPA format is presented as a function of spherical colatitude. We immediately observe a similar behavior of the curves for the three graphs with different FPA format. By comparing each graph to another one we can see that the corresponding curve is shifted vertically by a certain value. Extension of the range of real numbers, i. e. supposing more precise binary FPA format, the maximum degree of the ALFs is increasing by several tens or even several hundred orders of magnitude. Let us now focus on the interpretation according to the type of the ALFs. Considering unnormalized ALFs, the maximum degree for which overflow problems occur is decreasing towards the equatorial plane with only a slight change in the range $\theta \in \langle 15°, 90° \rangle$. Therefore a similar pattern for the selected spherical latitudes is visible in Fig. 2. Introducing normalization factors, the maximum degree indicating underflow problems increases towards the equatorial plane. Close to the poles a strong decrease of the maximum degree even below the values corresponding to the unnormalized ALFs can be seen. Jekeli et al. (2007)

Tab. 3: Minimum values corresponding to each curve plotted in Fig. 5.

FPA format / Spherical harmonics	Single	Double	Quadruple
Unnormalized	29	151	1606
Normalized	14	112	1789
Scaled	184	1475	23599

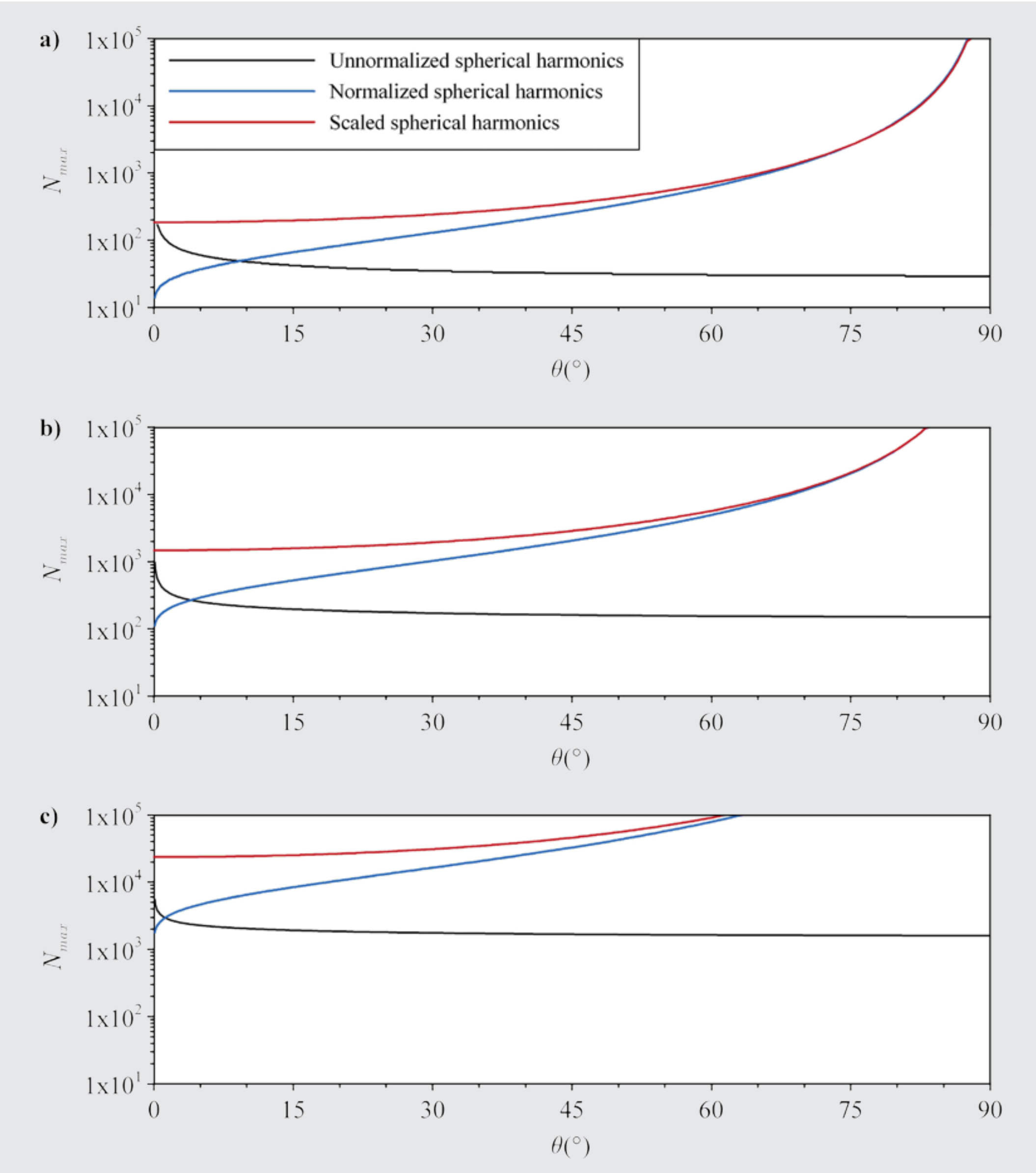

Fig. 5: Occurrence of overflow or underflow problems for the ALFs as a function of spherical colatitude: a) single, b) double, c) quadruple binary FPA basic format.

have assigned such a behavior as the pole singularity of the recursion formulae (12)–(14). However, the pole singularity disappears by introducing the scaled ALFs as seen in Fig. 5. In this case, the maximum degree indicating an overflow problem increases towards the equatorial plane. On the other hand only a slight change in the range $\theta \in \langle 0°, 30° \rangle$ is visible. Approaching the equatorial plane the curves representing normalized and scaled ALFs coincide. Usage of the scaled ALFs should be superior when the highest possible degree of SHE is required.

Interesting comparisons can be observed from Tab. 3 which contains the minimum values corresponding to each curve plotted in Fig. 5. Assuming unnormalized ALFs, SHEs of low and medium frequencies for single and double format up to degree 29 and 151, respectively, can be evaluated. However, in the case of quadruple format higher frequencies of the Earth's gravity field within the maximum degree exceeding the value 1600 can be achieved. According to the results in Fig. 5 and Tab. 3, the preference of the normalized ALFs is affected by their pole singularity. Neglecting this fact, normalized spherical harmonics should be superior to their unnormalized equivalent. On the other hand it is clear that scaled spherical harmonics overrun the previous two types by one order of the maximum degree of the SHE. Supposing quadruple format, SHEs up to degree and order 23599 may be evaluated which is even beyond the present possibilities in geodesy. Let us also mention that assuming the scaled spherical harmonics and quadruple format an identical value of the maximum degree has been mentioned by Jekeli et al. (2007). It is worth mentioning that another improvement of the maximum degree can be reached. As we have already shown in sections 2 and 4 spherical harmonics lead to overflow or underflow problems according to their type. In other words exponents of their magnitudes are having only positive or negative values. By setting initial values in an opposite direction on a numerical axis the maximum degree of the SHEs can be doubled. This simple manipulation was used by Wenzel (1998) who discussed the possibility of ultra high SHEs using normalized spherical harmonics.

6 Conclusions

In the present contribution, numerical problems of the spherical harmonics have been discussed. Evaluation of the unnormalized spherical harmonics leads to overflow problems when a high resolution Earth gravity field is desired. In general these problems can be avoided by numerical and algebraic methods. In numerical methods the range of real numbers is simply extended according to the principles of the FPA. At present three binary and two decimal FPA basic formats are provided by the IEEE Computer Society (2008). Single, double and quadruple binary FPA basic formats are well supported. In addition, these formats are implemented in the standard mathematical library of the programming language C and in GNU Compiler Collection. Therefore all of the standard binary FPA basic formats may be routinely used for the purpose of the determination of the Earth's gravity field. On the other hand, decimal FPA basic formats lack implementation in the mathematical library of the programming language C. Alternative numerical methods are based on the exploitation of the extended-range arithmetic and arbitrary precision libraries. Significant advantage of the extended-range arithmetic is the evaluation of extremely high degree and order SHEs. Comparing to the standardized FPA formats, computational time increases rapidly. Possibilities of arbitrary precision libraries have not yet been studied extensively in geodesy. Attenuation factors of the spherical harmonics are sought in algebraic methods. Supposing the global average of the normalized spherical harmonics equal to unity, normalization factors dependent on degree and order can be found. Despite the underflow problem, especially approaching the poles, normalized spherical harmonics became conventional in geodesy. The pole singularity disappears by introducing scaled spherical harmonics leading to an overflow problem. However, since attenuation factors depend on the spherical colatitude, the final evaluation of the gravitational potential has to be performed by Horner's scheme.

Assuming binary FPA basic formats, the limits of the numerical and algebraic methods have been tested by numerical experiments. Based on the occurrence of overflow and underflow problems in programming language C the maximum possible degrees of the spherical harmonics have been searched depending on the spherical colatitude. Extension of the range of the binary FPA basic format allows increasing of the maximum degree by one order for all types of the spherical harmonics. However, scaled spherical harmonics are superior to their unnormalized and normalized equivalents by an additional order of the maximum degree. When quadruple format is considered, scaled spherical harmonics can be evaluated up to degree and order 23599. Setting the initial values of the spherical harmonics in an opposite direction compared to their numerical problems, the maximum possible degree can be even doubled.

Despite of the numerical problems, many improvements in the knowledge of the Earth's gravity field have been achieved due to the spherical harmonics. It will be interesting to observe future progress in the modeling of the Earth's gravity field by this simple mathematical tool. Available computer facilities and simple algebraic operations allow us to consider extremely high SHEs even above degree 20000. Such a limit is sufficient enough to cover practical problems in geodesy and geophysics.

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