# zest

# **Zernike and Spherical harmonic Transforms**

Sebastian Sassi

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# 0.1 Getting started

#### 0.1.1 Installation

Before proceeding to installation, it is worth noting that zest mostly does not depend on libraries other than standard lbrary. However, an exception to this is that performing least squares fits of spherical harmonic and Zernike expansions requires linking with LAPACK.

For the installation you need to obtain the source code, e.g., by cloning the git repository. Then, navigate to the source directory

```
git clone https://github.com/sebsassi/zest.git
cd zest
```

If you are familiar with CMake, zest follows a conventional CMake build/install procedure. Even if not, the process is simple: first, create a directory where the library is built, say build, and then build the sources in that directory, e.g.,

```
cmake --preset=default cmake --build build
```

The default configuration here should be adequate. After that you can install the built library from the build directory to our desired location

```
cmake --install build --prefix <install directory>
```

Here install directory denotes your preferred installation location.

# 0.1.2 Basic Usage

To test the installation and take our first steps in using the library, we can create a short program that evaluates the spherical harmonic expansion of a function, rotates it, and prints out the rotated coefficients. Make a file rotate\_sh.cpp with the following contents

```
#include "zest/sh_glq_transformer.hpp"
#include "zest/rotor.hpp"
#include <cmath>
#include <cstdio>
int main()
    auto function = [](double lon, double colat)
        const double x = std::sin(colat)*std::cos(lon);
        return std::exp(-x*x);
    };
    // Evaluate the function on a Gauss-Legendre quadrature grid
    constexpr std::size_t order = 20;
    zest::st::SphereGLQGridPoints points{};
    zest::st::SphereGLQGrid grid
        = points.generate_values(function, order);
    // Transform the grid to obtain its spherical harmonic expansion
    zest::st::GLQTransformerGeo transformer{};
    zest::st::RealSHExpansion expansion
        = transformer.forward_transform(grid, order);
```

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```
// Euler angles
const double alpha = std::numbers::pi/2;
const double beta = std::numbers::pi/4;
const double gamma = 0;

// Rotate the expansion coefficients
std::array<double, 3> angles = {alpha, beta, gamma};
zest::WignerdPiHalfCollection wigner(order);
zest::Rotor rotor{};
rotor.rotate(expansion, wigner, angles);

for (std::size_t l = 0; l < expansion.order(); ++1)
{
    for (std::size_t m = 0; m <= 1; ++m)
        std::printf("f[%lu, %lu] = %f", l, m, expansion(l, m));
}
</pre>
```

Now, to compile the code, we use GCC in this example and link our code with zest

```
g++ -std=c++20 -03 -mfma -mavx2 -o rotate_sh rotate_sh.cpp -lzest
```

There are few things of note here. First, zest is built on the C++20 standard, and therefore requires a sufficiently modern compiler, which implements the necessary C++20 features. To tell GCC we are using C++20, we give the flag std=c++20.

Secondly, the performance of the library is sensitive to compiler optimizations. As a baseline, we use the optimization level -03 to enable all architecture-independent optimizations in GCC. On top of that, this example assumes that we are building for an x86 CPU, which supports floating point fused multiply-add operations (-mfma) and AVX2 SIMD operations (-mavx2). These options form a good performant baseline that should work for all modern x86 CPUs. In general, if you will be running your code on the system you compile it on -march=native should be a decent alternative to these options.

# 0.2 Theoretical background

This section aims to give a brief introduction to the mathematics that underlie this library. This introduction assumes basic mathematical knowledge of linear algebra, integration, and basis functions.

# 0.2.1 Spherical harmonics

Spherical harmonics, denoted  $Y_{lm}(\theta, \varphi)$ , are a collection of special functions defined on the sphere. They form a complete orthogonal basis on the sphere  $S^2$ , meaning that any square integrable function  $f(\theta, \varphi) \in L^2(S^2)$  can be represented as a linear combination of (possibly an infinite number of) spherical harmonics

$$f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{|m| \le l} f_{lm} Y_{lm}(\theta, \varphi),$$

such that

$$\int_{\mathbb{S}^2} Y_{lm}(\theta,\varphi)^* Y_{l'm'}(\theta,\varphi) \, d\Omega = N_{lm} \delta_{ll'} \delta_{mm'}.$$

Here  $\delta_{ij}$  is the Kroenecker delta, and  $N_{lm}$  is a normalization constant that depends on the normalization convention of spherical harmonics.

Spherical harmonics come in two forms: complex spherical harmonics, which we denote as  $Y_l^m$  with upper index m, and real spherical harmonics which we denote as  $Y_{lm}$  with upper index m. This library has been built around real spherical harmonics with currently no support for full complex spherical harmonics. Therefore

this introduction is presented in terms of real spherical harmonics, apart from cases where complex spherical harmonics are necessary. The real and complex spherical harmonics are related via a linear transformation

$$Y_{lm} = \begin{cases} \frac{i}{\sqrt{2}} (Y_l^m - (-1)^m Y_l^{-m}) & \text{if } m < 0, \\ Y_l^0 & \text{if } m = 0, \\ \frac{1}{\sqrt{2}} (Y_l^{-m} + (-1)^m Y_l^m) & \text{if } m > 0. \end{cases}$$

Spherical harmonics can be expressed in closed form using the associated Legendre polynomials  $R_l^m(x)$ . There are multiple possible conventions for writing the spherical harmonic functions depending on two factors: the normalization discussed above, and the presence of the so-called Condon–Shortley phase. For brevity, we do not write down all possible permutations of conventions here. Two conventions of note are the geodesy convention

$$Y_l^m(\theta,\varphi) = \sqrt{(2l+1)\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi},$$

and quantum mechanics convention

$$Y_l^m(\theta,\varphi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi}.$$

For the geodesy convention, the normalization constant is  $N_{lm} = 4\pi$ , whereas the quantum mechanics spherical harmonics are unit normalized with  $N_{lm} = 1$ . The quantum mechanics convention also includes the Condon–Shortley phase factor  $(-1)^m$ , whereas the geodesy convention doesn't.

This library is convention agnostic to an extent. It supports both Condon–Shortley phase conventions, and allows a choice between unit and  $4\pi$  normalization, but does not at present support all possible normalization conventions.

For completeness, we also write down the real spherical harmonics in the geodesy convention

$$Y_{lm}(\theta,\varphi) = \begin{cases} \sqrt{2(2l+1)\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) \sin(|m|\varphi) & \text{if } m < 0, \\ \sqrt{2l+1} P_l^m(\cos\theta) & \text{if } m = 0, \\ \sqrt{2(2l+1)\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) \cos(m\varphi) & \text{if } m > 0, \end{cases}$$

It is commonplace to absorb the normalization to the associated Legendre polynomials. Therefore we define

$$\bar{P}_{l}^{m}(x) = \sqrt{(2l+1)\frac{(l-m)!}{(l+m)!}}P_{l}^{m}(x),$$

for, e.g., the  $4\pi$  normalization convention.

# 0.2.2 Spherical harmonic transforms

Spherical harmonic transform here refers to the process of finding the expansion coefficients  $f_{lm}$  given a function  $f(\theta, \varphi)$ . This is in principle straightforward, since it is easy to check that the coefficients can be written as

$$f_{lm} = \frac{1}{N_{lm}} \int_{S^2} f(\theta, \varphi) Y_{lm}(\theta, \varphi) d\Omega.$$

If we express the spherical harmonics in terms of the associated Legendre polynomials and trigonometric functions, this can be written as

$$f_{lm} = \frac{1}{N_{lm}} \int_{-1}^{1} \bar{P}_{l}^{m}(\cos \theta) \int_{0}^{2\pi} \left\{ \frac{\cos(m\varphi)}{\sin(|m|\varphi)} \right\} f(\theta, \varphi) \varphi d \cos \theta.$$

The trigonometric functions inside the curly braces denote the two different options. It is worth noting that the inner integral over  $\varphi$  is a Fourier transform.

In practice, given an arbitrary function, the integrals won't generally have a closed form solution, which means that in practice the integrals have to be evaluated numerically. Naively, one could do this by providing a function that evaluates  $Y_{lm}(\theta, \varphi)$ , and use any numerical integration routine, but this is profoundly inefficient in all aspects.

Exact numerical evaluation of all expansion coefficients is impossible, because that would require evaluating  $f(\theta,\varphi)$  at an infinite number of points. To that end, we can seek an approximation given a finite set of points. Here we can rely on so-called numerical quadrature rules. The basic idea is that given a domain X, we can find a collection of points  $x_i \in X$ , with  $i = 1, 2, \ldots, N$ , and a corresponding set of weights  $w_i \in \mathbb{R}$ , such that for any polynomial such that we can approximate the integral of a function  $f: X \to \mathbb{R}$  with a sum

$$\int_X f(x) \, dx \approx \sum_{i=1}^N w_i f(x_i).$$

In particular, it is possible to find a quadrature rule that integrates polynomials up to some order exactly. That is, there exists an integer  $M \ge N$  such that for any polynomial  $P_M(x)$  of order M, we have an exact equality

$$\int_X P_M(x) dx \approx \sum_{i=1}^N w_i P_X(x_i).$$

A particular example of such a quadrature rule is Gauss–Legendre quadrature for functions defined on the interval [-1, 1], for which M = 2N - 1. The Gauss–Legendre quadrature rule is the basis of the fast spherical harmonic transform.

To return back to the spherical harmonic expansion coefficients, let  $\theta_i$ , with  $i=0,\ldots,L$ , be such that  $z_i=\cos\theta_i\in[-1,1]$  are the Gauss–Legendre quadrature nodes, and let  $\varphi_j=2\pi j/(2L+1)$ , with  $j=0,\ldots,2L$ . We can now write

$$f_{lm} \approx \sum_{i=0}^{\infty} Lw_i \bar{P}_l^m(z_i) \sum_{j=0}^{2L} \begin{Bmatrix} \cos(m\varphi_j) \\ \sin(|m|\varphi_j) \end{Bmatrix} f(\theta_i, \varphi_j).$$

Now, if  $f_L(\theta, \varphi)$  is a function which can be expressed as a finite linear combination of spherical harmonics such that

$$f_L(\theta, \varphi) = \sum_{l=0}^{\infty} L \sum_{|m| \le l} f_{lm} Y_{lm}(\theta, \varphi),$$

then the above relation will be exact. Therefore,  $f_L$  can be regarded as the best interpolating truncation approximation, up to degree L, for the function f on the grid defined by  $\theta_i$  and  $\varphi_i$ .

If we consider the number of operations it takes to evaluate all the coefficients up to degree L, we may note that there are  $(L+1)^2$  coefficients, and (L+1)(2L+1) grid points. Therefore it appears that it would take  $\mathcal{O}(L^4)$  operations to evaluate all coefficients. However, at closer inspection, we may observe that it is possible to first evaluate the intermediate coefficients

$$f_m(\theta_i) = \sum_{j=0}^{2L} \left\{ \frac{\cos(m\varphi_j)}{\sin(|m|\varphi_j)} \right\} f(\theta_i, \varphi_j).$$

This is nothing more than a discrete Fourier transform, and the intermediate coefficients can therefore be evaluated in  $\mathcal{O}(L^2 \log L)$  operations using a fast Fourier transform. After that, the sums

$$f_{lm} pprox \sum_{i=0}^{L} \bar{P}_{l}^{m}(z_{i}) f_{m}(\theta_{i})$$

can be evaluated in  $\mathcal{O}(L^3)$  operations, leaving us with an operation count that only grows as  $\mathcal{O}(L^3)$  to evaluate the spherical harmonic transform.

The inverse transform, from the coefficients back to the grid, can be performed using the same set of operations in reverse. That is, we can first compute the intermediate coefficients  $f_m(\theta_i)$  by summing  $f_{lm}$  over the associated Legendre polynomials, and then perform a fast Fourier transform to get the gridded values  $f(\theta_i, \varphi_i)$ .

#### 0.2.3 Zernike functions

The (3D) Zernike functions are a collection of functions that form an orthogonal basis on the unit ball B, defined as the points  $x \in \mathbb{R}^3$  such that  $||x|| \le 1$ . It is worth noting that, conventionally, "Zernike functions" or "Zernike polynomials", refers to an analogous collection of 2D functions that form a basis on the unit disk. Here we will refer to the 3D functions as simply "Zernike functions".

The Zernike functions can be written as

$$Z_{nlm}^{(\alpha)}(\rho,\theta,\varphi) = R_{nl}^{(\alpha)}(\rho)Y_{lm}(\theta,\varphi),$$

where the radial functions can be defined using Jacobi polyonomials  $P_n^{\alpha,\beta}(x)$  as

$$R_{nl}^{(\alpha)}(\rho) = (1 - \rho^2)^{\alpha} \rho^l P_{(n-l)/2}^{(\alpha,l+1/2)}(2\rho^2 - 1).$$

The parameter  $\alpha$  defines multiple families of Zernike polynomials. For practical purposes, the family defined by  $\alpha = 0$  is the simplest to deal with, and is what is used by this library. For this reason, we will denote the Zernike functions in this family simply by  $Z_{nlm}$ .

An important point about Zernike functions is that because the indices (n - l)/2 of the Jacobi polynomials must be nonnegative integers, n and l are restricted to having the same parity. That is, if n is even, then l must be even, and if n is odd, then l must be odd.

Since the Zernike functions form an orthogonal basis, any function on the unit ball can be written as

$$f(\rho,\theta,\varphi) = \sum_{\frac{1}{2}(n-l)\in\mathbb{N}} \sum_{|m|\leq l} f_{nlm} Z_{nlm}(\rho,\theta,\varphi),$$

and we have an orthogonality relation

$$\int_{B} Z_{nlm}(\rho, \theta, \varphi) Z_{n'l'm'}(\rho, \theta, \varphi) dV = N_{nlm} \delta_{nn'} \delta_{ll'} \delta_{mm'}.$$

The ambiquity about the phase and normalization of spherical harmonics naturally applies to Zernike functions, but there is an additional ambiquity over the normalization of the radial Zernike functions themselves. Per the definition of  $R_{nl}^{(\alpha)}(\rho)$  given above, we have an orthogonality relation

$$\int_{0}^{1} R_{nl}^{(\alpha)}(\rho) R_{n'l}^{(\alpha)}(\rho) \frac{\rho^{2} d\rho}{(1 - \rho^{2})^{\alpha}} = N_{nl}^{(\alpha)} \delta_{nn'}.$$

with

$$N_{nl}^{(\alpha)} = \frac{1}{2(n+\alpha+3/2)} \frac{((n-l)/2+1)_{\alpha}}{((n-l)/2+l+3/2)_{\alpha}}.$$

The notation  $(x)_{\alpha}$  is the Pochammer symbol, but we don't need to worry about it much, because under  $\alpha = 0$  the expression reduces to

$$N_{nl}^{(0)} = \frac{1}{2n+3}.$$

Like in the case of spherical harmonics, this normalization can be absorbed into the definition of  $R_{nl}^{(\alpha)}(\rho)$  to get unit-normalized Zernike functions. Both conventions are supported by zest.

#### 0.2.4 Zernike transforms

Just as we have the spherical harmonic transform to obtain the spherical harmonic expansion coefficients of a function defined on the sphere, we have a Zernike transform to obtain the Zernike expansion coefficients of a function on the ball. Similarly to the case of spherical harmonics, it is straightforward to see that the Zernike expansion coefficients of  $f(\rho, \theta, \varphi)$  are given by

$$f_{nlm} = \int_{B} f(\rho, \theta, \varphi) Z_{nlm}(\rho, \theta, \varphi) \rho^{2} d\rho d\Omega.$$

The numerical Zernike transform algorithm is effectively the same as the spherical harmonic transform presented earlier with an extra dimension on the grid. That is, in addition to the points  $\theta_i$ , and  $\varphi_j$ , we can define the points  $\rho_k$ , with  $k=0,\ldots,L+1$ , such that  $\rho_k=(x_k+1)/2$ , where  $x_k$  are Gauss–Legendre nodes. Note that the radial direction requires one node more than the  $\theta$  direction, because the radial integral comes with an extra factor of  $\rho$ . We can now write

$$f_{nlm} \approx \sum_{k=0}^{L+1} \sum_{i=0} Lw_k w_i \rho_k^2 R_{nl}(\rho_k) \bar{P}_l^m(z_i) \sum_{j=0}^{2L} \begin{Bmatrix} \cos(m\varphi_j) \\ \sin(|m|\varphi_j) \end{Bmatrix} f(\rho_k, \theta_i, \varphi_j).$$

As is the case with the spherical harmonic transform, this transform can be performed stepwise, first computing intermediate coefficients  $f_m(\rho_k, \theta_i)$ , by doing the innermost sum, then the intermediate coefficients  $f_{lm}(\rho_k)$  from the middle sum, and then finally  $f_{nlm}$  are obtained by doing the last sum. This means that the entire transformation can be performed with  $\mathcal{O}(L^4)$  operations.

#### 0.2.5 Rotations

It is common that we have a function expressed in terms of a spherical harmonic expansion

$$f(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{|m| \le l} f_{lm} Y_{lm}(\theta, \varphi).$$

and we express it in terms of coordinates  $(\theta', \varphi')$ , which are related to the coordinates  $(\theta, \varphi)$  by a rotation R. The challenge is then to find coefficients  $f'_{lm}$ , which express f in the rotated coordinate system,

$$f(\theta', \varphi') = \sum_{l=0}^{\infty} \sum_{|m| < l} f'_{lm} Y_{lm}(\theta', \varphi').$$

The spherical harmonics in the different coordinate systems are related by a linear transformation,

$$Y_l^m(\theta',\varphi') = \sum_{|m'| \leq l} D_{mm'}^{(l)}(R)^* Y_l^{m'}(\theta,\varphi).$$

Here  $D_{mm'}^{(l)}(R)$  are the elements of the Wigner D-matrix. Note that this relation is specifically for the complex spherical harmonics. There is a corresponding matrix for real spherical harmonics.

The above relation can be used to find the coefficients  $f_{l}^{m}$  of the complex sphericl harmonic expansion,

$$f'_{l}^{m} = \sum_{|m| \le l} D_{mm'}^{(l)}(R)^{*} f_{l}^{m}.$$

In principle, for a given rotation defined, e.g., by Euler angles, it is possible to compute the elements of the D-matrix and perform the matrix multiplication to get the rotation. However, an alternative approach used by zest avoids computing the D-matrix. This approach relies on two facts. First, that given Euler angles  $\alpha$ ,  $\beta$ , and gamma, the D-matrix can be expressed as

$$D_{mm'}^{(l)}(\alpha,\beta,\gamma) = e^{-im\alpha} d_{mm'}^{(l)}(\beta) e^{-im'\gamma},$$

where  $d_{mm'}^{(l)}(\beta)$  are coefficients of the Wigner (small) d-matrix. The Euler angles here specifically are in the ZYZ convention, where  $\alpha$  and  $\gamma$  correspond to rotations about the Z-axis, and  $\beta$  corresponds to a rotation about the Y-axis. The second fact is that a rotation about the Y-axis by angle  $\beta$  can be written as a rotation about the X-axis by 90 degrees, followed by a rotation about the Z-axis by the angle  $\beta$ , followed by another rotation about the X-axis by 90 degrees in the opposite direction to the first one. This is the ZXZXZ method, which has the property that all the rotations by variable angles are about the Z-axis, for which the D-matrix is diagonal. The X-rotations in turn can be expressed in terms of the d-matrix elements  $d_{mm'}^{(l)}(\pi/2)$ , which need to be computed once, and can be reused for all rotations.

When it comes to Zernike expansions, there is nothing special about the rotations compared to the spherical harmonic case, because the rotation only operates on the angular part. Therefore once we have determined how we apply the rotations to spherical harmonic coefficients, we get the corresponding rotations on Zernike coefficients for free.

# 0.3 Anatomy of zest

This section of the documentation outlines the core features of zest, and their usage, motivating some of the architectural decisions and giving guidance on best practices. Knowledge of the contents of the section on theoretical background is assumed in this section.

# 0.3.1 Layouts - complex multidimensional indexing

In dealing with spherical harmonic and Zernike expansions, one runs into nontrivial indexing schemes. Spherical harmonics are indexed by the pair of integers (l, m), for which the condition  $|m| \le l$  applies. With some cutoff  $l \le L$ , these index are organized in a triangle in the plane. The Zernike functions, on the other hand, are indexed by the triple (n, l, m), with not only the condition  $|m| \le l \le n$ , but also that (n - l)/2 must be an integer, which forces n and l to have the same parity. These indices are organized in a tetrahedron with holes in it where n and l do not satisfy the parity condition.

Mapping these multidimensional index schemes onto a one-dimensional buffer is a challenging endeavor. The simplest solution would be to use a conventional multidimensional array to store the elements corresponding to the indices, but this means that there will be elements in the buffer that are never accessed. For example, the index triple (1, 2, 3) doesn't correspond to any Zernike function, and therefore there is never need to access the corresponding element. For spherical harmonics, half of the elements in the buffer would never be accessed, and for Zernike functions up 83% of the elements would never be accessed. This is both wasteful in terms of memory usage, and bad for cache utilization.

Fortunately, it is relatively straightforward to create more compact schemes. for storing elements. For example, spherical harmonic coefficients can be stored sequentially by mapping the index pair (l, m) to the one-dimensional index i = l(l+1) + m without any wasted memory. An alternative is to map pairs  $\{|m|, -|m|\}$  onto the indices l(l+1)/2 + |m|. This wastes a small amount of memory because m = 0 maps to both elements of the pair, but has some desirable properties for iteration over the buffer.

To deal with differing indexing schemes in a unified and flexible manner, zest uses a system of *layouts*. A 2D layout, for example, is a type with the structure

```
struct SomeLayout
{
    using index_type;
    using size_type;
    using IndexRange;
    using SubLayout; // optional

    static constexpr LayoutTag layout_tag;

    static size_type size(size_type order);
    static size_type idx(index_type l, index_type m);
};
```

The function size gives the total number of elements in an index set as determined by the parameter order. The exact definition of order depends on the layout. For example, for spherical harmonic coefficients cut off at some degree L such that  $|m| \le l \le L$ , order is by convention equal to L+1. The case for Zernike functions is analogous. For the layout of a basic 1D array, order would just be the size. The convention is such that order =  $\emptyset$  always corresponds to an empty layout.

The function idx gives the index in the one-dimensional buffer corresponding to the pair (l, m), in this case. For example, it could return l(l+1) + m for a spherical harmonic layout.

The constant layout\_tag is used by zest to identify what type of index geometry the layout is intended to represent.

The member type SubLayout is a layout of one dimension lower to facilitate accessing lower-dimensional slices of the index set. For example, for a layout for spherical harmonic coefficients, it would be a 1D layout for to the row of m values that correspond to a single l.

Finally, the member type IndexRange leads to another concept in zest, the concept of *index ranges*. Because of potential nontrivial restrictions on indices—e.g., that n and l must have the same parity when dealing with Zernike functions—iterating through index sets by hand is error prone. Consider, for example, iterating l for Zernike functions

```
for (std::size_t 1 = n % 2; 1 < n; 1 += 2)
    // Do things</pre>
```

For someone used to writing C-style for-loops, it is easy to go through the motions and write 1 = 0 instead of 1 = n % 2, or ++1 instead of 1 += 2, either of which will lead to hard to diagnose bugs. Furthermore, this way it is difficult to write generic code, which can iterate both spherical harmonic and Zernike indices. Index ranges allow the use of range-based for-loops instead

```
SomeLayout::IndexRange indices;
for (auto 1 : indices)
   // Do things
```

#### 0.3.2 Containers and views

For handling expansion coefficients and quadrature grids, zest presents a number of containers and views. Containers are objects which own the underlying buffer they refer to, i.e., they are responsible for allocation and deallocation of the buffer. Views are objects which do not own the buffer they refer to; they simply give a *view* to a buffer owned by some other object.

The library comes with a number of containers for easy storage and manipulation of different types of data. For storing spherical harmonic and Zernike expansions of real functions, there are the classes zest::st::Re-alSHExpansion and zest::zt::RealZernikeExpansion respectively.

The template parameters of these containers primarily control the various normalization conventions. The parameter ElementType is the type of elements in the underlying buffer. There are two main choices here: if ElementType is a floating point type (e.g., double), this implies that the elements are stored sequentially with m going from -l to l. On the other hand, if ElementType is an array-like type of length two, e.g., std::array<double, 2>, then the elements are stored in pairs  $\{|m|, -|m|\}$  with |m| running from zero to l. The latter option is the default and recommended option when dealing with the quadrature-based transforms, but the former is mandatory for fitting an expansion to data.

For these classes, the library provides a number of convenient aliases for various common combinations of normalization and phase conventions. For spherical harmonics these aliases are

```
zest::st::RealSHExpansionAcousticszest::st::RealSHExpansionQMzest::st::RealSHExpansionGeo
```

For Zernike functions there are corresponding aliases for the unnormalized radial functions:

```
zest::zt::RealZernikeExpansionAcousticszest::zt::RealZernikeExpansionQMzest::zt::RealZernikeExpansionGeo
```

and furthermore for the normalized radial Zernike polynomials:

```
zest::zt::RealZernikeExpansionNormalAcousticszest::zt::RealZernikeExpansionNormalQMzest::zt::RealZernikeExpansionNormalGeo
```

For storage of function values on Gauss-Legendre quadrature grids there are the classes <code>zest::st::SphereGLQGrid</code> and <code>zest::zt::BallGLQGrid</code> for the sphere and ball, respectively. The ElementType parameter here is simply a floating point type. The parameter LayoutType, in turn, describes how the multidimensional grid is laid out in memory. This is not something a user of the library

generally needs to worry about, because the default layout is the layout that should be used for performing the transforms to expansion coefficients.

Mirroring the convention of the C++ standard library, views to buffers in zest are referred with the word "span". Each of the above containers has a corresponding view. Thus we have zest::st::RealSHSpan and zest::zt::RealZernikeSpan with the corresponding aliases for different normalization/phase conventions, and zest::st::SphereGLQGridSpan and zest::zt::BallGLQGridSpan for the quadrature grids.

In additon, for completeness it is worth mentioning the zest::MDSpan, which is a general multidimensional array view, and is the base of both zest::st::SphereGLQGridSpan and zest::zt::BallGLQGridSpan. It is a poor man's alternative to C++23's std::mdspan, replicating the part of its interface, which is necessary for this library.

Views are very useful, because they allow for more flexible storage of the expansions and grids. For example, zest does not offer a container for storage of multiple spherical harmonic expansions, and that is by design. If one needed to work with multiple spherical harmonic expansions at the same time—a scenario which is very easy to imagine—they might be tempted to use something like std::vector to store the expansions. But this involves multiple memory allocations, one for each expansion, and spreads the expansions across memory, which is not cache friendly and could negatively impact performance if the expansions are small.

Instead, what one should do is allocate one buffer of the expansion's underlying type, which stores all the expansions back to back in the same buffer, and then take views into that buffer to access the different expansions. For example

```
using ExpansionSpan = zest::st::RealSHExpansionQM;

constexpr std::size_t num_expansions = 100;
constexpr std::size_t order = 10;
constexpr std::size_t expansion_size = ExpansionSpan::size(order);

std::vector<std::array<double, 2>>
expansion_buffer(num_expansions*expansion_size);

for (std::size_t i = 0; i < num_expansions; ++i)
{
    ExpansionSpan expansion(expansion_buffer.data() + i*expansion_size, order);

    // ...
}</pre>
```

As is conventional in C++ libraries prior to C++23's multidimensional subscript operator, multidimensional views and containers can be indexed with the call operator operator ()

```
constexpr std::size_t order = 3;
zest::st::RealSHExpansion expansion(order);
expansion(0, 0) = {1.0, 0.0};
expansion(1, 0) = {0.5, 0.0};
expansion(1, 1) = {0.5, -0.5};
expansion(2, 0) = {0.25, 0.0};
expansion(2, 1) = {0.25, -0.25};
expansion(2, 2) = {0.25, -0.25};
```

All multidimensional containers and views in this library allow for lower dimensional subviews to be taken, which reproduce corresponding slices of the data. Specifically, the subscript operator operator[] provides access to the lower dimensional subview

(continued from previous page)

```
{
    expansion_1[m][0] += 0.1;
    expansion_1[m][1] -= 0.1;
}
```

This example also demonstrates the use of the index ranges discussed in the previous subsection. In fact, the above is the preferred way of iterating over an expansion, because it avoids the errors that could be made in writing the constraints for the indices by hand.

# 0.3.3 Gauss-Legendre quadrature transformers

At the heart of zest are the Gauss-Legendre quadrature grid based transforms of spherical harmonic and Zernike expansions. These transforms are implemented by the classes zest::st::GLQTransformer and zest::zt::GLQTransformer for spherical harmonic and Zernike transforms respectively. The normalization and phase convention parameters are the same as those to the respective expansion containers discussed above. To that end, both transformer classes have a set of aliases for some commond combinations of normalization and phase conventions. These are

```
zest::st::GLQTransformerAcousticszest::st::GLQTransformerQMzest::st::GLQTransformerGeo
```

for the spherical harmonic transformer as well as

```
zest::zt::GLQTransformerAcoustics
zest::zt::GLQTransformerQM
zest::zt::GLQTransformerGeo
zest::zt::GLQTransformerNormalAcoustics
zest::zt::GLQTransformerNormalQM
zest::zt::GLQTransformerNormalGeo
```

for the Zernike transformer. The final parameter GridLayoutType in turn is the same as for the corresponding grid containers.

It goes without saying that the transformer must have the same values for these template parameters as the expansion and grid. This is one of the ways zest protects consistency of conventions in transformations.

The transformers come with two methods for performing transformations: forward\_transform and back-ward\_transform. The forward transform transforms a grid to an expansion, and the backward transform is the inverse, transforming an expansion to a grid. Both of these methods have two primary overloads, one which takes both the input and output expansion/grid as arguments and modifies the output

```
transformer.forward_transform(grid, expansion);
transformer.backward_transform(expansion, grid);
```

and one which takes the input expansion/grid and returns the output container

```
auto expansion = transformer.forward_transform(grid, order);
auto new_grid = transformer.backward_transform(expansion, order);
```

Here the method takes the additional parameter order. In the case of the forward transform, this parameter is the order of the expansion. Note that the grid has its own order parameter, which is the maximum expansion order that can be taken with that grid. Therefore, the order of the output expansion is min(order, grid.order()). On the other hand, in the backward transform, the order parameter determines the point at which the summation of the expansion is truncated. The order of new\_grid will again be min(order, expansion.order()).

#### 0.3.4 Rotations

For understanding this subsection discussing the implementation of rotations in zest, reading the corresponding subsection in the theoretical background is highly recommended. In summary, zest implements rotations for both spherical harmonic and Zernike expansions using the ZXZXZ algorithm. This algorithm implements a rotation by Euler angles  $(\alpha, \beta, \gamma)$  as a series of rotations starting with a rotation about the z-axis by  $\gamma$ , followed by a 90 degree rotation about the new x-axis, followed by a rotation about the new z-axis by  $\beta$ , followed by a -90 degree rotation about the new x-axis, finally followed by a rotation about the new z-axis by  $\alpha$ ; hence ZXZXZ. This has the advantage that the general form of Wigner's D-matrices never needs to be evaluated. The x-axis rotations are expressible in terms of the d-matrix for a 90 degree rotation, and can be precomputed once, On the other hand, the z-rotations are just diagonal matrices of values  $e^{im\theta_i}$ , where  $\theta_i$  is one of  $(\alpha, \beta, \gamma)$ .

With this brief review of the essential facts, zest has a single class zest::Rotor for performing the rotations, which has the method rotate for performing general rotations and polar\_rotate for the special case of rotations about the z-axis

All rotations take as their last argument an enum of type zest::RotationType, which has two values zest::RotationType::object and zest::RotationType::coordinate. These express whether the rotation represents a rotation of an object in space (active rotation) or a rotation of the coordinate system (passive rotation). The polar rotation naturally takes as its argument a single angle, whereas the general rotation takes three Euler angles, given as a standard library array with three elements. Finally, the general rotation takes as its second argument an object of type zest::WignerdPiHalfCollection. This object contains the values of the d-matrix for a 90 degree angle, i.e.,  $\pi/2$ , up to some specified order.

# 0.4 Library reference

# 0.4.1 Spherical harmonic expansions

#### **Concepts**

```
template<typename T>
concept real_sh_expansion
```

#include < real sh expansion.hpp > Concept describing a conventional spherical harmonic expansion.

```
template<typename T>
concept row_skipping_real_sh_expansion
```

#include <real\_sh\_expansion.hpp> Concept describing a spherical harmonic expansion where every other row is skipped.

#### **Types**

```
template<SHNorm sh_norm_param, SHPhase sh_phase_param, typename ElementType =
std::array<double, 2>>
class RealSHExpansion
```

A container for purely real spherical harmonic data.

**Template Parameters** 

• **sh\_norm\_param** – normalization convention of the spherical harmonics

- **sh\_phase\_param** phase convention of the spherical harmonics
- **ElementType** type of elements

#### **Public Functions**

```
inline size_type order() const noexcept
```

Order of the expansion.

inline std::span<element\_type> flatten() noexcept

Flattened view of the underlying buffer.

inline std::span<const element\_type> flatten() const noexcept

Flattened view of the underlying buffer.

inline void resize(size\_type order)

Change the size of the expansion.

#### **Public Static Functions**

#### static inline constexpr size\_type size(size\_type order) noexcept

Number of data elements for size parameter order.

#### **Parameters**

**order** – parameter presenting the size of the expansion

template<typename ElementType, typename LayoutType, SHNorm sh\_norm\_param, SHPhase
sh\_phase\_param>

class SHLMSpan : public zest::TriangleSpan<ElementType, LayoutType>

A non-owning view for storing 2D data related to spherical harmonics.

#### **Template Parameters**

- **ElementType** type of elements
- **LayoutType** layout of the elements
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

template<typename ElementType, typename LayoutType, SHNorm sh\_norm\_param, SHPhase
sh\_phase\_param>

```
class SHLMVecSpan : public zest::TriangleVecSpan<ElementType, LayoutType>
```

A non-owning view for storing 3D data related to spherical harmonics.

#### **Template Parameters**

- **ElementType** type of elements
- **LayoutType** layout of the elements
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

#### **Type aliases**

#### using zest::st::RealSHExpansionAcoustics = RealSHExpansion<SHNorm::qm, SHPhase::none>

Convenient alias for RealSHExpansion with orthonormal spherical harmonics and no Condon-Shortley phase.

```
using zest::st::RealSHExpansionQM = RealSHExpansion<SHNorm::qm, SHPhase::cs>
```

Convenient alias for RealSHExpansion with orthonormal spherical harmonics with Condon-Shortley phase.

```
using zest::st::RealSHExpansionGeo = RealSHExpansion<SHNorm::geo, SHPhase::none>
```

Convenient alias for RealSHExpansion with 4-pi normal spherical harmonics and no Condon-Shortley phase.

template<sh\_packing PackingType, SHNorm sh\_norm\_param, SHPhase sh\_phase\_param>

using zest::st::PackedSHSpan = SHLMSpan<typename PackingType::element\_type, typename
PackingType::Layout, sh\_norm\_param, sh\_phase\_param>

A non-owning view of data modeling spherical harmonic data.

#### **Template Parameters**

- **PackingType** type of packing for the elements
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

template<typename ElementType, SHNorm sh\_norm\_param, SHPhase sh\_phase\_param>

using zest::st::RealSHSpan = PackedSHSpan<RealSHPacking<ElementType>, sh\_norm\_param,
sh\_phase\_param>

A non-owning view of data modeling purely real spherical harmonic data.

# **Template Parameters**

- **ElementType** type of elements
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

#### template<typename ElementType>

```
using zest::st::RealSHSpanAcoustics = RealSHSpan<ElementType, SHNorm::qm,
SHPhase::none>
```

Convenient alias for RealSHSpan with orthonormal spherical harmonics and no Condon-Shortley phase.

#### template<typename ElementType>

```
using zest::st::RealSHSpanQM = RealSHSpan<ElementType, SHNorm::qm, SHPhase::cs>
```

Convenient alias for RealSHSpan with orthonormal spherical harmonics with Condon-Shortley phase.

#### template<typename ElementType>

```
using zest::st::RealSHSpanGeo = RealSHSpan<ElementType, SHNorm::geo, SHPhase::none>
```

Convenient alias for RealSHSpan with 4-pi normal spherical harmonics and no Condon-Shortley phase.

# 0.4.2 Spherical harmonic transforms

#### **Concepts**

```
template<typename T>
concept sphere_glq_grid
```

#include <sh\_glq\_transformer.hpp> Concept enforcing a type to be either SphereGLQGrid or SphereGLQGridSpan.

template<typename AlignmentType = CacheLineAlignment>

```
struct LatLonLayout
     Longitudinally contiguous layout for storing a Gauss-Legendre quadrature grid.
          Template Parameters
             AlignmentType – byte alignment of the grid
     Public Static Functions
     static inline constexpr std::size_t size(std::size_t order) noexcept
          Number of grid points.
             Parameters
                 order - order of spherical harmonic expansion
     static inline constexpr std::array<std::size_t, 2> shape(std::size_t order)
                                                                   noexcept
          Shape of the grid.
             Parameters
                 order - order of spherical harmonic expansion
     static inline constexpr std::size_t fft_size(std::size_t order) noexcept
          Number of longitudinal Fourier coefficients.
     static inline constexpr std::array<std::size_t, 2> fft_stride(std::size_t order)
                                                                         noexcept
          Stride of the longitudinally Fourier transformed grid.
     static inline constexpr std::size_t lat_size(std::size_t order) noexcept
          Size in latitudinal direction.
     static inline constexpr std::size_t lon_size(std::size_t order) noexcept
          Size in latitudinal direction.
template<typename AlignmentType = CacheLineAlignment>
struct LonLatLayout
     Latitudinally contiguous layout for storing a Gauss-Legendre quadrature grid.
         Template Parameters
             AlignmentType – byte alignment of the grid
     Public Static Functions
     static inline constexpr std::size_t size(std::size_t order) noexcept
          Number of grid points.
             Parameters
                 order - order of spherical harmonic expansion
     static inline constexpr std::array<std::size_t, 2> shape(std::size_t order)
                                                                   noexcept
          Shape of the grid.
             Parameters
                 order - order of spherical harmonic expansion
     static inline constexpr std::size_t fft_size(std::size_t order) noexcept
          Number of longitudinal Fourier coefficients.
     static inline constexpr std::array<std::size_t, 2> fft_stride(std::size_t order)
          Stride of the longitudinally Fourier transformed grid.
```

```
static inline constexpr std::size_t lat_size(std::size_t order) noexcept
          Size in latitudinal direction.
     static inline constexpr std::size_t lon_size(std::size_t order) noexcept
          Size in longitudinal direction.
template<typename LayoutType = DefaultLayout>
class SphereGLQGridPoints
     Points defining a Gauss-Legendre quadrature grid on the sphere.
         Template Parameters
             LayoutType - memory layout of the grid
     Public Functions
     inline void resize(std::size_t order)
          Change the size of the corresponding grid.
     inline std::array<std::size_t, 2> shape() noexcept
          Shape of the corresponding grid.
     inline std::span<const double> longitudes() const noexcept
          Longitude values of the grid points.
     inline std::span<const double> glq_nodes() const noexcept
          Latitudinal Gauss-Legendre nodes.
     template<sphere_glq_grid GridType, typename FuncType>
     inline void generate_values(GridType &&grid, FuncType &&f)
          Generate Gauss-Legendre quadrature grid values from a function.
             Template Parameters
                 • GridType – type of grid
                 • FuncType – type of function
             Parameters
                 • grid - grid to place the values in
                 • f – function to generate values
     template<typename FuncType>
     inline auto generate_values(FuncType &&f, std::size_t order)
          Generate Gauss-Legendre quadrature grid values from a function.
             Template Parameters
                 FuncType – type of function
             Parameters
                 f – function to generate values
template<typename ElementType, typename LayoutType = DefaultLayout>
```

# class SphereGLQGrid

Container for Gauss-Legendre quadrature gridded data on the sphere.

#### **Template Parameters**

- **ElementType** type of elements in the grid
- LayoutType grid layout

```
Public Functions
     inline std::size_t order() const noexcept
          Order of spherical harmonic expansion.
     inline std::array<std::size_t, 2> shape() const noexcept
         Shape of the grid.
     inline std::span<const element_type> flatten() const noexcept
          Flattened view of the underlying buffer.
     inline std::span<element_type> flatten() noexcept
          Flattened view of the underlying buffer.
     inline void resize(std::size_t order)
         Change the size of the grid.
template<typename ElementType, typename LayoutType = DefaultLayout>
class SphereGLQGridSpan : public zest::MDSpan<ElementType, 2>
     A non-owning view on data modeling a Gauss-Legendre quadrature grid on the sphere.
         Template Parameters
               • ElementType – type of elements in the grid
               • LayoutType – grid layout
     Public Functions
     inline constexpr std::size_t order() const noexcept
          Order of spherical harmonic expansion.
     inline constexpr const std::array<std::size_t, 2> &shape() const noexcept
         Shape of the grid.
     inline constexpr std::span<element_type> flatten() const noexcept
          Flattened view of the underlying buffer.
     Public Static Functions
     static inline constexpr std::size t size(std::size t order) noexcept
         Number of grid points.
             Parameters
                 order - order of spherical harmonic expansion
     static inline constexpr std::array<std::size_t, 2> shape(std::size_t order)
                                                                   noexcept
         Shape of the grid.
             Parameters
                 order – order of spherical harmonic expansion
template<SHNorm sh_norm_param, SHPhase sh_phase_param, typename GridLayoutType =</pre>
```

#### class GLQTransformer

DefaultLayout>

Transformations between a Gauss-Legendre quadrature grid representation and spherical harmonic expansion representation of real data.

#### **Template Parameters**

- **sh\_norm\_param** normalization convention of spherical harmonics
- **sh\_phase\_param** phase convention of spherical harmonics

• **GridLayoutType** – memory layout of the grid

#### **Public Functions**

```
inline std::size_t order() const noexcept
Order of spherical harmonic expansion.
```

inline void resize(std::size\_t order)

Resize transformer for specified expansion order.

Forward transform from Gauss-Legendre quadrature grid to spherical harmonic coefficients.

#### **Parameters**

- values values on the spherical quadrature grid
- **expansion** coefficients of the expansion

Backward transform from spherical harmonic expansion to Gauss-Legendre quadrature grid.

#### **Parameters**

- **expansion** coefficients of the expansion
- values values on the spherical quadrature grid

Backward transform from spherical harmonic expansion of even or odd parity to Gauss-Legendre quadrature grid.



A spherical harmonic expansion has even/odd parity if the first index of all nonzero coefficients has even/odd parity.

```
Template Parameters

Expansion – type of expansion
```

#### **Parameters**

- **expansion** coefficients of the expansion
- values values on the spherical quadrature grid

Forward transform from Gauss-Legendre quadrature grid to spherical harmonic coefficients.

#### **Parameters**

- values values on the spherical quadrature grid
- order order of expansion

Backward transform from spherical harmonic coefficients to Gauss-Legendre quadrature grid.

#### **Parameters**

- values values on the spherical quadrature grid
- **expansion** coefficients of the expansion

Backward transform from spherical harmonic expansion of even or odd parity to Gauss-Legendre quadrature grid.



A spherical harmonic expansion has even/odd parity if the first index of all nonzero coefficients has even/odd parity.

# **Template Parameters Expansion** – type of expansion

#### **Parameters**

- **expansion** coefficients of the expansion
- values values on the spherical quadrature grid

```
template<st::SHNorm sh_norm_param, st::SHPhase sh_phase_param, typename
GridLayoutType = DefaultLayout>
class SHTransformer
```

High-level interface for taking SH transforms of functions on balls of arbitrary radii.

# **Template Parameters**

- **sh\_norm\_param** normalization convention of spherical harmonics
- **sh\_phase\_param** phase convention of spherical harmonics
- GridLayoutType -

#### **Public Functions**

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Get spherical harmonic expansion of a function expressed in spherical coordinates.

#### **Template Parameters**

FuncType – type of function

#### **Parameters**

- **f** function to transform
- expansion buffer to store the expansion

# template<spherical\_function FuncType>

Get spherical harmonic expansion of a function expressed in spherical coordinates.

#### **Template Parameters**

**FuncType** – type of function

#### **Parameters**

- **f** function to transform
- order order of the expansion

#### Returns

spherical harmonic expansion

```
template<cartesian_function FuncType>
```

Get spherical harmonic expansion of a function expressed in Cartesian coordinates.

#### **Template Parameters**

**FuncType** – type of function

#### **Parameters**

- **f** function to transform
- **expansion** buffer to store the expansion

#### template<cartesian\_function FuncType>

Get spherical harmonic expansion of a function expressed in Cartesian coordinates.

#### **Template Parameters**

**FuncType** – type of function

## **Parameters**

**f** – function to transform

#### Returns

spherical harmonic expansion

#### Type aliases

```
using zest::st::DefaultLayout = LonLatLayout<>
template<typename GridLayout = DefaultLayout>
using zest::st::GLQTransformerAcoustics = GLQTransformer<SHNorm::qm, SHPhase::none,
GridLayout>
```

Convenient alias for GLQTrans former with orthonormal spherical harmonics and no Condon-Shortley phase.

```
Template Parameters
GridLayout -
```

template<typename GridLayout = DefaultLayout>

using zest::st::GLQTransformerQM = GLQTransformer<SHNorm::qm, SHPhase::cs, GridLayout>

Convenient alias for GLQTransformer with orthonormal spherical harmonics with Condon-Shortley phase.

Template Parameters **GridLayout** –

template<typename GridLayout = DefaultLayout>

using zest::st::GLQTransformerGeo = GLQTransformer<SHNorm::geo, SHPhase::none,
GridLayout>

Convenient alias for GLQTransformer with 4-pi normal spherical harmonics and no Condon-Shortley phase.

Template Parameters GridLayout -

template<typename GridLayout = DefaultLayout>

using zest::st::SHTransformerAcoustics = SHTransformer<SHNorm::qm, SHPhase::none,
GridLayout>

Convenient alias for SHTransformer with orthonormal spherical harmonics and no Condon-Shortley phase.

Template Parameters
GridLayout -

template<typename GridLayout = DefaultLayout>

using zest::st::SHTransformerQM = SHTransformer<SHNorm::qm, SHPhase::cs, GridLayout>

Convenient alias for SHTransformer with orthonormal spherical harmonics with Condon-Shortley phase.

Template Parameters GridLayout –

template<typename GridLayout = DefaultLayout>

using zest::st::SHTransformerGeo = SHTransformer<SHNorm::geo, SHPhase::none,
GridLayout>

Convenient alias for SHTransformer with 4-pi normal spherical harmonics and no Condon-Shortley phase.

Template Parameters
GridLayout -

### 0.4.3 Zernike expansions

#### **Concepts**

template<typename T>
concept real\_zernike\_expansion

#include <zernike\_expansion.hpp> Concept enforcing a type to be either RealZernikeExpansion or RealZernikeSpan.

#### **Types**

template<ZernikeNorm zernike\_norm\_param, st::SHNorm sh\_norm\_param, st::SHPhase
sh\_phase\_param, typename ElementType = std::array<double, 2>>
class RealZernikeExpansion

A container for a Zernike expansion of a real function.

#### **Template Parameters**

- **sh\_norm\_param** normalization convention of spherical harmonics
- **sh\_phase\_param** phase convention of spherical harmonics

#### **Public Functions**

```
inline size_type order() const noexcept
```

Order of the expansion.

inline std::span<const element\_type> flatten() const noexcept

Flattened view of the underlying buffer.

inline std::span<element\_type> flatten() noexcept

Flattened view of the underlying buffer.

inline void resize(size\_type order)

Change the size of the expansion.

#### **Public Static Functions**

#### static inline constexpr size\_type size(size\_type order) noexcept

Number of data elements for size parameter order.

#### **Parameters**

**order** – parameter presenting the size of the expansion

template<typename ElementType, typename LayoutType, ZernikeNorm zernike\_norm\_param,
st::SHNorm sh\_norm\_param, st::SHPhase sh\_phase\_param>
class ZernikeSHSpan : public zest::TriangleSpan<ElementType, LayoutType>

A non-owning view of the Zernike expansion coefficients of a given radial index value.

#### **Template Parameters**

- **ElementType** type of elements in the view
- **zernike\_norm\_param** zernike function normalization convention
- **sh\_norm\_param** spherical harmonic normalization convention
- **sh\_phase\_param** spherical harmonic phase convention

template<typename ElementType, typename LayoutType, ZernikeNorm zernike\_norm\_param,
st::SHNorm sh\_norm\_param, st::SHPhase sh\_phase\_param>
class ZernikeNLMSpan : public zest::TetrahedronSpan<ElementType, LayoutType>

A non-owning view for storing 3D data related to Zernike functions.

#### **Template Parameters**

- **ElementType** type of elements
- LayoutType layout of the elements
- **zernike\_norm\_param** zernike function normalization convention
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

#### Type aliases

```
using zest::zt::RealZernikeExpansionAcoustics =
```

RealZernikeExpansion<ZernikeNorm::unnormed, st::SHNorm::qm, st::SHPhase::none>

Convenient alias for RealZernikeExpansion with unnormalized Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

#### using zest::zt::RealZernikeExpansionNormalAcoustics =

```
RealZernikeExpansion<ZernikeNorm::normed, st::SHNorm::qm, st::SHPhase::none>
```

Convenient alias for RealZernikeExpansion with orthnormal Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

```
using zest::zt::RealZernikeExpansionQM = RealZernikeExpansion<ZernikeNorm::unnormed,
st::SHNorm::qm, st::SHPhase::cs>
```

Convenient alias for RealZernikeExpansion with unnormalized Zernike functions, orthonormal spherical harmonics, and Condon-Shortley phase.

#### using zest::zt::RealZernikeExpansionNormalQM =

```
RealZernikeExpansion<ZernikeNorm::normed, st::SHNorm::qm, st::SHPhase::cs>
```

Convenient alias for RealZernikeExpansion with orthonormal Zernike functions, orthonormal spherical harmonics, and Condon-Shortley phase.

```
using zest::zt::RealZernikeExpansionGeo = RealZernikeExpansion<ZernikeNorm::unnormed,
st::SHNorm::geo, st::SHPhase::none>
```

Convenient alias for RealZernikeExpansion with unnormalized Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

#### using zest::zt::RealZernikeExpansionNormalGeo =

```
RealZernikeExpansion<ZernikeNorm::normed, st::SHNorm::geo, st::SHPhase::none>
```

Convenient alias for RealZernikeExpansion with orthonormal Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

```
template<zernike_packing PackingType, ZernikeNorm zernike_norm_param, st::SHNorm
sh_norm_param, st::SHPhase sh_phase_param>
using zest::zt::PackedZernikeSpan = ZernikeNLMSpan<typename
PackingType::element_type, typename PackingType::Layout, zernike_norm_param,
sh_norm_param, sh_phase_param>
```

A non-owning view of data modeling Zernike function data.

#### **Template Parameters**

- **PackingType** type of packing for the elements
- **zernike\_norm\_param** zernike function normalization convention
- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

```
template<typename ElementType, ZernikeNorm zernike_norm_param, st::SHNorm
sh_norm_param, st::SHPhase sh_phase_param>
using zest::zt::RealZernikeSpan = PackedZernikeSpan<RealZernikePacking<ElementType>,
zernike_norm_param, sh_norm_param, sh_phase_param>
```

A non-owning view of data modeling purely real Zernike function data.

#### **Template Parameters**

- **ElementType** type of elements
- **zernike\_norm\_param** zernike function normalization convention

- **sh\_norm\_param** normalization convention of the spherical harmonics
- **sh\_phase\_param** phase convention of the spherical harmonics

#### template<typename ElementType>

```
using zest::zt::RealZernikeSpanAcoustics = RealZernikeSpan<ElementType,
ZernikeNorm::unnormed, st::SHNorm::qm, st::SHPhase::none>
```

Convenient alias for RealZernikeSpan with unnormalized Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

#### **Template Parameters**

**ElementType** – type of elements in the view

#### template<typename ElementType>

```
using zest::zt::RealZernikeSpanNormalAcoustics = RealZernikeSpan<ElementType,
ZernikeNorm::unnormed, st::SHNorm::qm, st::SHPhase::none>
```

Convenient alias for RealZernikeSpan with orthonormal Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

#### **Template Parameters**

**ElementType** – type of elements in the view

#### template<typename ElementType>

```
using zest::zt::RealZernikeSpanQM = RealZernikeSpan<ElementType,
ZernikeNorm::unnormed, st::SHNorm::qm, st::SHPhase::cs>
```

 $Convenient\ alias\ for\ Real Zernike Span\ with\ unnormalized\ Zernike\ functions,\ orthonormal\ spherical\ harmonics,\ and\ Condon-Shortley\ phase.$ 

#### **Template Parameters**

**ElementType** – type of elements in the view

#### template<typename ElementType>

```
using zest::zt::RealZernikeSpanNormalQM = RealZernikeSpan<ElementType,
ZernikeNorm::normed, st::SHNorm::qm, st::SHPhase::cs>
```

Convenient alias for RealZernikeSpan with orthonormal Zernike functions, orthonormal spherical harmonics, and Condon-Shortley phase.

#### **Template Parameters**

**ElementType** – type of elements in the view

### template<typename ElementType>

```
using zest::zt::RealZernikeSpanGeo = RealZernikeSpan<ElementType,
ZernikeNorm::unnormed, st::SHNorm::geo, st::SHPhase::none>
```

Convenient alias for RealZernikeSpan with unnormalized Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

#### **Template Parameters**

**ElementType** – type of elements in the view

#### template<typename ElementType>

```
using zest::zt::RealZernikeSpanNormalGeo = RealZernikeSpan<ElementType,
ZernikeNorm::normed, st::SHNorm::geo, st::SHPhase::none>
```

Convenient alias for RealZernikeSpan with orthonormal Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

#### **Template Parameters**

**ElementType** – type of elements in the view

#### 0.4.4 Zernike transforms

```
Types
template<typename AlignmentType = CacheLineAlignment>
struct LonLatRadLayout
     Layout for storing a Gauss-Legendre quadrature grid.
         Template Parameters
             AlignmentType – byte alignment of the grid
     Public Static Functions
     static inline constexpr std::size_t size(std::size_t order) noexcept
         Number of grid points.
             Parameters
                 order - order of Zernike expansion
     static inline constexpr std::array<std::size_t, 3> shape(std::size_t order)
                                                                   noexcept
         Shape of the grid.
             Parameters
                 order - order of Zernike expansion
     static inline constexpr std::size_t fft_size(std::size_t order) noexcept
         Number of longitudinal Fourier coefficients.
     static inline constexpr std::array<std::size_t, 3> fft_stride(std::size_t order)
                                                                         noexcept
         Stride of the longitudinally Fourier transformed grid.
     static inline constexpr std::size_t lat_size(std::size_t order) noexcept
         Size in latitudinal direction.
     static inline constexpr std::size_t rad_size(std::size_t order) noexcept
         Size in radial direction.
     static inline constexpr std::size_t lon_size(std::size_t order) noexcept
         Size in latitudinal direction.
template<typename LayoutType = DefaultLayout>
class BallGLQGridPoints
     Points defining a grid in spherical coordinates in the unit ball.
         Template Parameters
             LayoutType - memory layout of the grid
     Public Functions
     inline void resize(std::size_t order)
         Change the size of the corresponding grid.
     inline std::span<const double> longitudes() const noexcept
          Longitude values of the grid points.
```

24 **CONTENTS:** 

inline std::span<const double> rad\_glq\_nodes() const noexcept

Radial Gauss-Legendre nodes.

# 

#### **Parameters**

- grid grid to place the values in
- **f** function to generate values

```
template<typename FuncType>
inline auto generate_values(FuncType &&f, std::size_t order)
```

Generate Gauss-Legendre quadrature grid values from a function.

```
Template Parameters
FuncType – type of function
```

#### **Parameters**

**f** – function to generate values

template<typename ElementType, typename LayoutType = DefaultLayout>

#### class BallGLQGrid

Container for gridded data in spherical coordinates in the unit ball.

#### **Template Parameters**

- **ElementType** type of elements in the grid
- LayoutType grid layout

#### **Public Functions**

```
inline std::size_t order() const noexcept
    Order of Zernike expansion.

inline std::array<std::size_t, 3> shape()
    Shape of the grid.

inline std::span<const element_type> flatten() const noexcept
    Flattened view of the underlying buffer.

inline std::span<element_type> flatten() noexcept
    Flattened view of the underlying buffer.

inline void resize(std::size_t order)
    Change the size of the grid.
```

#### **Public Static Functions**

```
static inline constexpr std::array<std::size_t, 3> shape(std::size_t order)
                                                                   noexcept
         Shape of the grid.
             Parameters
                 order - order of Zernike expansion
template<typename ElementType, typename LayoutType = DefaultLayout>
class BallGLQGridSpan : public zest::MDSpan<ElementType, 3>
     A non-owning view of gridded data in spherical coordinates in the unit ball.
         Template Parameters
               • ElementType – type of elements in the grid
               • LayoutType - grid layout
     Public Functions
     inline constexpr std::size t order() const noexcept
          Order of Zernike expansion.
     inline constexpr const std::array<std::size t, 3> &shape() const noexcept
         Shape of the grid.
     inline constexpr std::span<element type> flatten() const noexcept
         Flattened view of the underlying buffer.
     Public Static Functions
     static inline constexpr std::size_t size(std::size_t order) noexcept
         Number of grid points.
             Parameters
                 order - order of Zernike expansion
     static inline constexpr std::array<std::size_t, 3> shape(std::size_t order)
                                                                   noexcept
         Shape of the grid.
             Parameters
                 order - order of Zernike expansion
template<ZernikeNorm zernike_norm_param, st::SHNorm sh_norm_param, st::SHPhase</pre>
sh_phase_param, typename GridLayoutType = DefaultLayout>
class GLQTransformer
     Class for transforming between a Gauss-Legendre quadrature grid representation and Zernike polyno-
     mial expansion representation of data in the unit baal.
         Template Parameters
```

- **zernike\_norm\_param** normalization convention of Zernike functions
- sh norm param normalization convention of spherical harmonics
- **sh\_phase\_param** phase convention of spherical harmonics
- GridLayoutType –

#### **Public Functions**

```
inline std::size_t order() const noexcept
    Order of Xernike expansion.
inline void resize(std::size_t order)
```

Resize transformer for specified expansion order.

Forward transform from Gauss-Legendre quadrature grid to Zernike coefficients.

#### **Parameters**

- values values on the ball quadrature grid
- **expansion** coefficients of the expansion

Backward transform from Zernike expansion to Gauss-Legendre quadrature grid.

#### **Parameters**

- **expansion** coefficients of the expansion
- values values on the ball quadrature grid

inline RealZernikeExpansion<zernike\_norm\_param, sh\_norm\_param, sh\_phase\_param> forward\_transfo

Forward transform from Gauss-Legendre quadrature grid to Zernike coefficients.

### **Parameters**

- values values on the ball quadrature grid
- **order** order of expansion

Backward transform from Zernike coefficients to Gauss-Legendre quadrature grid.

#### **Parameters**

• values – values on the ball quadrature grid

• **expansion** – coefficients of the expansion

```
template<ZernikeNorm zernike_norm_param, st::SHNorm sh_norm_param, st::SHPhase
sh_phase_param, typename GridLayoutType = DefaultLayout>
class ZernikeTransformer
```

High-level interface for taking Zernike transforms of functions on balls of arbitrary radii.

#### **Template Parameters**

- **zernike\_norm\_param** normalization convention of Zernike functions
- **sh\_norm\_param** normalization convention of spherical harmonics
- **sh\_phase\_param** phase convention of spherical harmonics
- GridLayoutType –

#### **Public Functions**

```
inline void resize(std::size_t order)
```

Resize the transformer to work with expansions of different order.

Get Zernike expansion of a function expressed in spherical coordinates.

#### **Template Parameters**

FuncType – type of function

#### **Parameters**

- **f** function to transform
- radius radius of the ball f is defined on
- **expansion** buffer to store the expansion

```
template<spherical_function FuncType>
```

```
inline RealZernikeExpansion<zernike_norm_param, sh_norm_param, sh_phase_param> transform(Func-
Type
```

double radius, std:: or-

der)

&&f,

Get Zernike expansion of a function expressed in spherical coordinates.

#### **Template Parameters**

FuncType – type of function

#### **Parameters**

- $\mathbf{f}$  function to transform
- radius radius of the ball f is defined on
- order order of the expansion

#### Returns

Zernike expansion

template<cartesian\_function FuncType>

```
inline void transform(FuncType &&f, double radius,
```

RealZernikeSpan<std::array<double, 2>, zernike\_norm\_param, sh\_norm\_param, sh\_phase\_param> expansion)

Get Zernike expansion of a function expressed in Cartesian coordinates.

#### **Template Parameters**

FuncType – type of function

#### **Parameters**

- **f** function to transform
- radius radius of the ball f is defined on
- **expansion** buffer to store the expansion

#### template<cartesian\_function FuncType>

inline RealZernikeExpansion<zernike\_norm\_param, sh\_norm\_param, sh\_phase\_param> transform(Func-Type

> &&f, double radius, std:: or-

> > der)

Get spherical harmonic expansion of a function expressed in Cartesian coordinates.

#### **Template Parameters**

**FuncType** – type of function

#### **Parameters**

- **f** function to transform
- radius radius of the ball f is defined on
- order order of the expansion

#### Returns

Zernike expansion

#### Type aliases

```
using zest::zt::DefaultLayout = LonLatRadLayout<>
```

```
template<typename GridLayout = DefaultLayout>
```

```
using zest::zt::GLQTransformerAcoustics = GLQTransformer<ZernikeNorm::unnormed,
st::SHNorm::qm, st::SHPhase::none, GridLayout>
```

Convenient alias for GLQTransformer with unnormalized Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

# Template Parameters **GridLayout** –

template<typename GridLayout = DefaultLayout>

```
using zest::zt::GLQTransformerNormalAcoustics = GLQTransformer<ZernikeNorm::normed,
st::SHNorm::qm, st::SHPhase::none, GridLayout>
```

Convenient alias for GLQTransformer with orthonorml Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

```
Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::GLQTransformerQM = GLQTransformer<ZernikeNorm::unnormed,</pre>
st::SHNorm::qm, st::SHPhase::cs, GridLayout>
     Convenient alias for GLQTransformer with unnormalized Zernike functions, orthonormal spherical
     harmonics, and Condon-Shortley phase.
         Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::GLQTransformerNormalQM = GLQTransformer<ZernikeNorm::normed,</pre>
st::SHNorm::qm, st::SHPhase::cs, GridLayout>
     Convenient alias for GLQTransformer with orthonormal Zernike functions, orthonormal spherical
     harmonics, and Condon-Shortley phase.
         Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::GLQTransformerGeo = GLQTransformer<ZernikeNorm::unnormed,</pre>
st::SHNorm::geo, st::SHPhase::none, GridLayout>
     Convenient alias for GLQTransformer with unnormalized Zernike functions, 4-pi normal spherical
     harmonics, and no Condon-Shortley phase.
         Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::GLQTransformerNormalGeo = GLQTransformer<ZernikeNorm::normed,</pre>
st::SHNorm::geo, st::SHPhase::none, GridLayout>
     Convenient alias for GLQTransformer with orthonormal Zernike functions, 4-pi normal spherical
     harmonics, and no Condon-Shortley phase.
         Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::ZernikeTransformerAcoustics =
ZernikeTransformer<ZernikeNorm::unnormed, st::SHNorm::qm, st::SHPhase::none,</pre>
GridLayout>
     Convenient alias for ZernikeTransformer with unnormalized Zernike functions, orthonormal spher-
     ical harmonics, and no Condon-Shortley phase.
         Template Parameters
             GridLayout -
template<typename GridLayout = DefaultLayout>
using zest::zt::ZernikeTransformerNormalAcoustics =
ZernikeTransformer<ZernikeNorm::normed, st::SHNorm::qm, st::SHPhase::none,</pre>
```

GridLayout>

Convenient alias for ZernikeTransformer with orthonormal Zernike functions, orthonormal spherical harmonics, and no Condon-Shortley phase.

Template Parameters
GridLayout -

```
template<typename GridLayout = DefaultLayout>
```

```
using zest::zt::ZernikeTransformerQM = ZernikeTransformer<ZernikeNorm::unnormed,
st::SHNorm::qm, st::SHPhase::cs, GridLayout>
```

Convenient alias for ZernikeTransformer with unnormalized Zernike functions, orthonormal spherical harmonics, and Condon-Shortley phase.

Template Parameters **GridLayout** –

template<typename GridLayout = DefaultLayout>

```
using zest::zt::ZernikeTransformerNormalQM = ZernikeTransformer<ZernikeNorm::normed,
st::SHNorm::gm, st::SHPhase::cs, GridLayout>
```

Convenient alias for ZernikeTransformer with orthonormal Zernike functions, orthonormal spherical harmonics, and Condon-Shortley phase.

Template Parameters **GridLayout** –

template<typename GridLayout = DefaultLayout>

```
using zest::zt::ZernikeTransformerGeo = ZernikeTransformer<ZernikeNorm::unnormed,
st::SHNorm::geo, st::SHPhase::none, GridLayout>
```

Convenient alias for ZernikeTrans former with unnormalized Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

Template Parameters **GridLayout** –

template<typename GridLayout = DefaultLayout>

```
using zest::zt::ZernikeTransformerNormalGeo = ZernikeTransformer<ZernikeNorm::normed,
st::SHNorm::geo, st::SHPhase::none, GridLayout>
```

Convenient alias for ZernikeTransformer with orthonormal Zernike functions, 4-pi normal spherical harmonics, and no Condon-Shortley phase.

Template Parameters GridLayout –

# 0.4.5 Spherical harmonic and Zernike conventions

#### Enums

```
enum class zest::st::SHPhase
```

Spherical harmonic phase conventions.

Values:

enumerator none

enumerator cs

```
enum class zest::st::SHNorm
```

Spherical harmonic normalization conventions.

Values:

#### enumerator geo

geodesy (4 pi) normalization

#### enumerator qm

quantum mechanics (unit norm) normalization

#### enum class zest::zt::ZernikeNorm

Zernike polynomial normalizations.

Values:

enumerator normed

enumerator unnormed

#### 0.4.6 Rotations

#### **Enums**

#### enum class zest::RotationType

Describes whether rotation applies to object or coordinate system.

Values.

#### enumerator object

object is rotated

#### enumerator coordinate

coordinate system is rotated

#### **Types**

#### class Rotor

Rotations of spherical harmonic and Zernike coefficients.

#### **Public Functions**

General rotation of a real spherical harmonic expansion via Wigner's D-matrix.

The rotation uses an intrinsic ZYZ convention, where the first Euler angle rotates about the Z-axis, the second Euler angle rotates about the new Y-axis, and the third angle rotates about the new Z-axis again. In summary, the convention is: right-handed, intrinsic, ZYZ.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- expansion real spherical harmonic expansion
- wigner\_d\_pi2 Wigner d-matrices at pi/2
- euler\_angles Euler angles defining the rotation
- **type** type of rotation

template<st::row\_skipping\_real\_sh\_expansion ExpansionType>

General rotation of an even/odd real spherical harmonic expansion via Wigner's D-matrix.

The rotation uses an intrinsic ZYZ convention, where the first Euler angle rotates about the Z-axis, the second Euler angle rotates about the new Y-axis, and the third angle rotates about the new Z-axis again. In summary, the convention is: right-handed, intrinsic, ZYZ.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- **expansion** real spherical harmonic expansion
- wigner\_d\_pi2 Wigner d-matrices at pi/2
- euler\_angles Euler angles defining the rotation
- **type** type of rotation

General rotation of a real Zernike expansion via Wigner's D-matrix.

The rotation uses an intrinsic ZYZ convention, where the first Euler angle rotates about the Z-axis, the second Euler angle rotates about the new Y-axis, and the third angle rotates about the new Z-axis again. In summary, the convention is: right-handed, intrinsic, ZYZ.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- expansion real Zernike expansion
- wigner\_d\_pi2 Wigner d-matrices at pi/2
- euler\_angles Euler angles defining the rotation
- **type** type of rotation

General rotation of a real spherical harmonic expansion via Wigner's D-matrix.

The rotation uses an intrinsic ZYZ convention, where the first Euler angle rotates about the Z-axis, the second Euler angle rotates about the new Y-axis, and the third angle rotates about the new Z-axis again. In summary, the convention is: right-handed, intrinsic, ZYZ.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- **expansion** real spherical harmonic expansion
- wigner\_d\_pi2 Wigner d-matrices at pi/2
- **euler\_angles** Euler angles defining the rotation
- **type** type of rotation

template<zt::real\_zernike\_expansion ExpansionType>

General rotation of a real Zernike expansion via Wigner's D-matrix.

The rotation uses an intrinsic ZYZ convention, where the first Euler angle rotates about the Z-axis, the second Euler angle rotates about the new Y-axis, and the third angle rotates about the new Z-axis again. In summary, the convention is: right-handed, intrinsic, ZYZ.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- expansion real Zernike expansion
- wigner\_d\_pi2 Wigner d-matrices at pi/2
- euler\_angles Euler angles defining the rotation
- **type** type of rotation

Rotation about the Z-axis of a real spherical harmonic expansion.

#### **Template Parameters**

**ExpansionType** – type of expansion to rotate

#### **Parameters**

- expansion real spherical harmonic expansion
- angle polar rotation angle
- **type** type of rotation

Rotation about the Z-axis of a real Zernike expansion.

## **Template Parameters**

 $\textbf{ExpansionType} - type \ of \ expansion \ to \ rotate$ 

## **Parameters**

- expansion real spherical harmonic expansion
- **angle** polar rotation angle
- **type** type of rotation

#### class WignerdPiHalfCollection

Collection of Wigner (small) d-matrices at pi/2.

## template<typename ElementType>

## class WignerdSpan

Non-owning view of a Wigner (small) d-matrix at pi/2.

#### **Template Parameters**

**ElementType** – type of elements in the view

#### **Functions**

Translate rotation matrix into corresponding Euler angles.

#### **Parameters**

**rot** – rotation matrix

#### Returns

Euler angles in order alpha, beta, gamma

## 0.4.7 Uniform grids

### **Types**

#### class GridEvaluator

Class for evaluating spherical harmonic expansions on arbitrary grids.

#### **Public Functions**

```
explicit GridEvaluator(std::size_t max_order)
```

Reserves memory for an expansion of given order.

#### **Parameters**

**max\_order** – maximum order of spherical harmonic expansion.

```
GridEvaluator(std::size_t max_order, std::size_t lon_size, std::size_t lat_size)
```

Reserves memory for a combination of expansion and grid size.

#### **Parameters**

- max\_order maximum order of spherical harmonic expansion.
- lon\_size size of grid in the longitudinal direction.
- lat\_size size of grid in the latitudinal direction.

```
void resize(std::size_t max_order, std::size_t lon_size, std::size_t lat_size)
```

Resize for a combination of expansion and grid size.

#### **Parameters**

- max\_order maximum order of spherical harmonic expansion.
- **lon\_size** size of grid in the longitudinal direction.
- lat\_size size of grid in the latitudinal direction.

```
template<real_sh_expansion ExpansionType>
```

Evaluate spherical harmonic expansion on a grid.

#### **Parameters**

- **expansion** spherical harmonics expansion.
- longitudes longitude values defining the grid points.
- **colatitudes** colatitude values defining the grid points.

#### Returns

std::vector containing values of the expansion on the grid. The values are ordered as a 2D array with shape {longitudes.size(), colatitudes.size()} in
row-major order.

#### class GridEvaluator

#### **Public Functions**

```
explicit GridEvaluator(std::size_t max_order)
```

Reserves memory for an expansion of given order.

#### **Parameters**

max\_order - maximum order of spherical harmonic expansion.

Reserves memory for a combination of expansion and grid size.

#### **Parameters**

- max\_order maximum order of spherical harmonic expansion.
- lon\_size size of grid in the longitudinal direction.
- lat\_size size of grid in the latitudinal direction.
- rad\_size size of grid in the radial direction.

Resize for a combination of expansion and grid size.

#### **Parameters**

- max\_order maximum order of spherical harmonic expansion.
- lon\_size size of grid in the longitudinal direction.
- lat\_size size of grid in the latittudinal direction.
- rad\_size size of grid in the radial direction.

```
template<real_zernike_expansion ExpansionType>
```

Evaluate spherical harmonic expansion on a grid.

#### **Parameters**

- **expansion** spherical harmonics expansion.
- longitudes longitude values defining the grid points.
- **colatitudes** colatitude values defining the grid points.
- radii radius values defining the grid points.

## Returns

std::vector containing values of the expansion on the grid. The values are ordered
as a 3D array with shape {longitudes.size(), colatitudes.size(), radii.
size()} in row-major order.

## 0.4.8 Power spectra

#### **Functions**

#### namespace zest

#### namespace st

#### **Functions**

Compute cross power spectrum of two spherical harmonic expansions.

#### **Parameters**

- a spherical harmonic expansion
- **b** spherical harmonic expansion
- out output buffer for the cross power spectrum

```
template<st::real_sh_expansion ExpansionType>
std::vector<double> cross_power_spectrum(ExpansionType &&a, ExpansionType &&b)
```

Compute cross power spectrum of two spherical harmonic expansions.

#### **Parameters**

- a spherical harmonic expansions
- **b** spherical harmonic expansions

#### **Returns**

std::vector storing the the cross power spectrum

Compute power spectrum of a spherical harmonic expansions.

#### **Parameters**

- **expansion** spherical harmonic expansion
- **out** output buffer for the power spectrum

```
template<st::real_sh_expansion ExpansionType>
```

```
std::vector<double> power_spectrum(ExpansionType &&expansion)
```

Compute power spectrum of a spherical harmonic expansions.

## Parameters

**expansion** – spherical harmonic expansion

#### **Returns**

std::vector storing the power spectrum

#### namespace zt

## **Functions**

Compute power spectrum of a Zernike expansion.

#### **Parameters**

- **expansion** Zernike expansion.
- **out** place to store the power spectrum.

```
template<zt::real_zernike_expansion ExpansionType>
```

```
std::vector<double> power_spectrum(ExpansionType &&expansion)
             Compute power spectrum of a Zernike expansions.
                Parameters
                   expansion – Zernike expansion
                   std::vector storing the power spectrum.
0.4.9 Layouts
enum class zest::IndexingMode
     Enum for tagging the m indexing style for spherical harmonics related things.
     Values:
     enumerator negative
     enumerator nonnegative
enum class zest::Parity
     Values:
     enumerator even
     enumerator odd
enum class zest::LayoutTag
     Tag for easily differentiating various layouts.
     Values:
     enumerator linear
     enumerator triangular
     enumerator tetrahedral
Concepts
template<typename T>
concept one_dimensional_span
template<typename T>
concept two_dimensional_span
template<typename T>
concept two_dimensional_subspannable
template<typename T>
concept layout_2d
template<typename T>
concept triangular_layout
```

#### **Types**

template<IndexingMode indexing\_mode\_param>

#### struct StandardLinearLayout

Contiguous 1d layout, which is indexed exactly as you think it is.

```
0 1 2 3 4 5...
```

#### **Template Parameters**

indexing\_mode\_param - determines whether indexing may be negative

#### **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of elements in layout for size parameter order.

#### **Parameters**

order - parameter presenting the size of the layout

```
static inline constexpr std::size_t idx(index_type 1) noexcept
```

Linear index of an element in layout.

#### struct ParityLinearLayout

Contiguous 1d layout, with indexing according to certain parity.

```
0 2 4 6 8...
```

or

```
1 3 5 7 9...
```

## Warning

This indexing implies that adjacent even and odd indices map to the same memory slot. Indexing data with this layout mixing even and odd indices is an error.

#### **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of elements in layout for size parameter order.

#### **Parameters**

order - parameter presenting the size of the layout

```
static inline constexpr std::size_t idx(index_type 1) noexcept
```

Linear index of an element in layout.

template<IndexingMode indexing\_mode\_param>

## struct TriangleLayout

Contiguous 2D layout with indexing.

```
(0,0)
(1,0) (1,1)
(2,0) (2,1) (2,2)
(3,0) (3,1) (3,2) (3,3)
```

or

```
(0,0)

(1,-1) (1,0) (1,1)

(2,-2) (2,-1) (2,0) (2,1) (2,2)

(3,-3) (3,-2) (3,-1) (3,0) (3,1) (3,2) (3,3)

...
```

#### **Template Parameters**

indexing\_mode\_param - determines whether indexing may be negative

#### **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of elements in layout for size parameter order.

#### **Parameters**

**order** – parameter presenting the size of the layout

static inline constexpr std::size\_t idx(index\_type l, index\_type m) noexcept

Linear index of an element in layout.

## struct OddDiagonalSkippingTriangleLayout

Contiguous 2D layout with indexing.

```
(0,0)

(1,1)

(2,0) (2,2)

(3,1) (3,3)

(4,0) (4,2) (4,4)

...
```

## Warning

This indexing implies that some index combinations are simply not valid. It is erroneous to access data using this layout with indices whose sum is an odd number.

#### **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of elements in layout for size parameter order.

#### **Parameters**

order - parameter presenting the size of the layout

**static inline constexpr** std::size\_t **idx**(std::size\_t n, std::size\_t l) **noexcept**Linear index of an element in layout.

template<IndexingMode indexing\_mode\_param>

#### struct RowSkippingTriangleLayout

Contiguous 2D layout with indexing.

```
(0,0)
(2,0) (2,1) (2,2)
```

(continues on next page)

(continued from previous page)

```
(4,0) (4,1) (4,2) (4,3) (4,4)
```

or

```
(1,0) (1,1)
(3,0) (3,1) (3,2) (3,3)
(5,0) (5,1) (5,2) (5,3) (5,4) (5,5)
...
```

or alternatively

$$(0,0)$$

$$(2,-2) (2,-1) (2,0) (2,1) (2,2)$$

$$(4,-4) (4,-3) (4,-2) (4,-1) (4,0) (4,1) (4,2) (4,3) (4,4)$$
...

or

$$(1,-1) (1,0) (1,1)$$

$$(3,-3) (3,-2) (3,-1) (3,0) (3,1) (3,2) (3,3)$$

$$(5,-5) (5,-4) (5,-3) (5,-2) (5,-1) (5,0) (5,1) (5,2) (5,3) (5,4) (5,5)$$
...

## 1 Note

In this layout the index obtained from a pair (1,m) is unique only for 1 of the same parity. Otherwise the index is not unique, e.g., (0,0) and (1,0) fall on the same index.

## **Template Parameters**

indexing\_mode\_param - determines whether indexing may be negative

#### **Public Static Functions**

static inline constexpr std::size\_t size(std::size\_t order) noexcept

Number of elements in layout for size parameter order.

#### **Parameters**

order - parameter presenting the size of the layout

static inline constexpr std::size\_t idx(index\_type l, index\_type m) noexcept
Linear index of an element in layout.

template<IndexingMode indexing\_mode\_param>

## struct ZernikeTetrahedralLayout

Contiguous 3D layout with indexing.

```
(\emptyset,\emptyset,\emptyset)
```

(continues on next page)

(continued from previous page)

```
(1,1,0) (1,1,1)
(2,0,0)
(2,2,0) (2,2,1) (2,2,2)
...
```

#### **Template Parameters**

indexing\_mode\_param - determines whether indexing may be negative

#### **Public Static Functions**

#### static inline constexpr std::size\_t size(std::size\_t order) noexcept

Number of elements in layout for size parameter order.

#### **Parameters**

**order** – parameter presenting the size of the layout

Linear index of an element in layout.

#### template<typename ElementType, typename LayoutType>

#### class LinearSpan

A non-owning one-dimensional view of data elements.

#### **Template Parameters**

- **ElementType** type of data elements
- LayoutType type identifying the data layout

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
```

Order of data layout.

```
inline constexpr std::size_t size() const noexcept
```

Size of the underlying buffer.

#### inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

## **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of data elements for size parameter order.

#### **Parameters**

order – parameter presenting the size of the span

#### template<typename ElementType, typename LayoutType>

#### class LinearVecSpan

A non-owning one-dimensional view of one-dimensional segments of data.

## **Template Parameters**

- **ElementType** type of data elements
- LayoutType type identifying the data layout

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
   Order of data layout.
```

inline constexpr std::size\_t vec\_size() const noexcept

Size of a data segment.

inline constexpr std::size\_t size() const noexcept

Size of the underlying buffer.

inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

#### **Public Static Functions**

Number of data elements for size parameter order.

#### **Parameters**

- order parameter presenting the size of the span
- vec\_size number of elements in a single data segment

#### template<typename ElementType>

#### class ParitySpan

A non-owning view where adjacent even and odd indices refer to the same value. Given index i, the corresponding offset in the underlying buffer is given by i/2.

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
   Order of data layout.
```

inline constexpr std::size\_t size() const noexcept

Size of the underlying buffer.

inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

template<typename ElementType, typename LayoutType>

#### class TriangleSpan

A non-owning two-dimensional view of data elements with triangular layout.

#### **Template Parameters**

- **ElementType** type of data elements
- LayoutType type identifying the data layout

Subclassed by zest::st::SHLMSpan< ElementType, LayoutType, sh\_norm\_param, sh\_phase\_param >, zest::zt::ZernikeSHSpan< ElementType, LayoutType, zernike\_norm\_param, sh\_norm\_param, sh\_phase\_param >

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
   Order of data layout.
```

```
inline constexpr std::size_t size() const noexcept
```

Size of the underlying buffer.

#### inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

#### **Public Static Functions**

#### static inline constexpr std::size\_t size(std::size\_t order) noexcept

Number of data elements for size parameter order.

#### **Parameters**

order – parameter presenting the size of the span

## template<typename ElementType, typename LayoutType>

#### class TriangleVecSpan

A non-owning two-dimensional view of one-dimensional segments of data with triangular layout.

#### **Template Parameters**

- **ElementType** type of data elements
- LayoutType type identifying the data layout

Subclassed by zest::SHLMVecSpan < ElementType, LayoutType, sh\_norm\_param, sh\_phase\_param >

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
```

Order of data layout.

inline constexpr std::size\_t vec\_size() const noexcept

Size of a data segment.

#### inline constexpr std::size\_t size() const noexcept

Size of the underlying buffer.

## inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

#### **Public Static Functions**

Number of data elements for size parameter order.

#### **Parameters**

- order parameter presenting the size of the span
- vec\_size number of elements in a single data segment

## template<typename ElementType, typename LayoutType>

#### class TetrahedronSpan

A non-owning three-dimensional view of data elements with triangular layout.

#### **Template Parameters**

- **ElementType** type of elements in the view
- LayoutType layout of the elements

Subclassed by zest::zt::ZernikeNLMSpan< ElementType, LayoutType, zernike\_norm\_param, sh\_norm\_param, sh\_phase\_param >

#### **Public Functions**

```
\textbf{inline constexpr} \; \texttt{std::size\_t order()} \; \textbf{const noexcept}
```

Order of data layout.

inline constexpr std::size\_t size() const noexcept

Size of the underlying buffer.

inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

#### **Public Static Functions**

```
static inline constexpr std::size_t size(std::size_t order) noexcept
```

Number of data elements for size parameter order.

#### **Parameters**

order – parameter presenting the size of the span

#### template<typename ElementType, typename LayoutType>

## class TetrahedronVecSpan

A non-owning three-dimensional view of data elements with triangular layout.

#### **Template Parameters**

- **ElementType** type of elements in the view
- LayoutType layout of the elements

#### **Public Functions**

```
inline constexpr std::size_t order() const noexcept
```

Order of data layout.

inline constexpr std::size\_t size() const noexcept

Size of the underlying buffer.

inline constexpr element\_type \*data() const noexcept

Pointer to underlying buffer.

#### **Public Static Functions**

Number of data elements for size parameter order.

#### **Parameters**

- order parameter presenting the size of the span
- vec\_size number of elements in a single data segment

## 0.4.10 Indexing

## **Types**

template<std::integral IndexType, IndexType stride\_param>

#### class IndexIterator

Iterator presenting an infinite arithmetic sequence of integer indices with arbitrary stride.

**Template Parameters** 

```
• IndexType – type of the index
```

• **stride\_param** – stride of the index

#### **Public Functions**

inline constexpr IndexIterator & operator++() noexcept
Increment index by stride.

inline constexpr IndexIterator & operator -- () noexcept
 Decrement index by stride.

inline constexpr IndexIterator operator++(int) noexcept
 Increment index by stride.

inline constexpr IndexIterator operator--(int) noexcept
 Decrement index by stride.

inline constexpr IndexIterator & operator += (index\_type n) noexcept
Increment index by multiple strides.

inline constexpr IndexIterator & operator -= (index\_type n) noexcept
Decrement index by multiple strides.

inline constexpr IndexIterator operator+(difference\_type n) const noexcept
 Add n strides to index.

inline constexpr IndexIterator operator-(difference\_type n) const noexcept
Subtract n strides from index.

inline constexpr index\_type operator\*() noexcept
Get value of index.

inline constexpr index\_type operator[](index\_type n) noexcept
Get value of index n strides forward from current index.

inline constexpr index\_type index() const noexcept

Get value of index.

template<std::integral IndexType>

## class StandardIndexRange

Range of integer indices.

Template Parameters
IndexType – type of the index

#### **Public Functions**

## inline explicit constexpr StandardIndexRange(index\_type end)

Constructs a range of indices [0, end).

**Parameters** 

end - end of index range

inline constexpr StandardIndexRange(index\_type begin, index\_type end)

Constructs a range of indices [begin, end).

#### **Parameters**

- **begin** start of index range
- end end of index range

#### inline constexpr iterator begin() const noexcept

Iterator to the beginning of the range.

#### inline constexpr iterator end() const noexcept

Iterator to the end of the range.

#### template<std::integral IndexType>

#### class ParityIndexRange

Range of even or odd integer indices.

#### **Template Parameters**

**IndexType** – type of the index

#### **Public Functions**

## inline explicit constexpr ParityIndexRange(index\_type end)

Constructs a range of indices [end % 2, end).

#### **Parameters**

end – end of index range

#### inline constexpr ParityIndexRange(index\_type begin, index\_type end)

Constructs a range of indices [2\*floor(begin/2) + end % 2, end).

#### **Parameters**

- begin start of index range
- end end of index range

#### inline constexpr iterator begin() const noexcept

Iterator to the beginning of the range.

## inline constexpr iterator end() const noexcept

Iterator to the end of the range.

template<std::signed\_integral IndexType>

## class SymmetricIndexRange

Range of integer indices symmetric about zero.

#### **Template Parameters**

**IndexType** – type of the index

#### **Public Functions**

## inline explicit constexpr SymmetricIndexRange(index\_type end)

Constructs a range of indices (-end, end).

## **Parameters**

end – end of index range

#### inline constexpr SymmetricIndexRange(index\_type begin, index\_type end)

Constructs a range of indices [begin, end).

#### **Parameters**

- **begin** start of index range
- end end of index range

## inline constexpr iterator begin() const noexcept

Iterator to the beginning of the range.

#### inline constexpr iterator end() const noexcept

Iterator to the end of the range.

## 0.4.11 Multidimensional arrays

## **Types**

template<typename ElementType, std::size\_t rank\_param>

### class MDArray

Multidimensional array container.

**Template Parameters** 

- **ElementType** type of array elements
- rank\_param number of array dimensions

template<typename ElementType, std::size trank\_param>

#### class MDSpan

Poor man's mdspan for a non-owning multidimensional array view.

**Template Parameters** 

- **ElementType** type of array elements
- rank\_param number of array dimensions

## 0.4.12 Gauss-Legendre quadrature

#### **Enums**

```
enum class zest::ql::GLNodeStyle
```

Style of Gauss-Legendre nodes.

Values:

#### enumerator angle

nodes as angles in the interval [0,pi]

#### enumerator cos

nodes as consines of the angles in the interval [-1,1]

#### **Concepts**

# template<typename T> concept gl\_layout

#include <gauss legendre.hpp> Concept for restricting layout of Gauss-Legendre nodes.

## **Types**

#### struct PackedLayout

Packed layout of Gauss-Legendre nodes.

note Gauss-Legendre nodes on the interval [-1,1] are distributed symmetrically about 0, such that for any node x the point -x is also a node with the same weight. Therefore the nodes and weights only need to be produced for nonnegative x. For the negative portion of the interval the nodes are -x, and the weights are given by the corresponding weights.

#### struct UnpackedLayout

Unpacked layout of Gauss-Legendre nodes.

note Gauss-Legendre nodes on the interval [-1,1] are distributed symmetrically about 0, such that for any node x the point -x is also a node with the same weight. Therefore the nodes and weights only need to be produced for nonnegative x. For the negative portion of the interval the nodes are -x, and the weights are given by the corresponding weights.

#### **Functions**

```
template<gl_layout Layout, GLNodeStyle node_style_param,
std::ranges::random_access_range R>
constexpr void zest::gl::gl_nodes(R &&nodes, std::size_t parity) noexcept
```

For num\_nodes < 70 the nodes are read from a precomputed table. For greater numbers of nodes Bogaert's iteration-free method is used: I. Bogaert, Iteration-free computation of Gauss-Legendre quadrature nodes and weights, SIAM J. Sci. Comput., 36 (2014), pp. C1008-C1026).

The nodes returned are accurate to double macine epsilon.

Obtain Gauss-Legendre nodes for a given number of nodes.

#### **Template Parameters**

- Layout layout of nodes
- R type of the range for storing the nodes

#### **Parameters**

- nodes range for storing the nodes
- parity parity of the total number of nodes

```
template < gl_layout Layout, std::ranges::random_access_range R>
constexpr void zest::gl::gl_weights(R &&weights, std::size_t parity) noexcept
```

Obtain Gauss-Legendre weights for a given number of nodes.

For num\_nodes < 70 the nodes are read from a precomputed table. For greater numbers of nodes Bogaert's iteration-free method is used: I. Bogaert, Iteration-free computation of Gauss-Legendre quadrature nodes and weights, SIAM J. Sci. Comput., 36 (2014), pp. C1008-C1026).

The weights returned are accurate to double macine epsilon.

#### **Template Parameters**

- Layout layout of weights
- R type of the range for storing the weights

#### **Parameters**

- weights range for storing the weights
- parity parity of the total number of nodes

Obtain Gauss-Legendre nodes and weights for a given number of nodes.

For num\_nodes < 70 the nodes are read from a precomputed table. For greater numbers of nodes Bogaert's iteration-free method is used: I. Bogaert, Iteration-free computation of Gauss-Legendre quadrature nodes and weights, SIAM J. Sci. Comput., 36 (2014), pp. C1008-C1026).

The nodes and weights returned are accurate to double macine epsilon.

#### **Template Parameters**

- Layout layout of nodes and weights
- R type of the range for storing the nodes and weights

#### **Parameters**

- **nodes** range for storing the nodes
- weights range for storing the weights
- parity parity of the total number of nodes

## 0.4.13 Memory

## **Concepts**

```
template<typename T>
concept valid_simd_alignment
```

## **Types**

```
template<typename T, valid_simd_alignment Alignment>
```

### struct AlignedAllocator

Aligned memory allocator class.

#### **Template Parameters**

- T type of allocated object
- BYTE\_ALIGNMENT number of bytes to align to

## **Public Functions**

```
inline T *allocate(std::size_t n)
Allocate an aligned block of memory that fits n values of value_type.
```

 $\textbf{inline} \ void \ \textbf{deallocate} (\top \ \textbf{*p}, std::size\_t \ n) \ \textbf{noexcept}$ 

Free allocated memory.

template<typenameU>

struct rebind

template<std::size\_t byte\_alignment>

## struct VectorAlignment

Alignmnet descriptor for SIMD vector alignment.



byte\_alignment must be a power of two.

```
Template Parameters
byte_alignment - number of bytes to align to
```

#### **Public Static Functions**

```
template<typename T>
static inline constexpr std::size_t vector_size() noexcept
```

Number of elements that fit in a SIMD vector of given type.

## **Template Parameters**

**T** – type of elements

## struct NoAlignment

Alignmnet descriptor which doesn't specify any alignment.

#### **Public Static Functions**

```
template<typename T>
static inline constexpr std::size_t vector_size() noexcept
```

Number of elements that fit in a SIMD vector of given type.

## **Template Parameters**

T – type of elements

## Type aliases

```
using zest::SSEAlignment = VectorAlignment<16>
```

Alias for SSE (16 byte) alignment descriptor.

```
using zest::AVXAlignment = VectorAlignment<32>
```

Alias for AVX (32 byte) alignment descriptor.

## using zest::AVX512Alignment = VectorAlignment<64>

Alias for AVX512 (64 byte) alignment descriptor.

#### using zest::CacheLineAlignment = VectorAlignment<64>

Alias for cache line (64 byte) alignment descriptor.

## **Functions**

```
template<typename T, valid_simd_alignment Alignment>
constexpr std::size_t zest::aligned_size(std::size_t n) noexcept
```

Figure out the number of bytes needed to store a number of elements with given byte alignment.

## **Template Parameters**

- T type of allocated object
- BYTE\_ALIGNMENT number of bytes to align to

#### **Parameters**

**n** – number of elements

#### Returns

number of bytes

## **INDEX**

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