Representing three-dimensional cross fields using 4th order tensors

Alexandre Chemin, François Henrotte, Jean-François Remacle and Jean Van Schaftingen

Abstract This paper presents a new way of describing cross fields based on fourth order tensors. We prove that the new formulation is forming a linear space in $\mathbb{R}^9$. The algebraic structure of the tensors and their projections on SO(3) are presented. The relationship of the new formulation with spherical harmonics is exposed. This paper is quite theoretical. Due to pages limitation, few practical aspects related to the computations of cross fields are exposed. Nevetheless, a global smoothing algorithm is briefly presented and computation of cross fields are finally depicted.

1 Introduction

We call a cross f a set of 6 distinct unit vectors mutually orthogonal or opposite to each other (Fig. 1). This geometric object of vectorial nature lives in the tangent space of Euclidean spaces E^3. A cross field $F = \{x \in \Omega \subset E^3 \mapsto f(x)\}$, now, is a rule that associates a cross $f(x)$ to each point of a subset Ω of E^3. Cross fields are auxiliary in 3D mesh generation to define

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local preferred orientations for hexahedral meshes, or for the computation of the polycube decomposition of a solid. Automatic polycube decomposition is a necessary step for multiblock or isogeometric meshing of 3D domains.

Let the Euclidean space E^3 be equipped with a Cartesian coordinate system $\{x_1, x_2, x_3\}$. The six vectors $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$ and $(0, 0, \pm 1)$ form a cross, which we call the reference cross f_{ref}. Crosses being rigid objects, their orientation in space can be *identified* by a rotation respective to f_{ref}, that is a member of SO(3) represented by, e.g., the Euler angles α, β and γ, (Fig. 1). This *representation* of f is however not unique due to the symmetries of the cross, which are fully characterized by regarding the cross as set of six points at the summits of an octahedron. The symmetry group of this point set has 24 elements, which are the 24 rotations that apply the cross onto itself, and is called the octohedral point group O. We call attitude of the cross f its orientation in space up to the symmetries of the cross, and we have

$$f \in \mathrm{SO}(3)/\mathrm{O}.$$

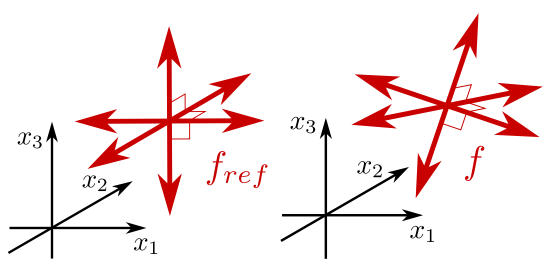

Fig. 1: 3D crosses representation. Left image shows the reference cross f_{ref} and right image shows a cross f that is a rotation of the reference cross.

The expansion of a discretized field F into coefficients and shape functions in finite element analysis is by definition a linear combination, leading then by orthogonalization in this linear space to a linear system of equations to solve. It is hence necessary in this finite element context to have a representation of the point value of the discretized field $F(x)$ in a linear space, i.e., a space containing the linear combinations (here with real coefficients) of all its members. This is however in general not the case with fields taking their values in non-trivial group manifolds like, e.g., SO(3)/O.

The sketch of the solution to this problem can be illustrated with a simple 2D example. Consider the unit circle S^1 and two points $e^{\imath\theta_1}$ and $e^{\imath\theta_2}$ on this manifold. Clearly, linear combinations

$$a\, e^{\imath\theta_1} + b\, e^{\imath\theta_2} \quad , \quad a, b \in \mathbb{R}$$

do not all belong to S^1. In order to have a practical representation of the elements of S^1 in a linear space amenable to finite element analysis, one has to expand S^1 to the enclosing complex plane, $\mathbb{C} \supset S^1$, which is a linear space. The finite element problem can so be formulated in terms of complex valued unknowns that are afterwards projected back into S^1 by means of a projection operator, e.g.,

$$\Pi : \mathbb{C} \mapsto S^1 \quad , \quad x + \imath y \mapsto e^{\imath \, \mathrm{atan2}(y,x)}.$$

A similar approach is followed in this paper for the 3D finite element smoothing of cross attitudes belonging to the group manifold SO(3)/O. The approach rely on a new way of representing 3D cross fields as a particular class of 4^{th} order tensors, themselves in close relations to 4^{th} degree homogeneous polynomials of the Cartesian coordinates. 3D cross field representations based on tensors have been used for 3D solid texturing and hex-dominant meshing [3, 6, 4, 5], but none of them was adressing symmetry issues or projections. The use of 4^{th} order tensors allows to build a 9-dimensional linear space $\mathcal{A}$, containing SO(3)/O as a subset, together with a projection operator

$$\Pi : \mathcal{A} \mapsto \mathrm{SO}(3)/\mathrm{O}.$$

The approach leads eventually to a very efficient smoother for cross fields, one order of magnitude faster than state-of-the art implementations. The proposed representation also allows easy computation of the distance between a finite element computed cross f, and its projection back into SO(3)/O. This distance indicates the presence of singular lines and singular points in the cross field in a straightforward fashion.

The paper is organized as follows. The 4^{th} order tensor representation for crosses is first inroduced, and the useful mathematical properties of this tensor space are then derived. The projection method is then presented and results obtained with a naive 3D crossfield smoothing on some benchmarks problem are finally discussed.

2 Cross representation with 4^{th} order tensors

2.1 The reference cross f_{ref}

Point groups, like O_h, are isometries leaving at least one point of space, the center, invariant. As such, they have very convenient and useful representations on the sphere, and hence also in terms of spherical harmonics. In [1, 2], spherical harmonics of degree 4 are proposed as a polynomial basis to represent 3D cross fields. They exhibit the required octahedral symmetry and span a linear polynomial space $\mathcal{H}_4$ of dimension 9. The projection operator

$$\Pi \; : \mathcal{H}_4 \mapsto \mathrm{SO}(3)/\mathrm{O},$$

however, is tedious as it relies on a complex minimization process that is not ensured to converge to the true projection. Moreover, the differential properties of spherical harmonics (they are solution of the laplacian operator) are of no use to the purpose of cross representation.

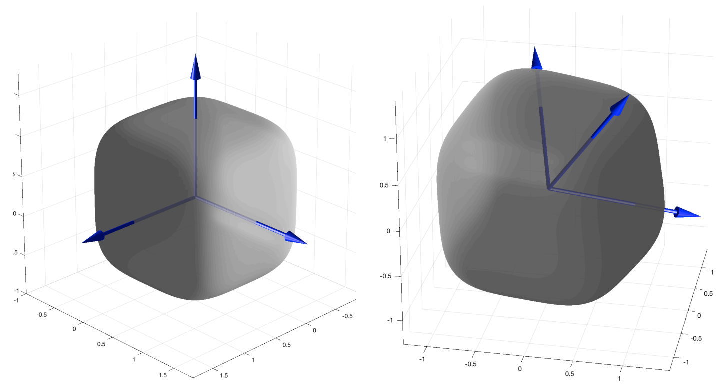

Fig. 2: Representation of the reference cross as a dice-shaped polynomial isovalue surface (left), and of a general cross attitude as a rotation of the latter (right)

The idea promoted in this paper is thus also to work with polynomials whose isovalues exhibit the sought octahedral symmetry but, instead of expanding them in a spherical harmonics basis, they are represented as explicit rotations of a reference polynomial

$$f_{ref}(x_1, x_2, x_3) = \|x\|_4^4 \equiv x_1^4 + x_2^4 + x_3^4, \tag{1}$$

whose isovalue $f_{ref} = 1$ is the dice-shaped surface depicted in Fig. 2 (left). Fourth order is the lowest polynomial order exhibiting distinctive octahedral symmetry, which is by the way rather natural in a Cartesian coordinate system, as it simply amounts to the invariance against any argument inversion and/or permutation :

$$f_{ref}(x_1, x_2, x_3) = f_{ref}(-x_1, x_2, x_3) = f_{ref}(x_2, -x_1, x_3) = \dots$$

In tensor notations, we have

$$f_{ref}(x_1, x_2, x_3) = \tilde{A}_{ijkl}\, x_i x_j x_k x_l$$

assuming Einstein's implicit summation over repeated indices. As a polynomial is characterized by its coefficients, not by the power terms which act as a basis, the 4^{th} order tensor

$$\tilde{A}_{ijkl} = \sum_{q=1}^{3} \delta_{iq}\delta_{jq}\delta_{kq}\delta_{lq}. \tag{2}$$

is another full-fledged representation of the reference cross f_{ref}. It has only three non-zero components

$$\tilde{\mathbb{A}}_{1111} = \tilde{\mathbb{A}}_{2222} = \tilde{\mathbb{A}}_{3333} = 1.$$

2.2 Rotation of the reference cross

The reference cross (1) exhibits octahedral symmetry and rotations, which are isometries, preserve this symmetry. It can therefore be stated that the space of all possible cross attitudes in E^3 is the set

$$f(x_1, x_2, x_3) = f_{ref}(R_{1i}x_i, R_{2j}x_j, R_{3k}x_k) \quad , \quad R_{ij} \in \mathrm{SO}(3), \tag{3}$$

whose corresponding tensor representation reads

$$\mathbb{A}_{ijkl} = R_{im}R_{jn}R_{ko}R_{lp}\,\tilde{A}_{mnop} = \sum_{q=1}^{3} R_{im}R_{jn}R_{ko}R_{lp}\,\delta_{iq}\delta_{jq}\delta_{kq}\delta_{lq} = \sum_{q=1}^{3} R_{iq}R_{jq}R_{kq}R_{lq}. \tag{4}$$

This tensor, noted $\mathbb{A}$, represents a general *attitude* of the cross in E^3, and the isovalue of the associated polynomial

$$f(x_1, x_2, x_3) = \mathbb{A}_{ijkl}\,x_ix_jx_kx_l = 1$$

is a rotation of the axis-aligned dice-shaped surface f_{ref}, Fig. 2.

Rotation matrices play a pivotal role in these definitions. For convenience, let us define the following nomenclature:

- The indices $1, 2, 3$ refer to the angles α, β and γ, i.e. the angles corresponding to the first, second and third elemental rotations, respectively.
- The matrices X, Y, Z represent the elemental rotations about the axes x_1, x_2, x_3 of the Cartesian reference cross in $\mathbb{R}^3$ (e.g., Y_1 represents a rotation about x_2 by an angle α).
- The shorthands s and c represent sine and cosine (e.g., s_1 represents the sine of α).

We have for example the rotation matrix in $\mathbb{R}^3$

$$R = Z_1 X_2 Z_3 = \begin{pmatrix} c_1c_3 - c_2s_1s_3 & -c_1s_3 - c_3c_2s_1 & s_2s_1 \\ c_1c_2s_3 + c_3s_1 & c_1c_2c_3 - s_1s_3 & -c_1s_2 \\ s_3s_2 & c_3s_2 & c_2 \end{pmatrix}, \tag{5}$$

which non-linearly depends on only three degrees of freedom : the angles α, β and γ.

2.3 Algebraic structure of $\mathbb{A}_{ijkl}$

A 4th order tensor in E^3 has at most $3^4 = 81$ independant components. The specific algebraic structure of (4) makes it so, however, that the tensor space of interest for cross fields is much smaller than that, and can be characterized as a linear space $\mathcal{A}$ of dimension 9, convenient for finite element interpolation, together with a non-linear projection operator

$$\Pi\ : \mathcal{A} \mapsto \mathrm{SO}(3)/\mathrm{O} \tag{6}$$

from the 9-dimensional linear space onto a 3-dimensional nonlinear manifold.

The demonstration of this algebraic structure is in several steps. First, the number of independent components of $\mathbb{A}$ cannot be larger than the dimension of the space of homogeneous polynomials of order 4 with 3 variables, i.e., $\binom{4+3-1}{4} = 15$. This is a mere consequence of the fact that the products of coordinates, as the product of real numbers, obviously commute, $x_i x_j = x_j x_i$, and that all terms associated with components of $\mathbb{A}$ whose indice sets are permutations of each other eventually contribute to the same term in the polynomial. In mathematical terms, it amounts to require the tensor $\mathbb{A}$ be *fully symmetric*, a condition usually written

$$\mathbb{A}_{ijkl} = \mathbb{A}_{(ijkl)}$$

with

$$\mathbb{A}_{(ijkl)} = \frac{1}{24}\left(\mathbb{A}_{ijkl} + \mathbb{A}_{jikl} + \dots\right)$$

where the 24 permutations of the set $ijkl$ are enumerated at the right-hand side.

The tensors (4) have however deeper structures, related with the unitary property

$$R^t R = I \quad , \quad R_{ik} R_{jk} = \delta_{ij}$$

of rotations matrices. The so called “partial traces”[1]

[1] Make sure to clearly distinguish sums over two repeated indices, which are implict in our notation, and sums over four repeated indices, which are explicitly written.

$$\mathbb{A}_{iikl} = \sum_{q=1}^{3} R_{iq} R_{iq} R_{kq} R_{lq} = \sum_{q=1}^{3} \delta_{qq} R_{kq} R_{lq} = R_{kq} R_{lq} = \delta_{kl} \qquad (7)$$

leads to the 6 additional relationships

$$\begin{aligned}
\mathbb{A}_{1111} + \mathbb{A}_{2211} + \mathbb{A}_{3311} &= 1, \\
\mathbb{A}_{1122} + \mathbb{A}_{2222} + \mathbb{A}_{3322} &= 1, \\
\mathbb{A}_{1133} + \mathbb{A}_{2233} + \mathbb{A}_{3333} &= 1, \\
\mathbb{A}_{1112} + \mathbb{A}_{2212} + \mathbb{A}_{3312} &= 0, \\
\mathbb{A}_{1113} + \mathbb{A}_{2213} + \mathbb{A}_{3313} &= 0, \\
\mathbb{A}_{1123} + \mathbb{A}_{2223} + \mathbb{A}_{3323} &= 0.
\end{aligned}$$

Other partial traces would give linearly dependent relationships, due to the full symmetry of the tensor mentioned above.

It is important to note that partial traces are conserved under affine combination of tensors. Tensors in $\mathbb{A}$ form thus a $15 - 6 = 9$ dimensional linear space, noted $\mathcal{A}$, convenient for finite element interpolation. Interestingly enough, this dimension is also that of the the space of 4th order spherical harmonics, used by some authors to represent crosses [2].

2.4 $\mathbb{A}$ *is a projector*

Let X be the set of symmetric 2^d order tensors in E^3. This is a linear space, and any tensor $\mathbf{d} \in X$ can be expanded in terms of rank one basis tensors

$$\mathbf{d} = d_{mn}\ e_m \otimes e_n \quad , \quad d_{mn} = d_{nm}$$

where e_m, $m, 1, 2, 3$, are the orthormal basis vectors of the Cartesian coordinate system. Alternatively, basis tensors rotated by a matrix $R \in SO(3)$ can be used as well,

$$\mathbf{d} = d'_{mn}\ r_m \otimes r_n \quad , \quad d'_{mn} = d'_{nm} \qquad (8)$$

with now

$$r_m = R(e_m) \quad , \quad (r_m)_i = R_{ij} \delta_{jm} = R_{im}$$

the m^{th} column vector of the rotation matrix R. The polynomials we are using in this paper to represent cross attitudes are built from special tensors in X for which one simply has $B'_{mn} = x_m x_n$.

Once the space X is appropriately characterized, the tensor $\mathbb{A}$ defined by (4) can be regarded as a linear application

$$\mathbb{A} : X \mapsto X,$$

and it is readily shown that it is a projection operator :

$$
\begin{aligned}
\mathbb{A}^2 = \mathbb{A} : \mathbb{A} \equiv \mathbb{A}_{ijmn}\mathbb{A}_{mnkl} \\
&= \sum_{q=1}^{3}\sum_{s=1}^{3} R_{iq}R_{jq}R_{mq}R_{nq}R_{ns}R_{ms}R_{ks}R_{ls} \\
&= \sum_{q=1}^{3}\sum_{s=1}^{3} R_{iq}R_{jq}R_{ks}R_{ls}\,\underbrace{R_{mq}R_{ms}}_{\delta_{qs}}\,\underbrace{R_{nq}R_{ns}}_{\delta_{qs}} \\
&= \sum_{q=1}^{3} R_{iq}R_{jq}R_{kq}R_{lq} = \mathbb{A}_{ijkl} = \mathbb{A},
\end{aligned}
\tag{9}
$$

To characterize this projection, the image by $\mathbb{A}$ of the basis tensors $r_m \otimes r_n$ in (8) is evaluated. One has

$$
\begin{aligned}
(\mathbb{A} : r_m \otimes r_n)\big|_{ij} &= \mathbb{A}_{ijkl}\ R_{km}R_{ln} \\
&= \sum_{q=1}^{3} R_{iq}R_{jq}R_{kq}R_{lq}R_{km}R_{ln} \\
&= \sum_{q=1}^{3} R_{iq}R_{jq}\delta_{qm}\delta_{qn},
\end{aligned}
$$

from where follows

$$
\mathbb{A} : (r_m \otimes r_m) = r_m \otimes r_m \quad m = 1, 2, 3 \text{ (no sum)} \tag{10}
$$

$$
\mathbb{A} : (r_m \otimes r_n) \quad = 0 \qquad \text{if } m \neq n. \tag{11}
$$

As expected for a projector, eigen values are either 0 or 1. The eigenspace corresponding to the eigenvalues $\lambda_1 = \lambda_2 = \lambda_3 = 1$ is

$$
\operatorname{range}\mathbb{A} = \operatorname{span}(r_1 \otimes r_1, r_2 \otimes r_2, r_3 \otimes r_3) \subset X
$$

whereas that corresponding to $\lambda_4 = \lambda_5 = \lambda_6 = 0$ is the kernel space

$$
\ker\mathbb{A} = \operatorname{span}(r_1 \otimes r_2 + r_2 \otimes r_1, r_2 \otimes r_3 + r_3 \otimes r_2, r_3 \otimes r_1 + r_1 \otimes r_3).
$$

Obviously, the *eigentensors* $\mathbf{d}^j$ are both symmetric ($\mathbf{d}^j_{mn} = \mathbf{d}^j_{nm}$), and orthonormal to each other ($\mathbf{d}^i : \mathbf{d}^j = \delta_{ij}$) under the Frobenius norm $\| \mathbf{d} \|_F^2 = \mathbf{d} : \mathbf{d} = d_{mn}d_{nm}$.

3 Three main results

The three main results of the paper are now presented in this section. We first prove that any tensor $\mathbb{A} \in \mathcal{A}$ (a fully symmetric tensor obeying (7)) corresponds to a cross attitude (i.e., a rotation of the reference cross) if it is a projector $\mathbb{A}^2 = \mathbb{A}$ onto a three-dimensional subspace of X. Then, we show how to project a tensor $\mathbb{A} \in \mathcal{A}$ that is not a projector onto another tensor in $\mathcal{A}$ verifying $\mathbb{A}^2 = \mathbb{A}$ with three non-zero eigenvalues. Finally, we show the direct relashionship between spherical harmonics and our representation on terms of 4^{th} order tensors.

3.1 Sufficiency

Theorem 1. *A tensor $\mathbb{A} \in \mathcal{A}$, (fully symmetric 4^{th} order tensor obeying the partial trace condition(7)) that is also a projector on a 3-dimensional subspace of X corresponds to a cross attitude (i.e., to a rotation of the reference cross)*

Proof. If $\mathbb{A}$ is a projector onto a 3-dimensional subspace of X, there exist three orthonormal symmetric second order tensors $\mathbf{d}^a, \mathbf{d}^b, \mathbf{d}^c \in X$ such that

$$\begin{aligned}\mathbf{d}^a \otimes \mathbf{d}^a + \mathbf{d}^b \otimes \mathbf{d}^b + \mathbf{d}^c \otimes \mathbf{d}^c &= \mathbb{A} \\ \mathbf{d}^l : \mathbf{d}^m &= \delta_{lm} \; l, m = a, b, c \\ \mathbf{d}^l_{ij} &= \mathbf{d}^l_{ji} \; l = a, b, c, \; i, j = 1, 2, 3.\end{aligned} \tag{12}$$

Note that there is no implicit summation on upper indices in this proof. The key point of the proof is to show that the eigentensors $\mathbf{d}^a$, $\mathbf{d}^b$ and $\mathbf{d}^c$ commute with each other. If this is the case, they are joint diagonalizable and share therefore the same set of eigenvectors. It is then easy to see that $\mathbb{A}$ is the 4^{th} order tensor representation of a cross.

Let
$$[\mathbf{d}^l, \mathbf{d}^m] = \mathbf{d}^l \cdot \mathbf{d}^m - \mathbf{d}^m \cdot \mathbf{d}^l$$
be the the commutator of $\mathbf{d}^l$ and $\mathbf{d}^m$, of which we have to prove the Frobenius norm is zero,
$$\| \, [\mathbf{d}^l, \mathbf{d}^m] \, \|_F^2 = [\mathbf{d}^l, \mathbf{d}^m] : [\mathbf{d}^l, \mathbf{d}^m] = 0.$$

One first notes that

$$\begin{aligned}(\mathbf{d}^a \cdot \mathbf{d}^b) : (\mathbf{d}^e \cdot \mathbf{d}^f) &= d^a_{ik} d^b_{kj} d^e_{il} d^f_{lj} = \operatorname{tr}(\mathbf{d}^a \mathbf{d}^b \mathbf{d}^f \mathbf{d}^e) \\ &= (\mathbf{d}^b \cdot \mathbf{d}^a) : (\mathbf{d}^f \cdot \mathbf{d}^e) \\ &= (\mathbf{d}^a \cdot \mathbf{d}^e) : (\mathbf{d}^b \cdot \mathbf{d}^f) \\ &= (\mathbf{d}^e \cdot \mathbf{d}^a) : (\mathbf{d}^f \cdot \mathbf{d}^b)\end{aligned} \tag{13}$$

exploiting the symmetry of the individual $\mathbf{d}^l$ tensors, and all possible reorganizations of the matrix products. As the contraction operator : is also symmmetric, there are thus 8 equivalent argument permutations (out of 24) for such scalar quantities. With this, one shows that

$$\begin{aligned}\| \, [\mathbf{d}^a, \mathbf{d}^b] \, \|_F^2 &= (\mathbf{d}^a \cdot \mathbf{d}^b - \mathbf{d}^b \cdot \mathbf{d}^a) : (\mathbf{d}^a \cdot \mathbf{d}^b - \mathbf{d}^b \cdot \mathbf{d}^a) \\ &= (\mathbf{d}^a \cdot \mathbf{d}^b) : (\mathbf{d}^a \cdot \mathbf{d}^b) - (\mathbf{d}^a \cdot \mathbf{d}^b) : (\mathbf{d}^b \cdot \mathbf{d}^a) - \\ &\quad (\mathbf{d}^b \cdot \mathbf{d}^a) : (\mathbf{d}^a \cdot \mathbf{d}^b) + (\mathbf{d}^b \cdot \mathbf{d}^a) : (\mathbf{d}^b \cdot \mathbf{d}^a) \\ &= 2(\mathbf{d}^a \cdot \mathbf{d}^a) : (\mathbf{d}^b \cdot \mathbf{d}^b) - 2(\mathbf{d}^a \cdot \mathbf{d}^b) : (\mathbf{d}^b \cdot \mathbf{d}^a) \end{aligned} \tag{14}$$

the last two terms being not reducible to each other by the permutation rules given above. As

$$(\mathbf{d}^a \cdot \mathbf{d}^b) : (\mathbf{d}^e \cdot \mathbf{d}^f) = \mathrm{tr}\,(\mathbf{d}^a \mathbf{d}^b \mathbf{d}^f \mathbf{d}^e),$$

the identity (14) can also be interpreted as

$$\| \, [\mathbf{d}^a, \mathbf{d}^b] \, \|_F^2 = \mathrm{tr}\,(\mathbf{d}^a \mathbf{d}^a \mathbf{d}^b \mathbf{d}^b - \mathbf{d}^a \mathbf{d}^b \mathbf{d}^a \mathbf{d}^b) = \mathrm{tr}\,\left((\mathbf{d}^a)^2 (\mathbf{d}^b)^2 - (\mathbf{d}^a \mathbf{d}^b)^2\right). \tag{15}$$

The identity tensor I being in the range of $\mathbb{A}$, it is an eigen tensor of $\mathbb{A}$, one has thus

$$\delta_{ij} = A_{ijkl}\delta_{kl} = A_{iklj}\delta_{kl}$$

where the full symmetry of $\mathbb{A}$ has been used. This reads, without components,

$$I = \mathbf{d}^a \mathbf{d}^a + \mathbf{d}^b \mathbf{d}^b + \mathbf{d}^c \mathbf{d}^c = (\mathbf{d}^a)^2 + (\mathbf{d}^b)^2 + (\mathbf{d}^c)^2,$$

wherefrom directly follows

$$(\mathbf{d}^a)^2 = (\mathbf{d}^a)^4 + (\mathbf{d}^a)^2 (\mathbf{d}^b)^2 + (\mathbf{d}^a)^2 (\mathbf{d}^c)^2. \tag{16}$$

On the other hand, using now the fact that $\mathbf{d}^a$ is an eigen tensor of $\mathbb{A}$, one has

$$d^a_{ij} = A_{ijkl} d^a_{kl} = d^a_{ij} d^a_{kl} d^a_{kl} + d^b_{ij} d^b_{kl} d^a_{kl} + d^c_{ij} d^c_{kl} d^a_{kl}$$

and, using again the full symmetry of $\mathbb{A}$

$$d^a_{ij} = d^a_{ik} d^a_{lj} d^a_{kl} + d^b_{ik} d^b_{lj} d^a_{kl} + d^c_{ik} d^c_{lj} d^a_{kl}$$

so that

$$\mathbf{d}^a = (\mathbf{d}^a)^3 + \mathbf{d}_b \mathbf{d}_a \mathbf{d}_b + \mathbf{d}_c \mathbf{d}_a \mathbf{d}_c$$

and premultiplying with $\mathbf{d}^a$

$$(\mathbf{d}^a)^2 = (\mathbf{d}^a)^4 + (\mathbf{d}_a \mathbf{d}_b)^2 + (\mathbf{d}_a \mathbf{d}_c)^2. \tag{17}$$

Substraction of (17) and (16) yields

$$0 = (\mathbf{d}_a\mathbf{d}_b)^2 + (\mathbf{d}_a\mathbf{d}_c)^2 - (\mathbf{d}^a)^2(\mathbf{d}^b)^2 + (\mathbf{d}^a)^2(\mathbf{d}^c)^2,$$

the trace of which gives, using (15),

$$0 = \| \ [\mathbf{d}^a, \mathbf{d}^b] \ \|_F^2 + \| \ [\mathbf{d}^a, \mathbf{d}^c] \ \|_F^2.$$

As this is a sum of positive terms, both terms are zero, and we have proven that $\mathbf{d}^a$ commutes with $\mathbf{d}^b$ and $\mathbf{d}^c$.

As $(\mathbf{d}^a, \mathbf{d}^b, \mathbf{d}^c)$ are symmetric and commute, there exist an othonormal basis $(r^1, r^2, r^3) \in (\mathbb{R}^3)^3$ such as:

$$\begin{aligned} \mathbf{d}^a &= \alpha_1 r^1 \otimes r^1 + \alpha_2 r^2 \otimes r^2 + \alpha_3 r^3 \otimes r^3 \;\; \alpha_1, \alpha_2, \alpha_3 \in \mathbb{R} \\ \mathbf{d}^b &= \beta_1 r^1 \otimes r^1 + \beta_2 r^2 \otimes r^2 + \beta_3 r^3 \otimes r^3 \;\; \beta_1, \beta_2, \beta_3 \in \mathbb{R} \\ \mathbf{d}^c &= \gamma_1 r^1 \otimes r^1 + \gamma_2 r^2 \otimes r^2 + \gamma_3 r^3 \otimes r^3 \;\; \gamma_1, \gamma_2, \gamma_3 \in \mathbb{R} \end{aligned} \tag{18}$$

We will now show that $r_i \otimes r_i$, $i \in \{1, 2, 3\}$ are eigentensors of $\mathbb{A}$. First, we know that $\mathbf{d}^l$ are orthogonal and of norm 1. So, $((\alpha_1, \alpha_2, \alpha_3), (\beta_1, \beta_2, \beta_3), (\gamma_1, \gamma_2, \gamma_3))$ forms an orthonormal basis of $\mathbb{R}^3$.

Therefore, it exists a unique vector $v \in \mathbb{R}^3$ such as :

$$\begin{pmatrix} \alpha_1 & \beta_1 & \gamma_1 \\ \alpha_2 & \beta_2 & \gamma_2 \\ \alpha_3 & \beta_3 & \gamma_3 \end{pmatrix} v = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \tag{19}$$

and we have

$$v_1\mathbf{d}^a + v_2\mathbf{d}^b + v_3\mathbf{d}^c = r_1 \otimes r_1 \tag{20}$$

As, $\mathbf{d}^l$ are eigentensors of $\mathbb{A}$ assiociated to eigenvalue 1,

$$\begin{aligned} \mathbb{A} : (r_1 \otimes r_1) &= \mathbb{A} : (v_1\mathbf{d}^a + v_2\mathbf{d}^b + v_3\mathbf{d}^c) \\ &= v_1\mathbf{d}^a + v_2\mathbf{d}^b + v_3\mathbf{d}^c \\ &= (r_1 \otimes r_1) \end{aligned} \tag{21}$$

Consequently, $r_1 \otimes r_1$ is an eigentensor of $\mathbb{A}$ assiociated to eigenvalue 1. We can show in the same way that $(r_2 \otimes r_2)$ and $(r_3 \otimes r_3)$ are also eigentensors of $\mathbb{A}$ assiociated to eigenvalue 1.

Thus, as $\mathbb{A}$ is a projector with only three non zero eigenvalues, we finally have :

$$\mathbb{A} = r_1 \otimes r_1 \otimes r_1 \otimes r_1 + r_2 \otimes r_2 \otimes r_2 \otimes r_2 + r_3 \otimes r_3 \otimes r_3 \otimes r_3 \tag{22}$$

Therefore, $\mathbb{A}$ is the representation of the cross with orthogonal directions (r_1, r_2, r_3).

3.2 Recovery

The representation that is advocated here relies heavily on the computation of eigentensors of fourth order tensors. Disappointingly, numerical tools for linear algebra are designed to manipulate vectors and matrices. Hopefully, it is possible to represent symmetric fourth order tensors as matrices.

A fourth order tensor $\mathbb{A}$ endowed with minor symmetry conditions $\mathbb{A}_{ijkl} = \mathbb{A}_{jikl} = \mathbb{A}_{ijlk}$ has 36 independant components. It is useful to write it in the so called Mandel notation as the following matrix 6×6 matrix:

$$A = \begin{pmatrix} \mathbb{A}_{1111} & \mathbb{A}_{1122} & \mathbb{A}_{1133} & \sqrt{2}\mathbb{A}_{1123} & \sqrt{2}\mathbb{A}_{1113} & \sqrt{2}\mathbb{A}_{1112} \\ \mathbb{A}_{2211} & \mathbb{A}_{2222} & \mathbb{A}_{2233} & \sqrt{2}\mathbb{A}_{2223} & \sqrt{2}\mathbb{A}_{2213} & \sqrt{2}\mathbb{A}_{2212} \\ \mathbb{A}_{3311} & \mathbb{A}_{3322} & \mathbb{A}_{3333} & \sqrt{2}\mathbb{A}_{3323} & \sqrt{2}\mathbb{A}_{3313} & \sqrt{2}\mathbb{A}_{3312} \\ \sqrt{2}\mathbb{A}_{2311} & \sqrt{2}\mathbb{A}_{2322} & \sqrt{2}\mathbb{A}_{2333} & 2\mathbb{A}_{2323} & 2\mathbb{A}_{2313} & 2\mathbb{A}_{2312} \\ \sqrt{2}\mathbb{A}_{1311} & \sqrt{2}\mathbb{A}_{1322} & \sqrt{2}\mathbb{A}_{1333} & 2\mathbb{A}_{1323} & 2\mathbb{A}_{1313} & 2\mathbb{A}_{1312} \\ \sqrt{2}\mathbb{A}_{1211} & \sqrt{2}\mathbb{A}_{1222} & \sqrt{2}\mathbb{A}_{1233} & 2\mathbb{A}_{1223} & 2\mathbb{A}_{1213} & 2\mathbb{A}_{1212} \end{pmatrix}. \tag{23}$$

Major symmetry conditions $\mathbb{A}_{ijkl} = \mathbb{A}_{klij}$ ensure that A is symmetric. Factors 2 and $\sqrt{2}$ in (23) allow to write the cross representation as the following usual quadratic form:

$$(x \otimes x)^t \ A \ (x \otimes x) = 1. \tag{24}$$

with

$$x \otimes x = \begin{pmatrix} x_1^2 & x_2^2 & x_3^2 & \sqrt{2}x_2x_3 & \sqrt{2}x_1x_3 & \sqrt{2}x_1x_2 \end{pmatrix}^t.$$

Let us now compute Mandel's representation of the reference cross $\tilde{\mathbb{A}}$ (see (1)):

$$\tilde{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{25}$$

In a previous section, we have shown that only 9 scalar parameters $(a_1, \ldots, a_9)$ are required to represent $\mathbb{A}$. Taking into account symmetries and partial traces, we can write

$$A = \begin{pmatrix} a_1 & & & & & \\ \frac{1}{2}(1 + a_3 - a_2 - a_1) & a_2 & & & \mathrm{SYM} & \\ \frac{1}{2}(1 + a_2 - a_3 - a_1) & \frac{1}{2}(1 + a_1 - a_2 - a_3) & a_3 & & & \\ -\sqrt{2}(a_4 + a_5) & \sqrt{2}a_4 & \sqrt{2}a_5 & 1 + a_1 - a_3 - a_2 & & \\ \sqrt{2}a_6 & -\sqrt{2}(a_6 + a_7) & \sqrt{2}a_7 & -2(a_8 + a_9) & 1 + a_2 - a_3 - a_1 & \\ \sqrt{2}a_8 & \sqrt{2}a_9 & -\sqrt{2}(a_8 + a_9) & -2(a_6 + a_7) & -2(a_4 + a_5) & 1 + a_3 - a_2 - a_1 \end{pmatrix} \tag{26}$$

with the following correspondances between the $\mathbb{A}_{ijkl}$'s and the a_i's:

$$a_1 = \mathbb{A}_{1111} \ , a_2 = \mathbb{A}_{2222}, \ a_3 = \mathbb{A}_{3333},$$

$$a_4 = \mathbb{A}_{2322}\ , a_5 = \mathbb{A}_{2333},\ a_6 = \mathbb{A}_{1311},$$

$$a_7 = \mathbb{A}_{1333}\ , a_8 = \mathbb{A}_{1211},\ a_9 = \mathbb{A}_{1222}.$$

Mandel's notation allows to write tensor contractions as matrix products. For example, $\mathbb{A} : \mathbb{A} = \mathbb{A}$ (see (9)) is written using Mandel's notation as $A \cdot A = A$.

Eigenvectors of A are the eigentensors of $\mathbb{A}$. Their 6 components are the 6 independent entries of eigentensors $\mathbf{d}^k$ that are symmetric second order tensors. The two following MATLAB functions allow to transform fourth order tensors $\mathbb{A}$ into Mandel's form and transform eigenvectors of A into second order tensors. We also see factors of $\sqrt{2}$ that accounts for the symmetry of A.

```
function D = Vec6ToTens2 (v)
    s = 2^(1./2.);
    D = [
       v(1) , v(6)/s , v(5)/s ;
       v(6)/s , v(2) , v(4)/s ;
       v(5)/s , v(4)/s , v(3) ;
        ];
end
```

```
function a = Tens4ToMat6 (A)
  s = 2^(1./2.);
  a = [
      A(1,1,1,1) , A(1,1,2,2) , A(1,1,3,3) , s*A(1,1,2,3), s*A(1,1,1,3), s*A(1,1,1,2) ;
      A(2,2,1,1) , A(2,2,2,2) , A(2,2,3,3) , s*A(2,2,2,3), s*A(2,2,1,3), s*A(2,2,1,2) ;
      A(3,3,1,1) , A(3,3,2,2) , A(3,3,3,3) , s*A(3,3,2,3), s*A(3,3,1,3), s*A(3,3,1,2) ;
      s*A(2,3,1,1) , s*A(2,3,2,2) , s*A(2,3,3,3) , 2*A(2,3,2,3), 2*A(2,3,1,3), 2*A(2,3,1,2) ;
      s*A(1,3,1,1) , s*A(1,3,2,2) , s*A(1,3,3,3) , 2*A(1,3,2,3), 2*A(1,3,1,3), 2*A(1,3,1,2) ;
      s*A(1,2,1,1) , s*A(1,2,2,2) , s*A(1,2,3,3) , 2*A(1,2,2,3), 2*A(1,2,1,3), 2*A(1,2,1,2) ;
      ];
end
```

Note that those MATLAB routines are made for testing and that 3D large codes will only manipulate the 9 nodal unknowns a_i.

Computing 3D cross fields implies to propagate tensors that have known values on the boundary of a 3D domain inside the domain. Assume a tensor $\mathbb{A}$ that has the right structure and that is such that $\mathbb{A} : \mathbb{A} = \mathbb{A}$. With such properties, we know that $\mathbb{A}$ is a rotation of $\tilde{\mathbb{A}}$. The first important issue is about backtracking R from $\mathbb{A}$ i.e. find the three orthonormal column vectors r^q of R that form $\mathbb{A}$ through Equation (4).

An eigentensor $\mathbf{d}^n$ of $\mathbb{A}$ that is associated with eigenvalue 1 is the linear combination

$$\mathbf{d}^n_{ij} = \sum_{q=1}^{3} c_{nq} r^q_i r^q_j.$$

We have

$$\mathbf{d}^n_{im} r^k_m = c_{nk} r^k_i$$

which means that the eigenvectors of $\mathbf{d}^n$ are indeed the r^k's. One issue here could be that $\mathbf{d}^n$ is not of full rank. Yet, the sum

$$\mathbf{d} = \sum_{k=1}^{3} \mathbf{d}^k$$

is of full rank. Eigenvectors of $\mathbf{d}$ are the wanted 3 directions. Assume a representation $\mathbb{A}$ in of the form (26) and let us recover rotation matrix R. The following MATLAB code recovers the rotation matrix R starting from a tensor $\mathbb{A}$ that is a rotation.

```
function R = Tens4ToRotation (A)
    a     = Tens4ToMat6 (A); % transform A into its matrix form
    [V,D] = eig (a)   ; % compute eigenspace
    [X,I] = sort(diag(D)); % sort eigenvalues
    % compute the sum of eigentensors of A associated
    % to eigenvalues equal to 1
    V2      = Vec6ToTens2 (V(:,I(4))+V(:,I(5))+V(:,I(6)));
    [R,d2] = eig(V2); % get rotation matrix R
end
```

This code has been tested to thousands of random rotations, giving the right answer in a 100% robust fashion.

The aim of our work is to build smooth cross fields in general 3D domains. For that, we will solve a boundary value problem for the 9 linearly independant components $(a_1, \ldots, a_9)$ of the tensor representation. Consider two representations X and Y with their representation vectors $(x_1, \ldots, x_9)$ and $(y_1, \ldots, y_9)$ Any smoothing procedure computes (weighted) averages of such representations. For example, representation vector

$$\frac{1}{2}(x_1 + y_1, \ldots, x_9 + y_9)$$

allows to build Mandel's representation $Z = \frac{1}{2}(X + Y)$ that as the same structure as matrix (26).

Assume a cross attitude $A(\alpha, \beta, \gamma)$ that depends on Euler angles α, β and γ. The projection of Z into the space of rotations of the reference cross is defined as the cross attitude A that verifies

$$A = \min_{\alpha,\beta,\gamma} \|A(\alpha, \beta, \gamma) - Z\|.$$

The following function

```
function P = projection (A)
    b_guess = [0 0 0];
    [b_guess(1) b_guess(2) b_guess(3)] = EulerAngles(Tens42Rotation (A));
    vA = Tensor4ToMat6 (A);
    fun = @(x) norm(Tensor4ToMat6(makeTensor (makeEulerRotation (x(1),x(2),x(3))))-vA) ;
    b_min = fminsearch(fun, b_guess);
    P = makeTensor (makeEulerRotation (b_min(1), b_min(2),b_min(3)));
end
```

allows to compute such a projection. In that function, we choose as an initial guess for Euler angles the value computed by `Tens4ToRotation` which uses the eigenspace of A relative to its three largest eigenvalues. Figure 3 shows that this initial guess is indeed a very good approximation of the projection. In reality, it is such a good approximation that it can be used as is without doing the exact minimization.

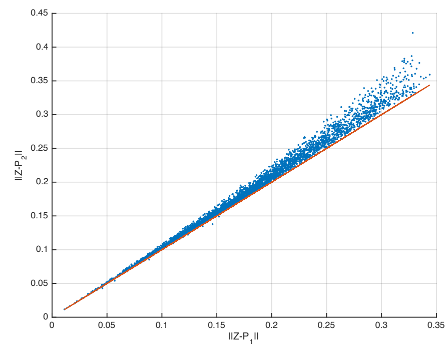

Fig. 3: Projection of 4000 random tensors Z. P_1 is the true projection while P_2 is the approximation computed using function `Tens42Rotation`.

On Figure 3, P_1 is the exact projection while P_2 is the approximation. We see that the approximation P_2 is always very good with respect to the projection, while being extremely simple and fast to compute.

3.3 Relation with spherical harmonics

Harmonic polynomials $h(x)$ are polynomials that are such $\nabla^2 h = 0$. Consider the rotated diced cube polynomial representation

$$\alpha(x) = \sum_{q=1}^{3} (r^q \cdot x)^4$$

We have

$$\nabla^2 \alpha = \sum_{j=1}^{3} \frac{\partial^2 \alpha}{\partial x_j^2} = 12 \sum_{q=1}^{2} (r^q \cdot x)^2 (r_j^q)^2 = 12 \sum_{q=1}^{3} \left[(r^q \cdot x)^2 \left((r_1^q)^2 + (r_2^q)^2 + (r_2^q)^2 \right) \right] = 12 \sum_{q=1}^{3} (r^q \cdot x)^2.$$

The equation $\sum_{q=1}^{3} (r^q \cdot x)^2$ is the one of the unit sphere that is invariant by rotation. Thus,

$$\nabla^2 \alpha = 12 \, |x|^2 \, .$$

Representation polynomial $\alpha(x)$ is thus not harmonic. Yet, acknowledging that

$$\nabla^2|x|^4 = 20|x|^2,$$

we can define the following projection operator of diced cubes onto harmonic polynomials

$$P_{\mathcal{H}_4}(\alpha(x)) = \alpha(x) - \frac{3}{5}|x|^4.$$

Operator $P_{\mathcal{H}_4}$ essentially remove three fifth of a sphere to the diced cube so that the representation retains its symmetry properties while becoming itself harmonic. Let us show that $P_{\mathcal{H}_4}$ is an orthogonal projector with respect to a norm that is related to spherical harmonics. Consider the unit sphere S^2 and compute

$$\int_{S^2} h(x)\left[P_{\mathcal{H}_4}(\alpha(x)) - \alpha(x)\right]dx = -\frac{3}{5}\int_{S^2} h(x)|x|^4 dx = -\frac{3}{5}\int_{S^2} h(x)dx.$$

Harmonic functions are endowed with the mean value property which states that the average of $h(x)$ over any sphere centered at c is equal to $h(c)$. So,

$$\int_{S^2} h(x)\left[P_{\mathcal{H}_4}(\alpha(x)) - \alpha(x)\right]dx = -\frac{3}{5}\int_{S^2} h(0)dx.$$

Harmonic polynomials are homogeneous so $h(0) = 0$ and operator $P_{\mathcal{H}_4}$ is an orthogonal projector onto fourth order spherical harmonics.

As an example, consider our reference diced cube that is represented by $\alpha(x) = x_1^4 + x_2^4 + x_3^4$. Its projection onto $\mathcal{H}_4$ is

$$P_{\mathcal{H}_4}(x_1^4 + x_2^4 + x_3^4) = \frac{2}{5}(x_1^4 + x_2^4 + x_3^4 - 3(x_1^2x_2^2 + x_1^2x_3^2 + x_2^2x_3^2))$$

This is indeed interesting to see that, for $x \in S^2$, we have

$$P_{\mathcal{H}_4}(x_1^4 + x_2^4 + x_3^4) = \sqrt{\frac{12\pi}{7}}\frac{16}{3}\left(\sqrt{\frac{7}{12}}Y_{4,0} + \sqrt{\frac{5}{12}}Y_{4,4}\right)$$

where $Y_{4,j}$, $j = -4, \ldots, 4$ are the orthonormalized real spherical harmonics. In [2], authors define their reference frame as

$$\tilde{F} = \sqrt{\frac{7}{12}}Y_{4,0} + \sqrt{\frac{5}{12}}Y_{4,4}$$

which is to a constant the orthogonal projection of our reference frame onto spherical harmonics.

4 Practical computations

Assume a domain Ω with its non smooth boundary Γ that may contain sharp edges and corners. Our aim is to find a crossfield F that is smooth, and such as for all $x ß \Gamma$, $F(x)$ has one direction aligned to the boundary normal $n(x)$. Here, a simple smoothing procedure that consist in locally averaging cross attitudes at every vertex of a mesh that covers Ω is proposed. The issue of boundary conditions is not treated here.

Let $\mathbf{a}_i \in \mathbb{R}^9$ the representation vector at vertex i. The energy function that is considered is pretty standard

$$E = \frac{1}{2} \sum_{ij} \|A_i - A_j\|_F^2 \tag{27}$$

where $\sum_{ij}$ is the sum over all edges of the mesh and $\|\cdot\|_F$ is the Frobenius norm. The energy is minimized in an explicit fashion. Tensor representations $\mathbf{a}_i \in \mathbb{R}^9$ are averaged at every vertex of the mesh and subsequently projected back to SO(3) in the approximate fashion developped above. The algorith is stopped when the global energy E has decreased by a factor of 10^4.

We have generated three uniform meshes of a unit sphere with different resolutions. Results are presented in Figure 4. The iterations were started with every node assigned to the reference frame aligned with the axis. Crosses with values of η in the range $\eta \in [0.3, 0.5]$ are drawn on the Figures. Figures show the usual polycube decomposition of the sphere with 12 singular lines made of “cylinders” that form an internal topological cube plus 8 singular lines connecting the corners of the topological cube to the surface. Refining the mesh allows to produce more detailed representation of the decomposition. Our method is significantly faster than the ones using spherical hamrmonics thanks to the efficient projection operator that only requires to compute eigenvectors and eigenvalues of 3×3 and 6×6 symmetric matrices.

5 Conclusion

The method to represent and compute crossfields on 3D domains offer a lot of advantages.At first, the new formulation is, to our opinion, way easier to understand geometrically: rotations of tensors, recovery procedures and projections have a clear geometrical representation. Then, we have shown that there exist a one-to-one relationship between our representation and 4th order spherical harmonics. It should be possible to build a 9×9 matrix that allow to change of base. The 4^{th} order tensor representation used allows to approximate in a very efficient way projections on the crosses space $\mathcal{F}$. The direct consequence is a fast resolution of the smoothing problem.

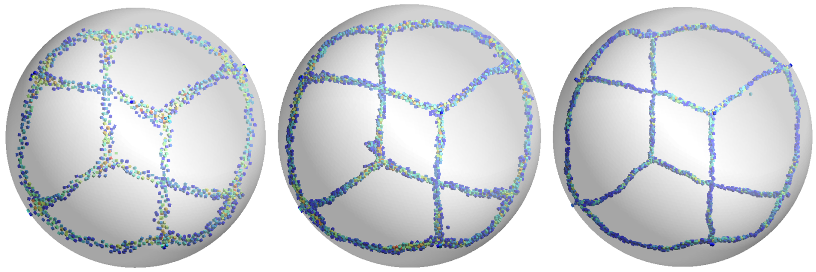

Fig. 4: Computation of cross field on a sphere meshed with tetrahedra. The three meshes used contain respectively 447,405, 2,124,801 and 6,128,555 tetrahedra. Resolution time for reducing the residual from 1 to 10^{-5} was respectively 3 seconds, 34 seconds and 81 seconds.

We are aware that this paper is quite theoretical: way more practical results about this new representation are in our hands: detection of singularities, boundary conditions, norms... Due to page limitations, we have deliberatley made the choice to present basic results. More practical aspects of that new representationas as well as computations of cross fields on complex geometries will appear in furthcoming papers.

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