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The SHA_SHS package

C, Fortran and MATLAB routines for ultra-high-degree spherical harmonic analysis (SHA) and synthesis (SHS) on the unit sphere

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1 Introduction

This document describes the SHA_SHS package. In Section 1.1, we start by listing and briefly describing all the source code files of the package. In Section 2, we introduce the notation and define surface spherical harmonics. Then, we describe the spherical harmonic analysis using point and mean values in Sections 3 and 4, respectively. Finally, Sections 5 and 6 introduce the surface sphere harmonic synthesis for point and mean values, respectively.

1.1 List of files

The source codes of the SHA_SHS package are organized in three folders depending on the programming language: `./src/C`, `./src/Fortran` and `./src/MATLAB`.

1.1.1 The SHA_SHS package in C

The C version of the package is organized as follows (the `./src/C` folder).

- `arr_calloc.c` – Initialization of an 1D array to zeros.
- `arr_malloc.c` – Allocation of an 1D array.
- `arr_min_dp.c` – Minimum value of an 1D array in double precision.
- `arr_min_qp.c` – Minimum value of an 1D array in quadruple precision.
- `fopen_create_path.c` – An auxiliary function; for details see the source code.
- `gl_grd_dp.c` – Generates the Gauss–Legendre grid and integration weights in double precision.
- `gl_grd_qp.c` – Generates the Gauss–Legendre grid and integration weights in quadruple precision.
- `mkdir_recursive.c` – An auxiliary function; for details see the source code.
- `sh_coeffs_free_dp.c` – Releases double-precision version of spherical harmonic coefficients from RAM.
- `sh_coeffs_free_qp.c` – Releases quadruple-precision version of spherical harmonic coefficients from RAM.
- `sh_coeffs_init_dp.c` – Initializes double-precision version of spherical harmonic coefficients to a structure required by the package.
- `sh_coeffs_init_qp.c` – Initializes quadruple-precision version of spherical harmonic coefficients to a structure required by the package.

- `sh_coeffs_read_bin_dp.c` – Reads double-precision version of spherical harmonic coefficients from a binary file to a structure required by the package.
- `sh_coeffs_read_bin_qp.c` – Reads quadruple-precision version of spherical harmonic coefficients from a binary file to a structure required by the package.
- `sh_coeffs_read_mtx_txt_dp.c` – Reads double-precision version of spherical harmonic coefficients from a text file to a structure required by the package.
- `sh_coeffs_read_mtx_txt_qp.c` – Reads quadruple-precision version of spherical harmonic coefficients from a text file to a structure required by the package.
- `sh_coeffs_write_bin_dp.c` – Writes double-precision version of spherical harmonic coefficients to a binary file.
- `sh_coeffs_write_bin_qp.c` – Writes quadruple-precision version of spherical harmonic coefficients to a binary file.
- `sh_coeffs_write_mtx_txt_dp.c` – Writes double-precision version of spherical harmonic coefficients to a text file.
- `sh_coeffs_write_mtx_txt_qp.c` – Writes quadruple-precision version of spherical harmonic coefficients to a text file.
- `sh_surf_analysis_mean_dp.c` – Surface spherical harmonic analysis (mean values) in double precision.
- `sh_surf_analysis_mean_qp.c` – Surface spherical harmonic analysis (mean values) in quadruple precision.
- `sh_surf_analysis_point_dp.c` – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature) in double precision.
- `sh_surf_analysis_point_qp.c` – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature) in quadruple precision.
- `sh_surf_synthesis_mean_dp.c` – Surface spherical harmonic synthesis of mean values at grids in double precision.
- `sh_surf_synthesis_mean_qp.c` – Surface spherical harmonic synthesis of mean values at grids in quadruple precision.
- `sh_surf_synthesis_point_dp.c` – Surface spherical harmonic synthesis of point values at grids in double precision.
- `sh_surf_synthesis_point_qp.c` – Surface spherical harmonic synthesis of point values at grids in quadruple precision.
- `test_run_dp.c` – Program to test the package in double precision.
- `test_run_qp.c` – Program to test the package in quadruple precision.

1.1.2 The SHA_SHS package in Fortran

The Fortran 95 version of the package is organized as follows (the ./src/Fortran folder).

- constants.f95 – Module defining numerical constants.
- FFTW3.f95 – Module related to the FFTW package.
- GL_grid_dp.f95 – Generates the Gauss–Legendre grid and integration weights in double precision.
- GL_grid_qp.f95 – Generates the Gauss–Legendre grid and integration weights in quadruple precision.
- Surface_SHA_dp.f95 – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature) in double precision.
- Surface_SHA_qp.f95 – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature) in quadruple precision.
- Surface_SHA_mean_dp.f95 – Surface spherical harmonic analysis (mean values) in double precision.
- Surface_SHA_mean_qp.f95 – Surface spherical harmonic analysis (mean values) in quadruple precision.
- Surface_SHS_dp.f95 – Surface spherical harmonic synthesis of point values at grids in double precision.
- Surface_SHS_qp.f95 – Surface spherical harmonic synthesis of point values at grids in quadruple precision.
- Surface_SHS_mean_dp.f95 – Surface spherical harmonic synthesis of mean values at grids in double precision.
- Surface_SHS_mean_qp.f95 – Surface spherical harmonic synthesis of mean values at grids in quadruple precision.
- Test_run_dp.f95 – Program to test the package in double precision.
- Test_run_qp.f95 – Program to test the package in quadruple precision.
- vartypes.f95 – Module defining data types.

1.1.3 The SHA_SHS package in MATLAB

Below is an overview of files related to the MATLAB version of the package (the ./src/MATLAB folder).

- GL_grid.m – Generates the Gauss–Legendre grid and integration weights.
- Surface_SHA.m – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature), non-parallel computation.
- Surface_SHA_sliced.m – Surface spherical harmonic analysis (point values, Gauss–Legendre quadrature), parallel computation.
- Surface_SHA_sliced_load.m – Loads data inside Surface_SHA_sliced.m.
- Surface_SHA_sliced_save.m – Saves data inside Surface_SHA_sliced.m.
- Surface_SHS.m – Surface spherical harmonic synthesis of point values at a grid.
- Surface_SHS_sliced.m – Surface spherical harmonic synthesis of point values at a grid inside
Surface_SHA_sliced.m.
- Test_run.m – Script to test the package, non-parallel computation.
- Test_run_sliced.m – Script to the package, parallel computation.

2 Preliminaries

2.1 Notation

The notation used throughout this document is explained in Table 1.

Table 1: Notation

Symbol	Definition
$\varphi \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$	Spherical latitude
$\lambda \in \left[0, 2\pi\right]$	Spherical longitude
$n = 0, 1, 2, \ldots$	Spherical harmonic degree
$m = 0, 1, 2, \ldots, n$	Spherical harmonic order
$n_{\max}$	Maximum spherical harmonic degree of the expansion
P_n	Legendre polynomial of degree n
$\bar{P}_{nm}$	Fully-normalized associated Legendre function of the first kind of degree n and order m
$\bar{Y}_{nm}$	Real-valued 4π-fully-normalized surface spherical harmonic of degree n and order m
$\{\bar{C}_{nm},\, \bar{S}_{nm}\}$	Real-valued 4π-fully-normalized surface spherical harmonic coefficients of degree n and order m
$f(\varphi, \lambda)$	Real-valued function on a sphere
$\tilde{f}$	Mean value of a real-valued function on a sphere over a grid cell
σ	Unit sphere
$\Delta\sigma$	Area of a grid cell on the unit sphere

2.2 Surface spherical harmonics

The following definition of real-valued 4π-fully-normalized surface spherical harmonics is adopted (e.g., Hoffmann-Wellenhof and Moritz, 2005):

$$\bar{Y}_{nm}(\varphi, \lambda) = \bar{P}_{nm}(\sin\varphi) \begin{cases} \cos(m\,\lambda), \\ \sin(m\,\lambda), \end{cases} \tag{1}$$

where (ibid.)

$$\bar{P}_{nm}(\sin\varphi) = \begin{cases} \sqrt{(2n+1)}\, P_n(\sin\varphi), & m = 0, \\ \sqrt{2(2n+1)\dfrac{(n-m)!}{(n+m)!}}\, \left(1 - \sin^2\varphi\right)^{m/2} \dfrac{\mathrm{d}^m P_n(\sin\varphi)}{\mathrm{d}(\sin\varphi)^m}, & 0 < m \leq n, \end{cases} \tag{2}$$

with

$$P_n(\sin\varphi) = \frac{1}{2^n\, n!}\, \frac{\mathrm{d}^n}{\mathrm{d}(\sin\varphi)^n} \left(\sin^2\varphi - 1\right)^n. \tag{3}$$

In the `SHA_SHS` package, the $\bar{P}_{nm}(\sin\varphi)$ terms are evaluated by the algorithm of Fukushima (2012), which is numerically stable up to ultra-high harmonic degrees and orders (tens of thousands and even well beyond).

3 Surface spherical harmonic analysis: point values

Surface spherical harmonic analysis is a numerical computation/estimation of surface spherical harmonic coefficients $\{\bar{C}_{nm},\, \bar{S}_{nm}\}$ of a function $f(\varphi, \lambda)$ defined on the unit sphere,

$$\left.\begin{matrix}\bar{C}_{nm}\\ \bar{S}_{nm}\end{matrix}\right\} = \frac{1}{4\pi} \iint_{\sigma} f(\varphi, \lambda)\, \bar{Y}_{nm}(\varphi, \lambda)\, \mathrm{d}\sigma. \tag{4}$$

Equation (4) can be computed *exactly*, provided that the signal f is band-limited (that is, possesses a finite number of non-zero surface spherical harmonics up to some maximum harmonic degree $n_{\max}$) and its sampling obeys some special scheme. For the latter, the `SHA_SHS` package uses the Gauss–Legendre quadrature (e.g. Sneeuw, 1994), as one of the most efficient quadrature schemes for surface spherical harmonic analysis. Another commonly used quadrature is due to Driscoll and Healy (1994). The Gauss–Legendre quadrature has been described several times in the literature (e.g., Sneeuw, 1994; Rexer and Hirt, 2015), so it is not repeated here.

The following routines compute Eq. (4) from point values of f (see also Section 1.1):

- `sh_surf_analysis_point_dp.c`,
- `sh_surf_analysis_point_qp.c`,
- `Surface_SHA_dp.f95`,
- `Surface_SHA_qp.f95`,
- `Surface_SHA.m`,
- `Surface_SHA_sliced.m`.

The points of the Gauss–Legendre grid and the respective weights can be computed using the following routines:

- `gl_grd_dp.c`,
- `gl_grd_qp.c`,
- `GL_grid_dp.f95`,
- `GL_grid_qp.f95`,
- `GL_grid.m`.

4 Surface spherical harmonic analysis: mean values

Surface spherical harmonic coefficients $\{\bar{C}_{nm}, \bar{S}_{nm}\}$ of $f(\varphi, \lambda)$ can also be estimated from mean values (block-means) of f sampled at suitable grid cells. This lead to the following equation

$$\left.\begin{matrix}\bar{C}_{nm}\\ \bar{S}_{nm}\end{matrix}\right\} = \frac{1}{4\pi} \sum_{i,j} \tilde{f}_{i,j} \int\limits_{\varphi_i^{\min}}^{\varphi_i^{\max}} \bar{P}_{nm}(\sin\varphi)\, \cos\varphi\, \mathrm{d}\varphi \int\limits_{\lambda_j^{\min}}^{\lambda_j^{\max}} \left\{\begin{matrix}\cos m\lambda\\ \sin m\lambda\end{matrix}\right\} \mathrm{d}\lambda, \tag{5}$$

where $\varphi_i^{\min}$, $\varphi_i^{\max}$, $\lambda_j^{\min}$ and $\lambda_j^{\max}$ denote the cell boundaries over which the mean value $\tilde{f}_{i,j}$ is given. Further details on the numerical evaluation of Eq. (5) can be found, for instance, in Colombo (1981).

The following routines compute Eq. (5) (see also Section 1.1):

- `sh_surf_analysis_mean_dp.c`,
- `sh_surf_analysis_mean_qp.c`,
- `Surface_SHA_mean_dp.f95`,
- `Surface_SHA_mean_qp.f95`.

5 Surface spherical harmonic synthesis: point values

Having surface spherical harmonic coefficients $\{\bar{C}_{nm}, \bar{S}_{nm}\}$ of a band-limited function $f(\varphi, \lambda)$, it is possible to reconstruct $f(\varphi, \lambda)$ at any point on the unit sphere by surface spherical harmonic synthesis,

$$f(\varphi, \lambda) = \sum_{n=0}^{n_{\max}} \sum_{m=0}^{n} \left(\bar{C}_{nm} \cos(m\,\lambda) + \bar{S}_{nm} \sin(m\,\lambda) \right) \bar{P}_{nm}(\sin\varphi). \tag{6}$$

If the evaluation points (φ, λ) form a regular grid, highly efficient FFT-based algorithms can be used to evaluate Eq. (6). These have been extensively discussed in the literature (e.g., Colombo, 1981; Sneeuw, 1994; Jekeli et al, 2007; Rexer and Hirt, 2015). The `SHA_SHS` package takes advantage of these algorithms in order to achieve an efficient grid-wise numerical computation.

The following routines compute Eq. (6) (see also Section 1.1):

- `sh_surf_synthesis_point_dp.c`,
- `sh_surf_synthesis_point_qp.c`,
- `Surface_SHS_dp.f95,`
- `Surface_SHS_qp.f95`,
- `Surface_SHS.m`,
- `Surface_SHS_sliced.m`.

6 Surface spherical harmonic synthesis: mean values

A mean value of $f(\varphi, \lambda)$ from Eq. (6) over $\varphi \in [\varphi_1, \varphi_2]$ and $\lambda \in [\lambda_1, \lambda_2]$ is given as follows,

$$\begin{aligned} \tilde{f}(\varphi_1, \varphi_2, \lambda_1, \lambda_2) &= \frac{1}{\Delta\sigma} \int\limits_{\varphi_1}^{\varphi_2} \int\limits_{\lambda_1}^{\lambda_2} f(\varphi, \lambda)\, \mathrm{d}\lambda\, \cos\varphi\, \mathrm{d}\varphi \\ &= \frac{1}{\Delta\sigma} \sum_{n=0}^{n_{\max}} \sum_{m=0}^{n} \left(\bar{C}_{nm} \int\limits_{\lambda_1}^{\lambda_2} \cos(m\,\lambda)\, \mathrm{d}\lambda + \bar{S}_{nm} \int\limits_{\lambda_1}^{\lambda_2} \sin(m\,\lambda)\, \mathrm{d}\lambda \right) \int\limits_{\varphi_1}^{\varphi_2} \bar{P}_{nm}(\sin\varphi)\, \cos\varphi\, \mathrm{d}\varphi, \end{aligned} \tag{7}$$

where $\Delta\sigma$ is the area of the spherical rectangle bounded by φ_1, φ_2, λ_1 and λ_2. The numerical implementation of Eq. (7) applied in `SHA_SHS` is described, for instance, in Colombo (1981).

The following routines compute Eq. (7) (see also Section 1.1):

- `sh_surf_synthesis_mean_dp.c`,
- `sh_surf_synthesis_mean_qp.c`,
- `Surface_SHS_mean_dp.f95`,
- `Surface_SHS_mean_qp.f95`.

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