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Christian Gruber

A study on the Fourier composition of the associated Legendre functions; suitable for applications in ultra–high resolution

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Christian Gruber

22. April 2008

Abstract

The associated Legendre functions were historically calculated as closed power series. With the growing need for higher degrees and associated orders recursive algorithms have been developed, highly efficient for numerical processing. As ground–based gravity measurements are available that can be combined with existing and upcoming datasets of satellite systems ultra-high degree spherical harmonic representation and transformation of the fields becomes a necessity. Moreover, for applications in spectral domain it is in general desirable to process the associated Legendre function directly, without a recursive antecessor that predefines the order of the sequence. The

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closed power series mentioned can not serve beyond certain degrees due to alternating signs with extraordinarily large rational numbers, leading to a considerable loss in numerical precision. The Fourier transform and recursive relations between the Fourier coefficients themselves instead turn out to be stable and widely useful.

Keywords: Fourier expansion, geopotential, ultra-high degree Legendre functions, Spherical Harmonics

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1 Introduction

The associated Legendre functions (hereinafter: Legendre functions) and their derivatives are of fundamental importance in various disciplines from classical to space Geodesy, in Geophysics or Astronomy and nowadays even in Biochemistry. Historically, they were calculated as closed power series, see Hobson (1931)[12]; Kaula (1966) [17]; Heiskanen and Moritz (1967)[11]. State of the art solutions are the fast and precise calculation by means of highly efficient recursive algorithms, see Holmes & Featherstone (2002) [14]; Claessens (2005) [4]. Available methods for the calculation of the Legendre functions have limited resolution, since they approach machine underflow in double precision arithmetic. Furthermore, derived functionals, useful for vector field calculations require adopted recursive schemes,

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as well. Using the spectral representation of the Legendre functions, their computation is straight forward since derivation in spectral domain reduces to a simple filter operation and is not as tedious as in time-domain.

Due to the recursive processing chain certain applications, such as product–sums of huge data–sets cannot be established most efficiently. The reader may consider the assembling of normal equation systems for the analysis of irregularly distributed ground– or satellite based data. The recursive processing chain for the computation of the respective spherical harmonic functions then always leads to outer (tensor) products of the observational equations. If random access to each degree/order of the spherical harmonic expansion exist, the processing of the inner product between two corresponding Legendre functions of huge data–sets becomes feasible and can be realized very efficiently through parallel algorithms.

The product–sums between Legendre functions have therefore already been investigated by (Balmino 1978) [1] and (Hwang 1995) [15] but could never be used beyond some low degrees of expansion due to well–known numerical problems.

Using the decomposition in terms of trigonometric series instead, it proves reliable concerning numerical issues and leads besides to a convenient 2D Fourier expansion for the surface harmonics, that gives the possibility of fast spherical transformation of a function on the sphere. Since in geodesy often directional derivatives are required, the distinction of the functionals assembling the spherical

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harmonics remains albeit useful in contrast to a concise transformation or convolution of a scalar function, see (Driscoll and Healey 1994 [6] and Schwartztrauber 1979 [21])

Many efforts have been made recently, see e.g. (Blais 2002 [2]; Wittwer et al. 2008 [24] and Jekeli 2006) [16] to develop stable algorithms for the computation of ultra-high degree Legendre functions, but they could not solve the problem of exceeding the range convention for the most common data type (double–precision, or DOUBLE). In quadrupol precision the under-/overflow problem can be deferred but not generally solved. To overcome the trouble of numerical instabilities for certain arguments a detailed insight to the problem is required. It can be obtained by a distinct, frequency-wise processing and scaling of the function.

In this article will be discussed two major approaches how to calculate the harmonic spectrum of the associated Legendre functions. Firstly, if there is a Legendre function as an equispaced signal available in space domain it can be decomposed by trigonometric base–functions. This can be done by either the discrete Fourier operator, (FFT) or numerical integration. Secondly, two recursive algorithms to calculate the Legendre functions will be assessed in spectral domain. It hereby turns out that computations to unlimited degree are feasible without use of extended precision numbers.

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2 Classification

In this paper we will use the definitions of resolution, according to Table 1. A classification is given, depending on degree or equivalent half wavelength for the corresponding resolution. The grading follows technical assumptions, i.e. with emphasize on calculations. Either power series, classical recursive equations or an inverse Fourier transform of the coefficients are considered. The power series are based on (Hobson 1931). Classic recursion in space domain comprises 'diagonal' computation of the sectorial function where $(m = l)$ and further recursion to $(m = 0)$. Forward recursion in the sequel of this manuscript means the development from $(m = 0)$, backward recursion starts from $(m = l)$, where m denotes the associated order and l is the degree of the Legendre function.

Since the computational cost for a direct expansion of the Legendre functions into Fourier coefficients increases rapidly, only moderate resolutions $(l \leq 360)$ will be addressed with a discrete Fourier transformation. For the higher degrees $(360 < l \leq 1800)$ or even ultra–high $(l > 1800)$ efficient algorithms based on the recursive calculation of the Fourier coefficients are recommended. With these algorithms at hand, expansions considerably larger than $l = 10800$ are feasible, leading to global resolutions below 1 arcmin $\times$ 1 arcmin.

The lowest degrees are computable in double precision by forward and backward recursion as well as the power series, despite their instability, (in double

Degree	Resolution ($\lambda/2$)	Attribute	Spatial	Spectral
$l \leq 30$	$6^\circ \quad \equiv 667km$	low	ps, fr, br	fr, br
$l \leq 360$	$0.5^\circ \equiv 55km$	moderate	br	fr*, br
$l \leq 1800$	$6' \quad \equiv 11km$	high	br	fr*, br
$l \leq 2700$	$4' \quad \equiv 7km$	ultra–high	br*	fr*, br*
$l > 2700$	$< 4'$	ultra–high	———	fr*, br*

Table 1: Classification of Legendre functions in view of their resolutions and usage within Spherical Harmonics. Resolution complies to half wavelenghts, *ps* denotes power series, *fr, br* are forward and backward recursion, $*$ indicates modifications to the standard algorithm are necessary, see also text for further explanation.

precision) Concerning moderate resolution space to frequency domain transformation can still be efficiently applied. For the higher resolutions, computation times increase rapidly; moreover modifications to the recursive formulas become necessary, (see Holmes & Featherstone 2006).

On the other hand, it is possible to apply the recursions directly to the Fourier coefficients of the Legendre functions. Forward recursion then reduces effectively to single precision if the under-/overflow is anticipated. A possible extention to gain double precision will be presented in the corresponding section about recursive algorithms for the Fourier coefficients of the Legendre funcions.

Backward recursion in spectral domain is capable to maintain DOUBLE numbers throughout all degrees/orders. But it requires special effort to compute the initial values originating from a binomial series and propagation of an adequate scaling factor.

3 The power series

The direct calculation of the Legendre functions stems from a power series

$$P_{lm}(x) = \sum_{j}^{\infty} a_{lm}^{j} x^{j}. \tag{1}$$

Hobson (1931) and Kaula (1966) give the solution of the Legendre diffential equation

$$P_{lm}(x) = (1 - x^2)^{m/2} \sum_{t=0}^{[\frac{l-m}{2}]} T_{lm}^{t} x^{l-m-2t}; \tag{2}$$

where $[.]-$ entier operator, $x = \sin\phi$ and a recursive procedure for the constants

$$T_{lm}^{t} = -\frac{(l-m-2t+1)(l-m-2t+2)}{2t(2l-2t+1)} T_{lm}^{t-1} \tag{3}$$

with an initial value

$$T_{lm}^{0} = \frac{(2l)!}{2^{l} l! (l-m)!}. \tag{4}$$

The constants T_{lm}^{t} then enable the calculation of any Legendre function independent from its recursive antecessor. For certain applications, e.g. the computation of normal equation systems, this can offer advantages over recursive computations.

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The coefficients T^t_{lm} are rational numbers emerging from equations with factorials or by eliminating them, from product series. Extremely large almost equal values with alternating signs occur, making it impossible to calculate any results in DOUBLE numbers beyond some low degrees ($l \geq 30$). To understand this, consider a number with 16 valid decimals and an exponent of 10^{17}. There exists no number in the same precision with an alternating sign that could be added, s.th. the result gives 1 (or is of dimension 10^0) because the last valid decimal already represents 10^1. Addition/ subtraction of numbers with different orders of magnitude has therefore to be strictly avoided but recursive manipulations of same order can be applied frequently.

In Table 2 the first terms of the Legendre functions P_{lm} of degree l and order m are given as harmonic polynomials.

The power series from Tab. 2 can now be decomposed by trigonometric theorems into Table 3. Introducing the corresponding Fourier series, it can be quickly assessed that to a certain degree l exclusively even or uneven frequencies $k = l-2p$ are required

$$\mathcal{F}(A) \Longleftrightarrow P_{lm}(\sin\phi) = \sum_{p=0}^{l} A_{lmp} \cdot e^{i\,k\phi}. \tag{5}$$

Moreover, since the complex (conjugate) constants A_{lmp} always take either an imaginary or real value (phase shift), the inverse Fourier transform can be evalu-

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P_0^0	$=$	1
P_1^0	$=$	$\sin\phi$
P_1^1	$=$	$\cos\phi$
P_2^0	$=$	$3/2\sin^2\phi - 1/2$
P_2^1	$=$	$3\cos\phi\sin\phi$
P_2^2	$=$	$3\cos^2\phi$
P_3^0	$=$	$5/2\sin^3\phi - 3/2\sin\phi$
P_3^1	$=$	$15/2\cos\phi\sin^2\phi - 3/2\cos\phi$
P_3^2	$=$	$15\cos^2\phi\sin\phi$
P_3^3	$=$	$15\cos^3\phi$
P_4^0	$=$	$35/8\sin^4\phi - 15/4\sin^2\phi + 3/8$
P_4^1	$=$	$35/2\cos\phi\sin^3\phi - 15/2\cos\phi\sin\phi$
P_4^2	$=$	$105/2\cos^2\phi\sin^2\phi - 15/2\cos^2\phi$
P_4^3	$=$	$105\cos^3\phi\sin\phi$
P_4^4	$=$	$105\cos^4\phi$

Table 2: Associated Legendre functions as power series

ated by real (8-Byte) coefficients a_{lm}^k, most suitable for computations and storage,

$$\bar{P}_{lm}(\sin\phi) = \mathrm{re}\left\{\sum_k (2-\delta_k^0)\cdot e^{ik\phi}\cdot a_{lm}^k \cdot i^{(l-m)\bmod 2}\right\}, k = (l \bmod 2)\ldots l, (2). \quad (6)$$

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where the overbar denotes normalization of the Legendre functions,

$$N_{lm} = \sqrt{(2-\delta_m^0)(2l+1)\frac{(l-m)!}{(l+m)!}}, . \tag{7}$$

such that

$$\bar{P}_{lm} = N_{lm}\ P_{lm}. \tag{8}$$

P_0^0	=	1
P_2^0	=	$1/4 - 3/4\cos(2\phi)$
P_2^1	=	$0 \quad + 3/2\sin(2\phi)$
P_2^2	=	$3/2 + 3/2\cos(2\phi)$
P_3^0	=	$3/8\sin\phi - 5/8\sin(3\phi)$
P_3^1	=	$3/8\cos\phi - 15/8\cos(3\phi)$
P_3^2	=	$15/4\sin\phi + 15/4\sin(3\phi)$
P_3^3	=	$45/4\cos\phi + 15/4\cos(3\phi)$
P_4^0	=	$9/64 - 20/64\cos(2\phi) + 35/64\cos(4\phi)$
P_4^1	=	$0 \quad + 10/16\sin(2\phi) - 35/16\sin(4\phi)$
P_4^2	=	$45/16 - 60/16\cos(2\phi) - 105/16\cos(4\phi)$
P_4^3	=	$0 \quad + 210/8\sin(2\phi) + 105/8\sin(4\phi)$
P_4^4	=	$315/8 + 420/8\cos(2\phi) + 420/8\cos(4\phi)$

Table 3: The associated Legendre functions in the Fourier–base

It can be clearly seen how the trigonometric decomposition follows a certain scheme, defining frequencies and phases. The phase depends on whether degree and order are even or odd. The following four cases can be distinguished, see Tab. 4.

$\ell \backslash m$		even				odd			
even	(I)	P_0^0							(II)
		P_2^0	P_2^2			P_2^1			
		P_4^0	P_4^2	P_4^4		P_4^1	P_4^3		
		P_6^0	P_6^2	P_6^4	P_6^6	P_6^1	P_6^3	P_6^5	
odd	(III)	P_1^0				P_1^1			(IV)
		P_3^0	P_3^2			P_3^1	P_3^3		
		P_5^0	P_5^2	P_5^4		P_5^1	P_5^3	P_5^5	

Table 4: Classification of Legendre functions by parity, degree and order

If all frequencies are known, a Fourier analysis to estimate the coefficients, can be applied. The general Fourier series of a periodic function $f(x+p) = f(x)$, with period p is given as

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left[a_k \cos\left(\frac{2\pi kx}{p}\right) + b_k \sin\left(\frac{2\pi kx}{p}\right) \right]. \qquad (9)$$

Taking the result of Tab. 4 into account, symmetric functions with respect to $x = 0$ arrise.

Symmetrical case $f(-x) = f(x)$

$$a_k = \frac{4}{p} \int_0^{p/2} f(x) \cos\left(\frac{2\pi k x}{p}\right) \cdot dx; \; b_k = 0, \; k = 0, 1, 2, \ldots \tag{10}$$

Anti–symmetrical case $f(-x) = -f(x)$

$$b_k = \frac{4}{p} \int_0^{p/2} f(x) \sin\left(\frac{2\pi k x}{p}\right) \cdot dx; \; a_k = 0, \; k = 0, 1, 2, \ldots \tag{11}$$

Eq.(10) can be used whenever degree and order of the Legendre functions are in parity, i.e. $(l - m)$ even, and Eq. (11) in the case $(l - m)$ odd. Consider $l = 4, m = 0, \; k = 0, 2, 4$ and a period $p = \pi$

$$a_0 = \frac{4}{\pi} \int_0^{\pi/2} \left(T_{40}^0 \sin^4 \phi + T_{40}^1 \sin^2 \phi + T_{40}^2\right) \cdot d\phi = 2 \cdot 9/64 \tag{12}$$

$$a_1 = \frac{4}{\pi} \int_0^{\pi/2} \left(T_{40}^0 \sin^4 \phi + T_{40}^1 \sin^2 \phi\right) \cos 2\phi \cdot d\phi = -20/64 \tag{13}$$

$$a_2 = \frac{4}{\pi} \int_0^{\pi/2} T_{40}^0 \sin^4 \phi \cos 4\phi \cdot d\phi = 35/64, \tag{14}$$

and for $l = 4, m = 1$ and $k = 0, 2, 4$ analoguously Eq. (11).

The constant a_0 is obviously doubled compared to the results in Tab. 3; this is compensated by introducing complex notation

$$A_k = \begin{cases} \frac{a_0}{2} & k = 0 \\ \frac{1}{2}\left(a_k - i b_k\right) & k > 0 \\ \frac{1}{2}\left(a_{-k} + i b_{-k}\right) & k < 0 \end{cases} \tag{15}$$

The decomposition is then well defined and the constants T^t_{lm} can be converted into Fourier coefficients by multiplication with the integrals of the powers of the trigonometric functions. Yet there is no true advantage in this, since the alternating series to determine the coefficients of the power series are still being used. The usually introduced full–normalization, Eq. (7) can be incorporated into calculations but does not improve numerical stability, substantially. Different approaches will be therefore discussed in order to provide fast and reliable calculation of the Fourier coefficients for different applications.

In (Brovelli und Sansò 1990) [3] it is indicated, that the Inclination functions for inclination $I = \pi/2$ represent the Fourier coefficients of the Legendre functions. A possible choice would be therefore the recursive calculation of Inclination functions for $I = \pi/2$, but this will almost certainly lead to instabilities for higher degrees, see Gooding and Wagner (2008) [8] for a detailed discussion. The following fruitfull methods will be proposed instead:

- time $\Rightarrow$ frequency

- Discrete numerical Integration of the Legendre functions

- Applying the FFT operator to the Legendre functions

- frequency $\Rightarrow$ frequency

- Application of a direct recursion to the Fourier coefficients starting with

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($m = 0$) and disregarding divergent components in the course of the recursion

- Application of a direct recursion to the Fourier coefficients starting from ($m = l$).

Since the discrete numerical integration can be applied very simple it will be introduced first. The corresponding concept based on the use of an FFT operator will be discussed subsequently. The processing by recursive algorithms applied directly to the Fourier coefficients follows in chapter 6.

Fig. 1 illustrates the processing of the Fourier coefficients, that will be discussed in the following sections.

4 Fourier Analysis by discrete numerical integration

In this approach equispaced Legendre function values of a specific $\bar{P}_{lm}(t)$ are transformed into their respective Fourier spectrum. To calculate the function values standard recursive formulas are applied, cf. Holmes and Featherstone (2006), Koop and Stelpstra (1989) [18]. By minimizing the norm of the residuals in a least squares sense, $\|\bar{P}_{lm}(t) - \sum\limits_{k} a_{lm}^{k} e^{ik\phi}\|_{L2}$ with empirical values $\bar{P}_{lm}(t)$ and parameters

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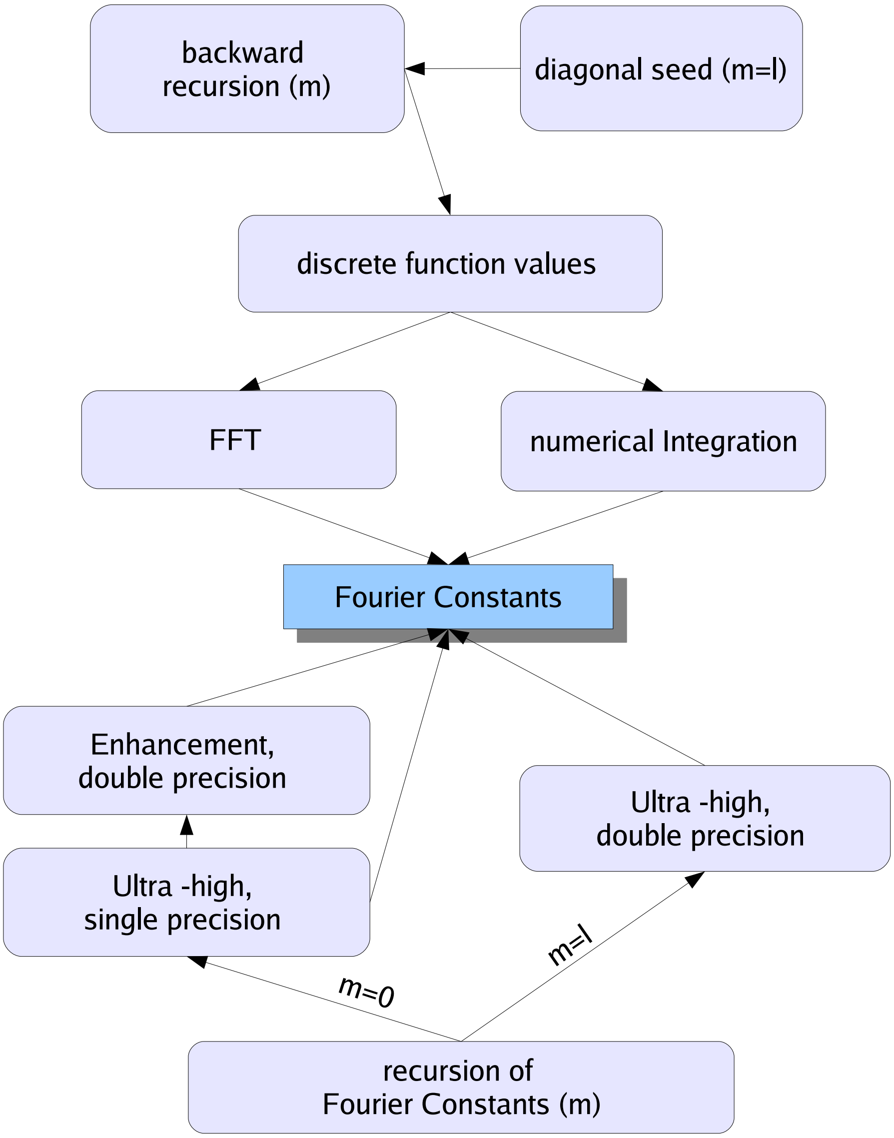

Figure 1: Different processing chains to obtain Fourier coefficients for the associated Legendre functions

$a^k_{lm} \in \mathbb{R}$, $t_i = \sin\phi_i$, and $0 \leq \phi \leq \pi/2$, one can generally apply

$$a^k_{lm} = (B^T B)^{-1} B^T \overline{P}^m_l(t_i). \qquad (16)$$

The Jakobi matrix B of the form (**I**) according to Tab. 4, for $l = 6$

$$B = \begin{pmatrix} \cos 6\phi_i & \cos 4\phi_i & \cos 2\phi_i & 1 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}_{[N\times K]}, \qquad i = 1, \ldots, N. \tag{17}$$

where N is the total number of samples for the function and K spans a subspace according to all possible frequencies $k = (l \mod 2), \ldots, l$, step 2. It is intended to find $C = (B^T B)^{-1}$, where

$$C^{-1} = \left(B^T B\right) = \begin{pmatrix} (\cos 6\phi, \cos 6\phi) & (\cos 4\phi, \cos 6\phi) & (\cos 2\phi, \cos 6\phi) & (1, \cos 6\phi) \\ & (\cos 4\phi, \cos 4\phi) & (\cos 2\phi, \cos 4\phi) & (1, \cos 4\phi) \\ & & (\cos 2\phi, \cos 2\phi) & (1, \cos 2\phi) \\ \textbf{symm}. & & & N \end{pmatrix}. \tag{18}$$

The matrix C will be diagonally dominant occupied, due to the orthogonality relations in Eq. (19). These can be listed for $(0 \le \phi < 2\pi)$

$$\begin{aligned} \sum_{i=0}^{N-1} \cos k\phi_i \cos h\phi_i &= \begin{cases} 0 & k \neq h \\ N/2 & k = h \neq 0 \\ N & k = h = 0 \end{cases} \\ \sum_{i=0}^{N-1} \sin k\phi_i \sin h\phi_i &= \begin{cases} 0 & k \neq h \\ N/2 & k = h \neq 0 \\ 0 & k = h = 0 \end{cases} \\ \sum_{i=0}^{N-1} \cos k\phi_i \sin h\phi_i &= 0 \quad \forall \quad k, h. \end{aligned} \tag{19}$$

with the number of samples N and an equi spaced sampling interval.

Comparing these results to the analytical counterpart of the matrix $B^T B$, corresponding to the products in Eq. (18) where the scalar product in the sense of a metric $\boldsymbol{\rho}: \boldsymbol{M} \times \boldsymbol{M} \to \mathbb{R}$, with $u, v \in \boldsymbol{M}$ is given as

$$\rho(u,v) = \frac{2}{p} \int_a^b u(x)\overline{v(x)}dx, \quad p = b - a := \pi \tag{20}$$

leads for the trigonometric functions to $\boldsymbol{\rho}(u,v) = \delta^v{}_u$, the Kronecker function. Integrating according to Eq. (20), over $x := \phi \in [0, \pi/2]$, one obtains for the given example analytically (a), whereas for the equispaced, discrete sampling in Eq. (18), (b)

$$C^{-1} = \underset{\text{(a)}}{\begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 \\ & \frac{1}{2} & 0 & 0 \\ & & \frac{1}{2} & 0 \\ \textbf{symm}. & & & 1 \end{pmatrix}}, C^{-1} = \underset{\text{(b)}}{\begin{pmatrix} \frac{N+1}{2} & 0 & +1 & 0 \\ & \frac{N+1}{2} & 0 & +1 \\ & & \frac{N+1}{2} & 0 \\ \textbf{symm}. & & & N \end{pmatrix}}. \tag{21}$$

By multiplying B with a diagonal matrix

$$B' = d \cdot B, \quad d = \begin{pmatrix} 1/\sqrt{2} & & & \\ & 1 & & \\ & & 1 & \\ & & & 1/\sqrt{2} \end{pmatrix}, \tag{22}$$

or equivalently by dividing the first and last row

$$B'_{1,j} = B_{1,j}/\sqrt{2}, \; B'_{N,j} = B_{N,j}/\sqrt{2} \quad \text{where} \;\; i,j = 1,\ldots,N \tag{23}$$

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and using a determined system, i.e. delimiting the number of samples to $N = l / 2 + 1$, the matrix C^{-1} takes a diagonal shape and results in the inverse

$$C^{-1} = B'^T B' = \begin{pmatrix} N-1 & & & 0 \\ & \frac{N-1}{2} & & \\ & & \frac{N-1}{2} & \\ \textbf{symm}. & & & N-1 \end{pmatrix} \Longleftrightarrow C = 2/l \cdot \begin{pmatrix} 1 & & & 0 \\ & 2 & & \\ & & 2 & \\ \textbf{symm}. & & & 1 \end{pmatrix}. \tag{24}$$

The right hand side of the system must be eqally adopted. One obtains with

$$a_{lm}^k = CB^T D \bar{P}_l^m(t_i), \quad D = d^T d. \tag{25}$$

a set of k coefficients a_{lm}^k according to Eq. (16). The product $CB^T D$ can be also written as $4/l \cdot B''$ if the first & last row as well as first and last columns are modified, accordingly

$$\begin{aligned} B'_{1,j} &= B_{1,j}/2, \; B'_{N,j} = B_{N,j}/2 \\ B''_{i,1} &= B'_{i,1}/2, \; B''_{i,N} = B'_{i,N}/2. \end{aligned} \tag{26}$$

For the odd orders there is no (DC) frequency. The matrix for the case (**II**), with $l = 6$, $m = 1, 3, 5$, $\phi \in [0, \pi/2]$ will take the form

$$C^{-1} = \begin{pmatrix} (\sin 6\phi, \sin 6\phi) & (\sin 4\phi, \sin 6\phi) & (\sin 2\phi, \sin 6\phi) \\ & (\sin 4\phi, \sin 4\phi) & (\sin 2\phi, \sin 4\phi) \\ \textbf{symm}. & & (\sin 2\phi, \sin 2\phi) \end{pmatrix} = \begin{pmatrix} \frac{N}{2} & & 0 \\ & \frac{N}{2} & \\ \textbf{symm}. & & \frac{N}{2} \end{pmatrix}. \tag{27}$$

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Again using a minimum of samples $N = l/2$ only then yields

$$C^{-1} = \begin{pmatrix} \frac{N+1}{2} & & 0 \\ & \frac{N+1}{2} & \\ \textbf{symm}. & & \frac{N+1}{2} \end{pmatrix} = 4/(l+2) \cdot I \tag{28}$$

and can be effectively applied as a scalar to B^T in Eq. (16)

$$a_{lm}^k = 4/(l+2) \cdot B^T \bar{P}_l^m(t_i) \tag{29}$$

For the odd degrees and even orders, case (**III**) $l = 7$, $m = 2, 4, 6$, $\phi \in [0, \pi/2]$, $k = 1, 3, 5, \ldots, l$

$$C^{-1} = \begin{pmatrix} (\sin 7\phi, \sin 7\phi) & (\sin 5\phi, \sin 7\phi) & (\sin 3\phi, \sin 7\phi) & (\sin \phi, \sin 7\phi) \\ & (\sin 5\phi, \sin 5\phi) & (\sin 3\phi, \sin 5\phi) & (\sin \phi, \sin 5\phi) \\ & & (\sin 3\phi, \sin 3\phi) & (\sin \phi, \sin 3\phi) \\ \textbf{symm}. & & & (\sin \phi, \sin \phi) \end{pmatrix} \tag{30}$$

with $N = (l+1)/2 + 1$ we obtain a chessboard structure in the off diagonals

$$C^{-1} = \begin{pmatrix} \frac{N}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ & \frac{N}{2} & -\frac{1}{2} & \frac{1}{2} \\ & & \frac{N}{2} & -\frac{1}{2} \\ \textbf{symm}. & & & \frac{N}{2} \end{pmatrix}. \tag{31}$$

Dividing the last row in matrix B by $\sqrt{2}$ erases the off diagonal elements and leads to $C = 4/(l+1) \cdot \boldsymbol{I}$. Adopting also the right hand side further results in

$$a_{lm}^k = 4/(l+1) \cdot B'' \bar{P}_l^m(t_i) \tag{32}$$

with modified last row and column

$$B'_{N,j} \;= B_{N,j}/\sqrt{2}, \quad B''_{i,N} = \;\; B'_{i,N}/\sqrt{2}, \quad \text{where} \;\; i,j = 1,\ldots,N \tag{33}$$

The forth case (**IV**), with $l = 7$, $m = 1, 3, 5, 7$, $\phi \in [0, \pi/2]$

$$C^{-1} \;\; = \begin{pmatrix} (\cos 7\phi, \cos 7\phi) & (\cos 5\phi, \cos 7\phi) & (\cos 3\phi, \cos 7\phi) & (\cos\phi, \cos 7\phi) \\ & (\cos 5\phi, \cos 5\phi) & (\cos 3\phi, \cos 5\phi) & (\cos\phi, \cos 5\phi) \\ & & (\cos 3\phi, \cos 3\phi) & (\cos\phi, \cos 3\phi) \\ \textbf{symm}. & & & (\cos\phi, \cos\phi) \end{pmatrix} \tag{34}$$

is analoguous to case (**III**), with

$$C^{-1} \;\; = \begin{pmatrix} \frac{N+1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ & \frac{N+1}{2} & \frac{1}{2} & \frac{1}{2} \\ & & \frac{N+1}{2} & \frac{1}{2} \\ \textbf{symm}. & & & \frac{N+1}{2} \end{pmatrix}. \tag{35}$$

Changing first row and column in B then leads to $C = 4/(l+3) \cdot \boldsymbol{I}$ and therefore

$$a^k_{lm} = 4/(l+3) \cdot B'' \bar{P}^m_l(t_i), \quad k = 1, 3, 5, \ldots, l \tag{36}$$

where

$$B'_{1,j} \;= B_{1,j}/\sqrt{2} \;\; \text{and} \;\; B''_{i,1} = \;\; B'_{i,1}/\sqrt{2}. \tag{37}$$

In Tab. 5 the corresponding cases (**I-IV**) are listed

case	range	sampling $\Delta\phi$	N	base function
I	$0 \leq \phi \leq \pi/2$	π/l	$l/2$+1	cosinus
II	$0 < \phi < \pi/2$	$\pi/(l+2)$	$l/2$	sinus
III	$0 \leq \phi \leq \pi/2$	$\pi/(l+1)$	$(l+1)/2+1$	sinus
IV	$0 \leq \phi \leq \pi/2$	$\pi/(l+1)$	$(l+1)/2+1$	cosinus

Table 5: Definition of the determining sampling for the decomposition of the Legendre functions.

The presented method is suitable for the simultaneous calculation of all coefficients of the associated orders m to a certain degree l, since beside the function values at the right hand side nothing changes for different orders. Since for every degree a matrix vector operation over $l^2/4$ elements has to be calculated, a total count of $\mathcal{O}(l^3/4)$ is necessary for all respective orders. Using at this point the fast Fourier FFT operator instead, only $(l \log l)$ operations for each order are required, in total thus $\mathcal{O}(l^2 \log l)$ per degree. Since the number of samples for use of the FFT method has to be doubled there is no gain in moderate resolutions.

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5 The fast Fourier–operator applied to the associated Legendre functions

In analogy to the previous method the computation of the Fourier coefficients from equispaced Legendre function samples can be achieved by fast Fourier transformation, FFT. The integral, with $t = \sin\phi$, $t \in [-1;1]$ is given by

$$A_{lmk} = \frac{1}{\pi} \int\limits_{-\pi/2}^{\pi/2} e^{-ik\phi} \bar{P}_{lm}(t) d\phi. \tag{38}$$

The discrete case with equispaced samples is then

$$A_{lmk} \equiv \frac{1}{N} \sum_{k=0}^{N-1} e^{-i2\pi kn/N} \bar{P}_l^m(t_n), \quad n = 0, \ldots, N-1 \tag{39}$$

where a real input signal will produce a complex (periodical) spectrum

$$A_{-k} = A_{N-k} = A_k^*, \tag{40}$$

such that it is sufficient to store only coefficients with positive indexes. The following symmetry properties can be used to keep the number of required samples of Legendre functions low and get the most efficient scheme to compute the coefficients for this application,

1. the Legendre functions are periodic on $[0 : \pi]$,
2. the Legendre functions of even order are symmetric to $\pi/2$ and of odd order anti-symmetric to $\pi/2$.

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A real input signal can be cut in two halves and assigned both as a real and imaginary signal to the FFT operator. The complex result can then be assembled in an inverse manner. The use of this efficient FFT method for the Legendre functions, sampled between $\phi = [0 : \pi/2]$ with the step size

$$\Delta\phi = \begin{cases} \pi/l_{\max} & l_{\max} : \textbf{even} \\ \pi/(l_{\max}+1) & l_{\max} : \textbf{odd} \end{cases} \tag{41}$$

is demonstrated as follows:

i *assemble the signal,* with $N = [l_{\max}/2] + 1$

$$\begin{aligned} \alpha &= (-1)^m \\ \beta &= (-1)^l \\ \gamma &= \alpha \cdot \beta \end{aligned}$$

$$\begin{aligned} p_j &= \bar{P}_{lm}(t_j), j = 0, \ldots, N(\mathit{1.quadrant}) \\ p_{2N-k} &= \alpha \cdot p_k, k = 1, \ldots, N-1(\mathit{2.quadrant}) \\ p_{2N+j} &= \beta \cdot p_j, (\mathit{3.quadrant}) \\ p_{4N-k} &= \gamma \cdot p_k, (\mathit{4.quadrant}) \end{aligned} \tag{42}$$

ii *decompose two halves into complex values*

$$h_n = p_{2n} + i p_{2n+1}, \quad n = 0, \ldots, 2N-1$$

iii *apply the* FFT*–operator*

$$H_n = \mathcal{F}[h_n]$$

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iv *add the last value* (due to periodicity)

$$H_{2N} = H_1$$

v *merge the real and imaginary solution,* see Numerical recipies (1992) [20] for further details

$$a^k_{lm} = \frac{1}{2}(H_n + H^*_{M/2-n}) - \frac{i}{2}\left(H_n - H^*_{M/2-n}\right) e^{i2\pi n/M}$$

where $M = 4 \cdot [l_{\max}/2], \quad n = 0, 1, \ldots, M/2$

vi *save only those constants* a^k_{lm}, where $k = \begin{cases} 0, 2, \ldots, l & l : \textbf{even} \\ 1, 3, \ldots, l & l : \textbf{odd} \end{cases}$

For the calculation of all coefficients up to degree/order $l = 1080$ by FFT, in total

$$L = \sum_{l=1}^{1080} 4l^2 \log 2l \;\approx\; 1.2 \;\times\; 10^{10} \tag{43}$$

operations are required, whereas in the case of the numerical integration $l^4/16 \approx 8.5 \times 10^{10}$.

6 Recursive computation of the Fourier coefficients to unlimited degree

Other than in the previous section, where explicit, discrete Legendre function values have been transformed from time to Fourier domain, in this section the recursive processing of the coefficients themselves will be discussed. Dilts (1985) [5] describes such recursive relations between the constants with regard to degree–wise recursion and elaborates an algorithm purely in integer arithmetics. His numerical calculation extends until degree $l = 14$ and no normalization has been applied. Elovitz et al. (1989) [7] have therefore included a normalization and extend computations with spherical harmonic coefficients up to degree $l = 250$. From today's view the conclusion that processing of spherical harmonic models by Fourier coefficients for the Legendre functions would be too costly compared to a standard quadrature method is not sustainable any longer, since the spherical harmonic model coefficients can be aggregated into lumped harmonics and then applied to a 2D FFT operator to generate high resolution global data grids within best performance.

Considering the order–wise recursion based on the associated Legendre differential equation, Heiskanen and Moritz (1967) [11]

$$-P_l^{m+1}(\sin\phi) + (l+m)(l-m+1)P_l^{m-1}(\sin\phi) = 2\frac{\partial}{\partial\phi}P_l^m(\sin\phi), \qquad (44)$$

it is straight forward to plug in Fourier coefficients from Tab. 3, since the trigonometric base functions cancel on both sides and the number of coefficients belonging to a certain degree does not change during recursion. If we wish the $a_{l,m}^k$ introduced in Eq. (6) to be fully normalized coefficients, we first "denormalize" by Eq. (7) in order to fulfill Eq. (44),

$$-a^k_{l,m+1}/N_{l,m+1} + (l+m)(l-m+1) \cdot a^k_{l,m-1}/N_{l,m-1} = \beta_{l-m} \cdot 2k \cdot a^k_{l,m}/N_{l,m}, \tag{45}$$

with an auxiliary

$$\beta_{l-m} = \begin{cases} -1 & \text{for } (l-m \ \ \textbf{even}) \\ 1 & \text{for } (l-m \ \ \textbf{odd}). \end{cases} \tag{46}$$

The equation can be solved as an initial value problem with $(m = 0)$. For this purpose further auxiliaries will be computed, following from the decomposition of the factorials in Eq. (7) into product series

$$\begin{aligned} j_m &= 1 + \delta^0_m \\ d_{l,m} &= \sqrt{(l+m)(l-m+1)} \\ e_{l,m} &= \sqrt{(l-m)(l+m+1)}. \end{aligned} \tag{47}$$

Normalization can then be considered implicit within recursions. The constants a^k_{lm} to a certain degree l can be computed reversely according to the following scheme,

$$\begin{aligned} a^k_{l,m+1} &= \sqrt{j_m} \cdot \beta_l \cdot k \cdot a^k_{l,m} & (m = 0) \\ a^k_{l,m+1} &= \left(\beta_{l-m} \cdot k \cdot a^k_{l,m} + d_{l,m} \cdot a^k_{l,m-1}\right)/e_{lm} & (l \geqslant m > 0) \end{aligned} \tag{48}$$

starting with a^k_{l0} for the Legendre polynomial, determined in a direct manner. We follow a direct trigonometric expansion, see Hoffsommer and Potters (1960) [13]

$$P_l(\sin\phi) = \sum_{k=0}^{l} p_k \cdot p_{l-k} \cdot \sin(l-2k)\phi \tag{49}$$

thence for the coefficients, including normalization

$$a_{l0}^k = \sqrt{2l+1} \cdot p_k \cdot p_{l-k}. \tag{50}$$

The constants p_j can be obtained by

$$p_{j+1} = (1 - 1/(2j)) \cdot p_j, \quad p_0 = 1. \tag{51}$$

The recursive scheme in Eq. (48) is suitable for simultaneous computations of all frequencies k belonging to the next associated order of a certain degree l. Unfortunately the process becomes instable for higher degrees ($l > 30$) due to earlier described numerical problems. Hofsommer and Potters (ibid) therefore suggested to introduce a second boundary to the differential equation (44) in order to stabilize calculations. This can be done successfully and leads to a stable solution but the equations cannot be solved in a recursive manner. In order to understand the principles and extend this idea later on we first consider the equivalent of Eq.

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(48), for $l = 4$, newly expressed as a matrix operation, $N \cdot x = 0$

$$\begin{pmatrix} *| & -1 & 0 & 0 & 0 \\ *| & * & -1 & 0 & 0 \\ 0| & * & * & -1 & 0 \\ 0| & 0 & * & * & -1 \end{pmatrix} \cdot \begin{pmatrix} a^k_{\ell,0} \\ --- \\ a^k_{\ell,1} \\ a^k_{\ell,2} \\ a^k_{\ell,3} \\ a^k_{\ell,4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{52}$$

and a rank defect of 1. The $*$ serve as placeholders for individual numbers according to the recursion. Swapping the first column to the right-hand-side then gives a solvable (determined) system

$$\begin{pmatrix} -1 & 0 & 0 & 0 \\ * & -1 & 0 & 0 \\ * & * & -1 & 0 \\ 0 & * & * & -1 \end{pmatrix} \cdot \begin{pmatrix} a^k_{\ell,1} \\ a^k_{\ell,2} \\ a^k_{\ell,3} \\ a^k_{\ell,4} \end{pmatrix} = -a^k_{\ell,0} \cdot \begin{pmatrix} * \\ * \\ 0 \\ 0 \end{pmatrix}. \tag{53}$$

It can be shown, how instabilities evolve with the system if the inversion is carried out by respective Gauss-matrices. To avoid them the introduction of a second constraint to the right-hand-side will result in an overdetermined system that is capable to deliver stable results,

$$\begin{pmatrix} -1 & 0 & 0 \\ * & -1 & 0 \\ * & * & -1 \\ 0 & * & * \end{pmatrix} \cdot \begin{pmatrix} a^k_{\ell,1} \\ a^k_{\ell,2} \\ a^k_{\ell,3} \end{pmatrix} = \begin{pmatrix} -a^k_{\ell,0} \cdot * \\ -a^k_{\ell,0} \cdot * \\ 0 \\ +a^k_{\ell,4} \end{pmatrix}. \tag{54}$$

The solution of a full inverse is now required, resulting in substantially higher numerical workload. Specifically, to each frequency k a solution has to be found for $(m = 2, \ldots, l-1)$ unknown coefficients by a matrix inversion. Moreover the last value as second constraint in Eq. (53) has to be introduced and thus stable calculated as well. However, since this value approaches zero it can in practice be set to zero for most cases, without the need to calculate it; the other cases, will be discussed in the next section. A combined solution between forward recursion until the anticipated instability and an additional estimation for a few "enhancement coefficients" replacing and/or completing deficient orders will be introduced in the section for proposed calculation schemes.

Beforehand, recursive relations can also be reversed and thus the initial value replaced by the final one. This approach turns out to provide numerically stable results to the ultra–high degree and can be used efficiently. The processing steps are briefly outlined in the following. From Eq. (2) the final value $\bar{P}_{ll}(\sin\phi)$ is obtained by

$$\bar{P}_{ll}(\sin\phi) = N_{ll} \cdot T^0_{ll} \cdot \cos^l \phi, \tag{55}$$

where the coefficients T^0_{ll} are calculated from

$$T^0_{ll} = (2l-1) \cdot T^0_{l-1,l-1} \tag{56}$$

with an initiale value $T^0_{11} = 1$. The normalization from Eq. (7) becomes

$$N_{ll} = \sqrt{\frac{(4l+2)}{\Pi^l_{n=1} n(l+n)}} \tag{57}$$

and can be included in the recursion in Eq. (56) to obtain fully normalized coefficients,

$$\begin{aligned}
\bar{T}^0_{ll} &= (2l-1) \cdot \bar{T}^0_{l-1,l-1} \cdot \left(\frac{\Pi^{l-1}_{n=1} n(l-1+n)}{\Pi^l_{n=1} n(l+n)} \cdot \frac{2l+1}{2l-1} \right)^{\frac{1}{2}} \\
&= (2l-1) \cdot \bar{T}^0_{l-1,l-1} \cdot \left(\frac{\Pi^{l-1}_{n=1}(l-1+n)/(l+n)}{2l^2} \cdot \frac{2l+1}{2l-1} \right)^{\frac{1}{2}} \\
&= (2l-1) \cdot \bar{T}^0_{l-1,l-1} \cdot \left(\frac{1}{2l(2l-1)} \cdot \frac{2l+1}{2l-1} \right)^{\frac{1}{2}} \\
&= \left(\frac{2l+1}{2l} \right)^{\frac{1}{2}} \bar{T}^0_{l-1,l-1}.
\end{aligned} \tag{58}$$

The initial value is $\bar{T}^0_{11} = \sqrt{3}$. To obtain the Fourier constants we need further to decompose the power series of the cosine function into a trigonometric series, accordingly

$$\cos^j y = \sum_{k=0}^{j} \bar{c}_k \cos ky = 2^{(-l+1)} \sum_{k=0,2}^{l} \frac{1}{(1+\delta^0_k)} \begin{pmatrix} l \\ \left[\frac{l-k}{2}\right] \end{pmatrix} \cos ky, \tag{59}$$

where $[\ldots]$ denotes the entier operator. Thus the coefficients $\bar{c}_k$ can be generated from the binomial series

$$\begin{pmatrix} l \\ \left[\frac{l-k}{2}\right] \end{pmatrix} = \frac{l!}{\left(l - \left[\frac{l-k}{2}\right]\right)! \left[\frac{l-k}{2}\right]!}, \tag{60}$$

Note that due to the factorials again numerical under–/overflow is imminent but can be circumvented by appropriate choice of a calculation scheme, see the subsequent section on backward recursion. The Fourier coefficient for the order $(m = l)$ then become

$$a_{ll}^k = \bar{c}_k \bar{T}_{ll}^0, \quad k = 0, \ldots, l \quad \vee \quad (l-k)\,\mathbf{mod}\ 2 = 0, \tag{61}$$

and the reversed solution of Eq. (48), derived from Eq. (45) yields,

$$\begin{aligned} a_{l,l-1}^k &= -2\ k \cdot a_{ll}^k \ / \ \sqrt{2l} & (1 \leqslant m = l) \\ a_{l,m-1}^k &= \left(e_{lm}\ a_{l,m+1}^k - \beta_{l-m} \cdot 2\ k \cdot a_{lm}^k / d_{lm}\right) / \sqrt{j_{m-1}} & (1 \leqslant m < l). \end{aligned} \tag{62}$$

This method computes stable for $l \leq 1023$ using DOUBLE numbers. An underflow occurs for higher degrees in the starting values a_{ll}^k. The reason is found in the constant $2^{(-l+1)}$ in Eq. (59), having strongest impact on the frequenies for $k = l$ that approach roughly 10^{-300}, thus becoming close to the limiting boundary of the IEEE standards for DOUBLE numbers. Using $\sqrt{2^{-l+1}}$ instead, which is effectively an upscale, the maximum degree can be elevated to $l = 2048$ and in each recursive step m, it has to be again downscaled by $\sqrt{2^{-m}}$. For the ultra–high degrees beyond, either a frequency depended scaling is advisory or the extension of the used data type to 16 Bytes. The corresponding range of the data type considerably extends if 128-bit numbers (EXTND) are used, Tab. 6

Name:	Single	Double	Extnd
kind:	*4*	*8*	*16*
digits:	*24*	*53*	*113*
radix:	*2*	*2*	*2*
minexponent:	*-125*	*-1021*	*-16381*
maxexponent:	*128*	*1024*	*16384*
precision:	*6*	*15*	*33*
range:	*37*	*307*	*4931*
epsilon:	*1.192E-07*	*2.220E-16*	*1.926E-34*
huge:	*3.403E+38*	*1.798+308*	*1.190+4932*
tiny:	*1.175E-38*	*2.225-308*	*3.362-4932*

Table 6: Floating point numbers according to IEEE, digits are the number of bits in the mantisse, exponent gives the range of the binary exponent, e.g. $2^{1023} \simeq 9 \times 10^{307}$.

Usage of the EXTND type enables the stable calculation of the Fourier constants for the Legendre functions up to at least degree/order 16.000 without any scaling but is of course adjunctive to large memory and computational requirements, cf. Wittwer et al. (2007) [24] for a study on extended–range arithmetic and its strong impact on performance. Jekeli et al. (2008) [16] gives the upper bound for Legendre functions calculated in time domain by use of the EXTND type to $L = 23599$.

Since a frequency–wise scaling is in principle not complicated and leads to stable results throughout the use of the DOUBLE data type, it will be introduced in the next section.

7 Two calculation schemes for the associated Legendre functions

In this section forward and backward calculation is introduced that can both supply spectral coefficients for the Legendre functions to unlimited degree with DOUBLE data. In the case of the forward recursion 7 significant digits are reached before failure of the algorithm is anticipated and computations will be stopped. An efficient correction based on the boundary value proposal from the previous section then will enhance the solution, without ever getting close to under-/overflow of the calculated coefficients. The backward recursion is numerically capable to unlimited degree but requires frequency depended scaling to circumvent underflow and a stable, pre–calculated value for the binomial seed in Eq. (60).

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Since the Fourier coefficient series in each frequency asymptotically converges with increasing order towards zero, the numerical instabilities can be anticipated during recursive processing. In Eq. (48) it can be steadily evaluated in each processing step whether amplitudes belonging to a respective frequency continuously decrease

$$|a^k_{l,m+1}| < |a^k_{lm}| \tag{63}$$

and recursion interrupted, if not. By setting the remaining values to zero only a small omission error is introduced. Fig. 2 shows the occurrence of the instability with higher orders and high frequencies at some SINGLE/DOUBLE changeover level.

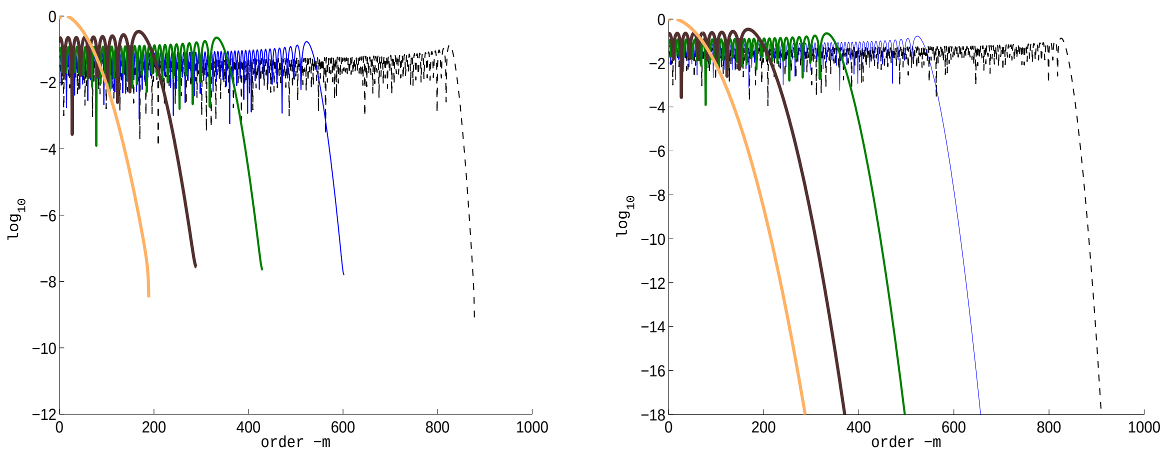

Figure 2: Left panel: when coefficient power fails to decrease during forward order-wise processing, recursion is stopped and the respective DOUBLE solution after manipulation, right panel. The amplitude series belong to the frequencies $k = \{1000, 984, 940, 848, 558\}$ for $l = 1000$ from left to right.

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Neglecting the higher frequencies for higher orders of the Legendre functions has the same impact as if these functions were calculated to single precision only.

$$P_\ell^m \Longleftrightarrow \mathcal{F}(A) \begin{cases} A_{\ell m}^k & \textbf{for} |a_{\ell m}^k| > 10^{-7} \\ 0 & \textbf{for} |a_{\ell m}^k| < 10^{-7}. \end{cases} \tag{64}$$

Applying such spectral truncated Legendre functions within a spherical harmonic synthesis to coefficients of physical data in Earth sciences, e.g. the gravity potential field has very low impact due to attenuation of the model coefficients with increasing resolution. Following Kaula's rule of thumb for the average coefficient per degree $\sigma_l = 10^{-5} \cdot l^{-2}$ the calculation e.g. of geoid heights N computed from a geopotential model, using single precision Legendre functions would result in an error per degree

$$\sigma_{N,l} = R \cdot 10^{-7} \cdot 10^{-5} \cdot l^{-2} [m] \tag{65}$$

where $R = 6378km$, and accumulates to

$$\sigma_{N,c} = 6,378/3 \cdot 10^{-7} [m]. \tag{66}$$

keeping in mind that instabilities commence at $l \geq 30$. This cumulative error is stil far below the precision of available global gravitational models. Concerning data synthesis it is therefore meaningless whether to use the full spectrum of the associated Legendre functions or just a truncated approximation. An advantage of the truncation scheme is that it is by far the fastest method to compute ultra–high degree Legendre functions on a grid since no initial seeds are required, no

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scaling of the frequencies by additional exponents has to be applied and besides the total number of effective coefficients to be computed in each step decreases gradually with the increasing number of excluded frequencies after failing the test of convergence in Eq. (63).

Nevertheless, and in order to recover inputs from the inverse orthogonal transform this truncation might not be acceptable and is therefore to be enhanced in the following section.

7.1 Enhancement of the forward solution

Recalling the solutions a_{lm}^k belonging to a certain degree l and frequency k, $\forall$ $(m = 2, \ldots, l-1)$ are based on the solution of a tridiagonal system where the first and last equations $(m = 0 \vee m = l)$ have to be reduced as boundary values, an enormous computational task would have to be solved for each frequency, respectively. Fortunately, the number of unknown coefficients of orders m can be substantially reduced from m_u, denoting a valid coefficient shortly before the suspension in Eq. (63) to m_d some 10^{th} of values after this break, just far enough to assume the remaining coefficients to have already asymptotically approached algrebraical zero.

Now, for each frequency k, a system according to Eq. (53) is to be established, estimating correction values for the coefficients a_{lm}^k, where $(m_u \leq m \leq m_d)$. In

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Fig 3 the error-belt that has to be corrected by additional, enhanced estimates is shown. It is important to notice, that the system matrix in the following remains equal throughout all frequencies, except from the diagonal elements that can be updated by a factor. What remains to be done is to subtract the previous, already computed coefficients $a^k_{l,m}$, where $(m < m_u)$ that will remain uncorrected, from the right-hand-side, as it was done in Eq. (53). The final value a^k_{l,m_d+1} then completes the shortened tridiagonal system with two boundaries,

$$\begin{pmatrix} -1 & 0 & 0 & \cdots & 0 \\ * & -1 & 0 & & 0 \\ * & * & -1 & & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & & & -1 \\ & & & * & * \\ 0 & 0 & 0 & 0 & * \end{pmatrix} \cdot \begin{pmatrix} a^k_{l,m_u} \\ a^k_{l,m_u+1} \\ \vdots \\ a^k_{l,m_d} \end{pmatrix} = -\begin{pmatrix} * & -1 & 0 & \cdots & 0 \\ * & * & - & & 0 \\ 0 & * & * & \ddots & 0 \\ \vdots & & \ddots & \ddots & -1 \\ 0 & 0 & 0 & * & * \end{pmatrix} \cdot \begin{pmatrix} a^k_{l,0} \\ a^k_{l,1} \\ \vdots \\ a^k_{l,m_u-1} \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ a^k_{l,m_d+1} \end{pmatrix}, \tag{67}$$

where it is either set to numerical zero or, in case of approaching algebraically relevant values, e.g. if $(m_d + 1 = l)$ it can be calculated as described in the next section about the starting seeds for $(m = l)$. The multiplications thus effectively reduce to

$$N_{[:,m_u \ldots m_d]} \cdot \begin{pmatrix} a^k_{l,m_u} \\ a^k_{l,m_u+1} \\ \vdots \\ a^k_{l,m_d} \end{pmatrix} = -N_{[:,0 \ldots m_u-1]} \cdot \begin{pmatrix} a^k_{l,0} \\ a^k_{l,1} \\ \vdots \\ a^k_{l,m_u-1} \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ a^k_{l,m_d+1} \end{pmatrix}. \quad (68)$$

Due to the tridiagonal structure in Eq.(52), the reduction term on the right-hand-side simplifies to two scalar entries at the indexes $m_u - 1$ and m_u

$$-N_{[:,0 \ldots m_u-1]} \cdot \begin{pmatrix} a^k_{l,0} \\ a^k_{l,1} \\ \vdots \\ a^k_{l,m_u-1} \end{pmatrix} = N[m_u - 1 \ldots m_u, 0 \ldots m_u - 1] \cdot \begin{pmatrix} a^k_{l,0} \\ a^k_{l,1} \\ \vdots \\ a^k_{l,m_u-1} \end{pmatrix} \quad (69)$$

and can thus be processed even for ultra-high degrees very efficiently.

7.2 Backward recursion

This approach avoids the enhancement step since no instabilities occur compared to the forward processing, but requires initial values and book–keeping of additional integer exponents.

Thus for the purpose of the calculating either initial values in $(m = l)$ for backward recursion or providing non–zero final values to enhance the forward recursion as discussed in the previous section we will introduce a general computational

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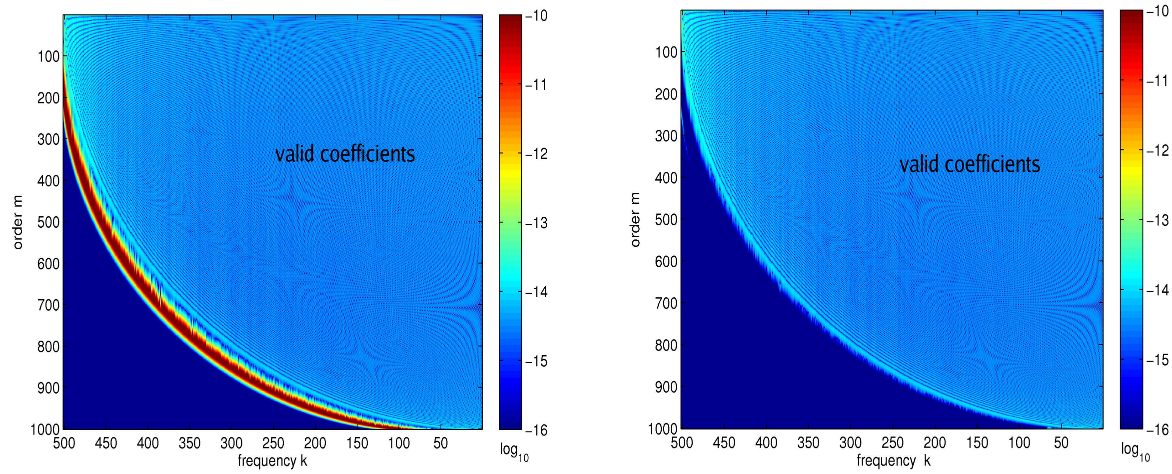

Figure 3: Left panel: error belt (red) in the vicinity of algorithm cut-off before and after correction (right panel) by additional estimates for each frequency k and those respective orders of interest (inside the belt).

scheme, that can provide results to unlimited degree l. The scheme has to fulfill the following requirements:

- manipulate (absolute) numbers $< 2^{-1021}$
- maintain consistency when exceeding under-/overflow values

The first requirement can be met by separating an additional scaling parameter from the result. This parameter can then be used in the course of computations of the Fourier coefficients for the Legendre functions, scaling thus intermediate results always inside the suitable numerical range that is represented by DOUBLE numbers. The second requirement demands special attention during the processing

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of the product sums in the binomial equations, i.e. to avoid that multiplications cannot be committed in under-/overflow domain.

Recalling Eq. (59) and changing the term 2^{-l+1} to 2^{-l} to obtain compliance with Eq. (6) s.th. all coefficients have to be doubled except when $k = 0$. We can then write

$$a_{ll}^{k} = \; 2^{-l} \begin{pmatrix} l \\ f \end{pmatrix}, f = \left[\frac{l-k}{2} \right]. \tag{70}$$

The binomial formula is now converted into a division and a product sequence

$$2^{-l} \begin{pmatrix} l \\ f \end{pmatrix} = \frac{\Pi_{l-f+1}^{l}}{2^{l} \cdot \Pi_{1}^{f}} = \Pi \left(\frac{l-f+1}{2^{l/f}}, \ldots, \frac{l}{f 2^{l/f}} \right), \tag{71}$$

whence before calculating the product we expand Eq. (71) into a series of rational numbers

$$\begin{aligned} 2^{-l} \begin{pmatrix} l \\ f \end{pmatrix} \;\; &= \;\; (l-f+1)/2^{l/f} \cdot (l-f+2)/(2 \cdot 2^{l/f}) \cdot \ldots \cdot \\ & \;\;\;\;\;\; (l-1)/((f-1) \cdot 2^{l/f}) \cdot l/(f \cdot 2^{l/f}). \end{aligned} \tag{72}$$

Instead of multiplying then sequentially, we can alternately combine the rationals from both sides,

$$(l-f+1)/2^{l/f} \cdot l/(f \cdot 2^{l/f}) \cdot (l-f+2)/(2 \cdot 2^{l/f}) \cdot (l-1)/((f-1) \cdot 2^{l/f}) \cdot \ldots \cdot \tag{73}$$

and continue to do so recursively as long as the exponent of the first term remains below a threshold, i.e. the order of magnitude does not drop below e.g. 2^{-700}.

The resulting sequence then cannot be shortened any further by using DOUBLE numbers. As an example, consider the binomial sequence for $(l = m = 8046), k = 7046)$ after several multiplications from both sides, it becomes

$$\begin{aligned}
a^{7046}_{8046,8046} &= 25.6761235136699 \times 10^{-207} \quad \text{first term} \\
&\times \; 13.0972864271867 \times 10^{-207} \\
&\times \; 9.02613352518573 \times 10^{-207} \\
&\times \; 7.09475992352919 \times 10^{-207} \\
&\times \; 6.03558284701099 \times 10^{-207} \\
&\times \; 5.43316669809149 \times 10^{-207} \\
&\times \; 5.11866122428050 \times 10^{-207} \\
&\times \; 70.8558172718808 \times 10^{-105} \\
&\times \; 224.030023870168 \times 10^{-054} \\
&\times \; 95.5221219093371 \times 10^{-015}.
\end{aligned}$$

At this point the scaling factor is drawn from the remaining 9 numbers,

$L_g(i) = [\log a_i / \log 2] = -\{684, 684, 685, 685, 685, 685, 343, 172, 43\}; \quad i = 2, \ldots, 10$

where $[\ldots]$ is again the entier operator, and applies as reduction $2^{\sum_{i=2}^{10} L_g(i)} = 2^{-4666}$ that has to be registered separately.

The reduced (stored) value without the scaling is,

$$a^{*k}_{ll} = a_1 \cdot \Pi^{10}_{i=2} \left(a_i \cdot 2^{-L_g(i)} \right) = 2.1219974676090 \times 10^{-207} \qquad (74)$$

and its true value, $a_{ll}^k = a_{ll}^{*k} \times 2^{-4666}$ but of no practical relevance since algebraically zero. During the recursion the mantissa has then to be periodically updated by the appropriate re–scaling ($2^x > 2^{-1021} > 2^{-4666}$) as soon as algebraically relevant values ($> 2^{-53}$) are approached. In Fig. (4) it is shown how each frequency starts from its reduced value, unwinds from 2^{-700} towards 0 during recursive processing and becomes several times re–scaled until the registered exponent has vanished. After the external exponent is cleared, valid coefficients in DOUBLE remain.

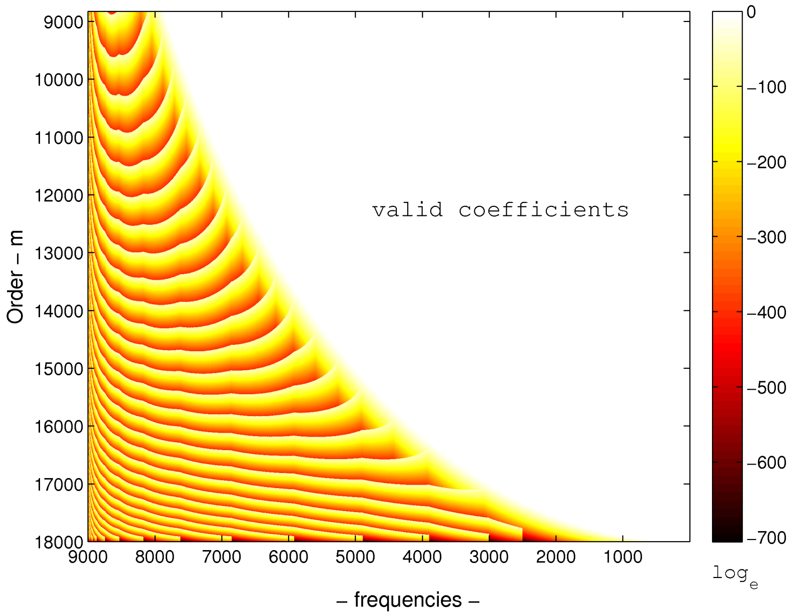

Figure 4: Frequencies for $0 \leqslant m \leqslant l = 18.000$ with additional external exponents. Whenever algebraically relevant coefficients during the recursion are approached, the mantissa is reset as long as an external exponent is still registered.

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8 Comparison of results

An important test of plausibility follows the ideas of Wagner (1983) [23]. It provides the overall errors in the coefficients and therefore the stability during recursion. The test is a general invariance for all degrees and has been coined by the authors Gooding and Wagner (2008) the *relative deficit* (R.D) meaning in fact an absolute numerical deficit. It was initially discovered in the framework of inclination functions. Adoption due the symmetry for the Legendre function results in

$$R.D = 1 - \left\{ \sum_{m,k} \left(2 - \delta_k^0 \left(1 - l \ \mathbf{mod} \ 2\right)\right) \left(a_{lm}^k\right)^2 \right\} / (2l+1), \tag{75}$$

and should assert in Tab. 7 to machine precision, cf. *epsilon* from Tab. 6.

Fig. 5 compares the presented spectral methods to originally computed Legendre functions by standard recursive algorithms, each in the co-latitude range between $(0° \leq \theta \leq 180°)$. The Fourier coefficients have been used in Eq. (6). Underflow errors can be observed during conventional recursive processing in time–domain, starting at $(\theta = 20°)$ as well as $(\theta = 160°)$. The synthesis of Legendre functions from their Fourier coefficients instead proofs stable and reliable up to the very high degree over the entire definition range.

Two distinct analytical formulations will be used in conclusion to affirm our concept. Firstly, the Legendre function of a certain order (Legendre polynomial,

$0 \leqslant m \leqslant l$	10^{16}R.D	Run t(s)
30	-4	0.00
360	60	0.08
1.080	153	0.28
2.160	155	0.75
5.400	42	3.23
7.200	227	9.41
10.800	443	10.8
21.600	325	43.2
36.000	414	125
43.200	546	180
54.000	486	281
64.800	-346	457
81.000	722	638
108.000	868	1159

Table 7: Validation of coefficients via the general invariance. As a rule of thumb $10^{-16}R.D. \sim 2\sqrt{l}$ can be observed. Runtime for relative performance.

$m = 0$) from a direct formula can be used to compare with the result after initial computation of the sectorial solution by Eq.(61) and recursive backward processing

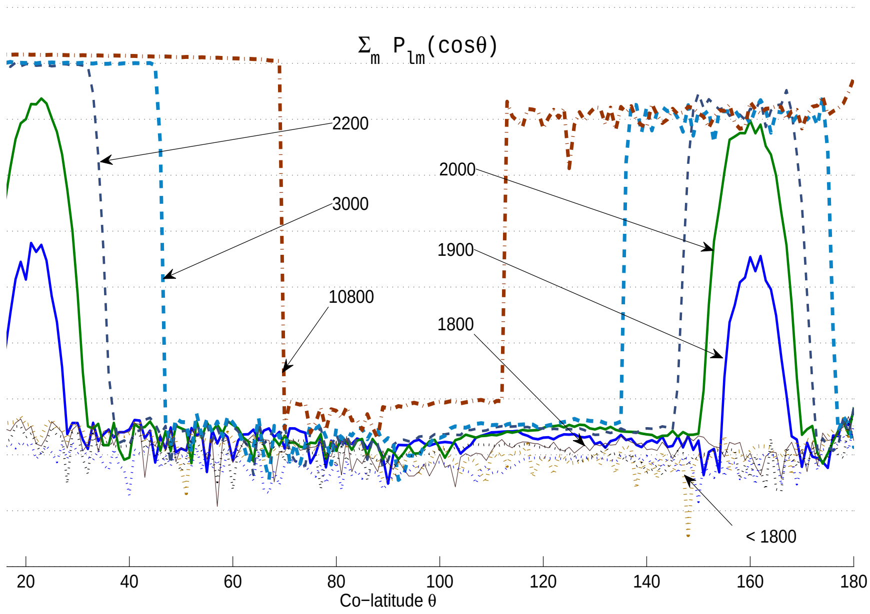

Figure 5: Comparison between spectrally composed Legendre functions vs. classical recursive computation, in terms of the order-wise sum for each degree, respectively. The underflow error from computation in data domain gradually increases with higher degrees, eventually spreading over all latitudes.

thru all associated orders, Tab 8.

A second test compares order–wise recursive processing to the direct solution for a certain frequency ($k = 1$), see Gooding and Wagner (2008). Neglecting their sign–convention and supplying normalization to their Eq. (28a) and Eq. (28b) yields for our purpose

Degree	Resolution $\lambda/2$	$\sigma_p = \sqrt{\frac{[\epsilon\epsilon]}{n^2-n}}$
5.400	$2'$ (3700m)	*3.1d-13*
7.200	$1.5'$ (2500m)	*3.8d-13*
10.800	$1'$ (1800m)	*5.5d-13*
21.600	$30''$ (900m)	*1.3d-12*
36.000	$18''$ (555m)	*2.1d-12*
43.200	$15''$ (460m)	*2.6d-12*
54.000	$12''$ (370m)	*3.1d-12*
64.800	$10''$ (310m)	*3.0d-12*
81.000	$8''$ (247m)	*4.3d-12*
108.000	$6''$ (185m)	*6.2d-12*

Table 8: Final test after synthesis of Legendre functions from Fourier coefficients: comparison to each degree and ($m = 0$) in the sample-range ($0° \leqslant \theta \leqslant 180°$) after backward recursion from ($m = l$) with the initial values calculated by a closed analytic expression, Eq. (49). Resolution in equivalent half-wavelength (length on the Earth surface). σ_p ist the standard deviation for the single Legendre function sample after synthesis from the coefficients. The test shows good correspondence even for the highest resolution.

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$(l + m \text{ even})$ (76)

$$a_{\ell m}^{k=1}\left(\frac{\pi}{2}\right) = \frac{m(l+m)!(l-1)!\sqrt{(2-0^m)(2l+1)}}{2^{2l-1}\sqrt{\prod_{l-m+1}^{l+m}(l+1)[1/2(l-m)]![1/2(l+m)]!\left\{[1/2(l-1)]!\right\}^2}}$$

$(l + m \text{ odd})$ (77)

$$a_{\ell m}^{k=1}\left(\frac{\pi}{2}\right) = \frac{\sqrt{(2-0^m)(2l+1)}(l+m)!(l-1)!}{2^{2l-1}\sqrt{\prod_{l-m+1}^{l+m}[1/2(l-m-1)]![1/2(l+m-1)]![1/2(l-1)]![1/2(l+1)]!}}.$$

Both expressions can be computed by decomposing the factorials into product – loops with special attention to overflow. Fig. 6 shows the result of the comparison for this selected frequency in both equations at the degree $l = 100.001$. The result shows good correspondence throughout all recursive orders.

9 Conclusions on the use of the Fourier–base for the Legendre functions

In order to obtain stable Legendre functions in time domain, a frequency wise consideration of numerical under-/overflow is presented in this article. It is shown that 4 basic methods to calculate the Fourier coefficients of the Legendre functions can be applied. They can be distinguished in the transformation from time to frequency domain or by direct recursions about the Fourier coefficients themselves. Usage of the primary method is for moderate resolutions sufficient, but for higher resolutions the direct recursions applied to the Fourier coefficients are the method

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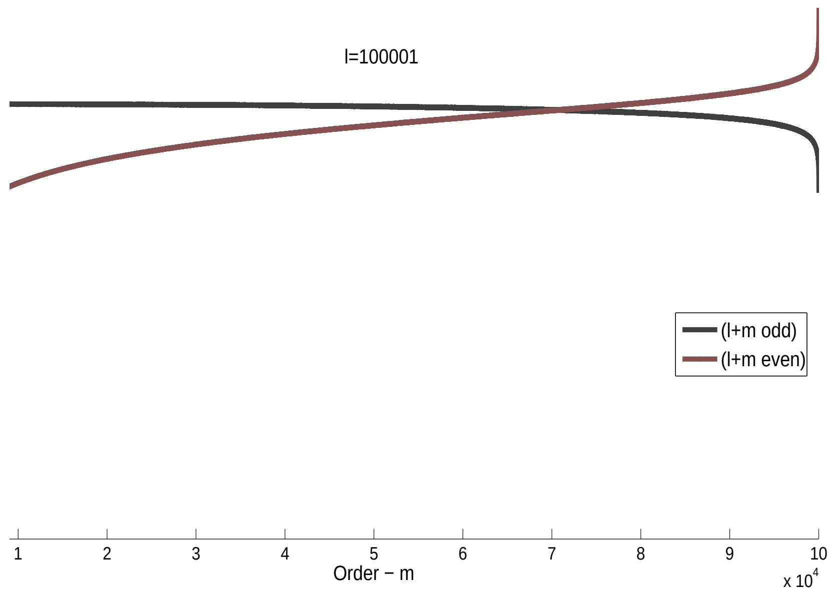

Figure 6: Error difference between recursive results for $k = 1$ belonging to $l = 100001$, $0 \leqslant m \leqslant l$, compared to the direct, analytical solution via the factorial Eq. (70) and Eq. (71).

of choice. Forward recursion delivers the fastest solutions to single precision that can be enhanced by least squares estimates for deficient orders in each frequency, respectively. No numerical problems occur, no re–scaling is required. Backward recursion performs reliable in ultra-high degrees as well, but in order to stable compute the recursions, additional, external exponents have to be introduced and applied in the course of computations if double precision arithmetic is applied. A decay in precision of merely $(10^{-16} 2\sqrt{l})$ can be observed for the Legendre functions after re-transformation into time-domain.

Derivation of the Legendre functions can be conveniently applied in spectral domain. When using non-singular expressions, see Petrovskaya (2006) [19] full gravity gradients can be realized. After transformation of the spherical harmonic model coefficients into lumped Harmonics highly efficient global model synthesis can be achieved by 2D-FFT, see Sneeuw and Bun (1996) [22] and Gruber (2010) [10]. The product–sums of spherical Harmonics for unevenly distributed data analysis on a sphere can be processed efficiently by direct scalar products between the trigonometric base functions, Gruber (2008) [9]

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