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Tangent vectors to a 3-D surface normal: A geometric tool to find orthogonal vectors based on the Householder transformation

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ABSTRACT

An important geometric and linear algebraic problem denoted as vector orthogonalization, fundamental to handle contact detection and contact force descriptions in engineering applications, is here considered. The problem is to find a set of linearly independent vectors that span the entire R^3 Euclidean space given only one of the base vectors. This paper contains the explanation on how the Householder transformation, which is extensively used for matrix orthogonalization, provides an elegant analytical expression that solves the vector orthogonalization problem. Based on the QR matrix factorization method, the orthogonal vectors are produced using a Householder reflection that transforms the given vector into a multiple of the unit vector whose entries are all zero with the exception of the first. Based on efficiency, accuracy and numerical robustness criteria, the proposed technique is compared to other vector orthogonalization methods. The numerical results show that the Householder vector orthogonalization formula is the most efficient when it comes to outputting a set of orthonormal vectors, presenting speedups close to 1.017 times faster when compared to other efficient techniques. In addition, when dealing with C^n continuous implicit surfaces, with $n > 1$, the Householder vector orthogonalization formula reveals to be particularly useful for vector calculus since it provides a set of differential operators to calculate, not only the normal, but also the tangent and binormal surface vector fields which can be used to calculate surface curvatures. The major contribution of this paper is to explicitize how the Householder transformation holds an analytical expression that calculates the tangent and binormal vectors from a given normal at a surface point vector, which is computationally efficient and numerically robust for real-time computational geometry and computer graphics applications, namely, for contact mechanics applications with implicit surfaces of engineering problems with multiple contacts. Such a vector orthogonalization technique also has direct applications in several CAD/CAM processes, ranging from the elaboration of rough solid models to the precise manufacturing of a product.

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1. Introduction

In linear algebra, orthogonalization consists of finding a set of orthogonal vectors, called the basis, which spans an entire space or a particular subspace [1]. The vectors that form a basis are linearly independent, meaning that they are mutually orthogonal and that any vector can be expressed as a linear combination of the vectors that compose the basis. To construct a basis considering solely a non-null vector demands an orthogonalization process capable of generating the remaining linearly independent vectors. The operation to build such base vectors is here designated as vector orthogonalization. In $\mathbb{R}^3$ Euclidean space, the vector orthogonalization problem can be stated by the following question:

How to determine a vector that is orthogonal to an explicitly given arbitrary, fixed, real, and non-null 3-D vector?

Such a geometric problem emerges naturally in contact mechanics, not only from the necessity to calculate the minimum distance between surfaces based on the common normal concept [2,3], but also from the need to guarantee continuous control of the tangential friction forces for smooth surfaces [4]. In 3-D contact detection, vector orthogonalization is a frequently used and fundamental operation: each point of contact demands the determination of an orthogonal reference system composed by the normal, tangent and binormal surface vectors which is then used to formulate the minimum distance between surfaces for which the contact force magnitude is directly proportional [5,6]. Since normal reaction and friction forces are time dependent, this referential must be calculated and updated with maximum efficiency. Depending on the complexity of the mechanical system, the number of contact pairs can be small (e.g., articular joint biomechanics [7]), medium (e.g., human biomechanics of impact [8], vehicle crashworthiness

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analysis [9], rail-wheel simulations [10]), or large (e.g., particle collision in geomechanical studies [11,12]) where millions of contact pairs may occur in a single contact detection simulation. Thus, techniques that increase contact detection efficiency are greatly welcomed. Besides contact detection, efficient vector orthogonalization calculation encounters applications in other fields of computational geometry and computer graphics, namely, mesh generation [13], continuation methods for implicit surface polygonization or vector field plotting [14], curve and surface metrics (e.g., perimeter, area, curvature), distance computation between objects [4,15–17], calculation of tangential direction fields [18] and surface fitting [19–21]. As for computer-aided design and manufacturing (CAD/CAM) processes, several applications make use of a vector orthogonalization operation and would benefit from an efficient technique such as shape interrogation [22,23], modeling of generalized cylinders [24,25] and minimizing reference frame computation [26,27].

There are several approaches to orthogonalize a vector. A first and naïve approach for vector orthogonalization consists of encountering a non-collinear vector, $\mathbf{v}$, whose cross-product with a given arbitrary non-null vector $\mathbf{n}$ would provide an orthogonal vector, $\mathbf{t}$, with $\mathbf{v}, \mathbf{n}, \mathbf{t} \in \mathbb{R}^N$. By applying a cross-product between $\mathbf{n}$ and $\mathbf{t}$ a second vector of the base is obtained, $\mathbf{b}$, with $\mathbf{b} \in \mathbb{R}^N$. In order to avoid vanishing vectors or quasi-null vectors, the angle between the given vector, $\mathbf{n}$, and the auxiliary vector, $\mathbf{v}$, must be sufficiently large so that the cross-product does not output a quasi-null vector. An example of this approach is presented in [28] where an orthonormal set in several dimensions is computed based on the cross-product between the given vector and the column of the identity matrix whose unit component value corresponds to the entry of the given vector with the least magnitude. This approach is also applied in [2] where a set of non-collinear vectors is obtained based on the analogy with a square plate mechanism. A second approach for vector orthogonalization consists of writing an orthogonal matrix (e.g., the projection matrix of the given vector, $\mathbf{nn}^T$) and rotating its column vectors so that one of them is collinear to the given vector. Since this matrix is orthogonal, its columns form a basis which can be rotated so that one of the basis vectors becomes aligned with the given vector. By evaluating the angles formed between the given vector and with each of the basis vectors, one can determine the desired rotation by simply choosing a basis vector that makes a sufficiently large angle with the given vector, and the axis of rotation is given by their cross-product. This approach has been used for calculating curvatures of implicit surfaces [29]. Note that these two approaches do not provide a direct mathematical formula for the desired vector base. They rather consist of geometric processes involving testing for eventual singularities and malformed vectors. A third approach consists of applying the first stage of a full form of the QR decomposition to construct an orthonormal basis, namely, a variant that uses either Givens rotations or Householder reflections. These variants output a matrix Q whose first column is collinear to the given vector. As for the most common variant, i.e., the reduced form using the Gram–Schmidt process is not applicable since, by definition, it only outputs a collinear vector when given a matrix with a column form. Among Givens rotations and Householder reflections, the latter is preferable since it exhibits the lowest computational cost for QR decomposition (Givens QR has twice more flop count than Householder QR). Most frequently in the literature, these variants are presented only for square matrices [30] although the decomposition exists for a generic rectangular matrix [31]. Here, the particular case of the input matrix defined as a 3×1 column is considered. A fourth approach for vector orthogonalization, which is only applicable to normal vectors derived from implicit and parametric surfaces, consists of calculating the eigenvalues and eigenvectors of the normal vector gradient (i.e., the Jacobian of the normal vector) since these are the principal curvatures and principal directions at the surface point, respectively [32]. The eigenvectors form an orthogonal basis where one of the vectors is collinear to the given normal. Despite the richness of geometric attributes associated with this approach, it is only valid for C^2 continuous surfaces and solving the eigenvalue/eigenvector problem is computationally costly as it demands the calculation of the Jacobian matrix and to solve the characteristic polynomial. In addition, the eigenvectors are numerical solutions, and thus cannot be directly applied for analytical analyses. All the mentioned approaches are valid for contact detection purposes but only the Householder transformation may provide the continuity control necessary to calculate friction forces in a continuous manner. Therefore, in this paper, the strategy explored to orthogonalize a vector makes use of the transformation proposed by Alston Scott Householder for the inversion of nonsymmetric matrices [33] which offers an explicit proposal to find perpendicular vectors. Such a transformation consists of a matrix that performs a reflection of a vector along a (hyper)plane containing the origin. The (hyper)plane is defined by an auxiliary vector whose components make part of the transformation matrix. Note that a reflection is a special case of an orthogonal transformation. Rotation matrices are another type of orthogonal transformations [1,34]. Numerically, the Householder transformation introduces blocks of zeros into vectors or columns of matrices in an extremely stable manner regarding round-off errors. Due to its column-zeroing functionality, the Householder transformation is extensively used in linear algebra and numerical analysis. Besides QR decomposition, there are several applications of the Householder transformation for solving different mathematical problems formulated as systems of linear equations: upper-triangularization of symmetric and nonsymmetric matrices, computation of determinants, computation of matrix inverses, factorization of matrices (SVD), approximation by linear least squares, and computation of eigenvalues and eigenvectors of real symmetric matrices [1,34,35].

In order to solve the vector orthogonalization problem via Householder transformations, a specific Householder matrix $\mathbf{H}$, with $\mathbf{H} \in \mathbb{R}^{NxN}$, is designed so that it annihilates all elements of a given vector $\mathbf{n}$ (e.g., a normal 3-D vector at a surface point), with the exception of the first, when premultiplied by this matrix. Such a system of equations is equivalent to a set of collinear and orthogonal vector relationships between the given vector $\mathbf{n}$, with $\mathbf{n} \in \mathbb{R}^N \setminus \{\mathbf{0}\}$, and the columns of the matrix $\mathbf{H}$. This set of vector relationships may be written as the linear algebraic equation $\mathbf{Hn} = \lambda \mathbf{e}_1$, with $\lambda \in \mathbb{R}$ and $\mathbf{e}_1 \in \mathbb{R}^N$, where $\mathbf{e}_1$ is the first column of the identity matrix, $\mathbf{I} \in \mathbb{R}^{NxN}$. By making the first column of $\mathbf{H}$ collinear to $\mathbf{n}$, and since $\mathbf{H}$ is orthogonal, the remaining columns are perpendicular to the given vector. So, it is the content of the Householder matrix rather than the reflected vector itself that is of interest to solve the problem.

Note that, for the particular case of $\mathbf{n}$ being a 3-D normal vector to a surface, this Householder transformation discloses an explicit geometric meaning as the second and third columns (or lines) provide formulae for calculating a tangent vector basis to the given 3-D normal vector. This geometric meaning is extremely relevant for contact detection formulations [2] since the system of equations $\mathbf{Hn} = \lambda \mathbf{e}_1$ consists of a set of collinear and orthogonal conditions formulated by the common normal concept [3]. Consequently, this geometric meaning raises a couple of practical questions: (i) given a 3-D normal vector to a surface, $\mathbf{n} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$, which is the vector $\mathbf{h} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$ that defines the Householder matrix that contains the tangent vector basis? (ii) is it possible to deduce an analytical expression for this vector $\mathbf{h}$?

One goal of this paper is to exploit the geometric meaning of the Householder transformation for the vector orthogonalization of the 3-D case and its application framework within contact mechanics, namely, using the formula for improving the efficiency of contact detection methodologies and making use of its analyticity for granting continuous contact forces. Hence, this paper complements a previous work where the Householder reflection or transformation was solely used as an explicit formula readily prepared to be applied for vector orthogonalization within a contact detection methodology [2]. Here, the theoretical background and necessary demonstrations, along with some examples, are presented in order to show the usefulness and to exemplify the purpose of applying the Householder transformation for solving the vector orthogonalization problem. The computational efficiency, numerical robustness, and accuracy of the Householder formula is also investigated by comparing the Householder technique to other vector orthogonalization methods [2,28]. The benchmarked results shall then reveal the most efficient algorithm(s) for vector orthogonalization, an important feature for several engineering applications in which contact detection of extremely large numbers of interactions is necessary [17]. Another goal of this paper is to highlight the utility of the Householder formula to calculate vector tangential vector fields given an implicit surface functional and, consequently, surface curvature. It is indeed an important geometric application of the formula in contact detection with implicit surfaces, as the Householder transformation provides an elegant, straightforward, and analytical formula to calculate a local orthogonal basis of a plane tangential to a surface point, thus finding the tangent and binormal vectors. In fact, the Householder vector orthogonalization formula offers a set of differential operators to calculate the normal, tangent, and binormal vector fields of a given scalar field described by an implicit surface function.

The remainder of this paper is organized as follows. Section 2 provides a brief description of CAD/CAM applications that could benefit from the calculation of orthogonal vectors by the Householder approach. In Section 3, the orthogonal vectorization within the contact mechanics is contextualized revealing the importance of this vectorial operation for calculating the minimum distance between surfaces and for defining contact and friction forces. Section 4 provides the seminal mathematical ideas that led us to consider the Householder transformation as the key object to solve the vector orthogonalization problem in contact detection. Section 5 reviews some preliminaries on orthogonal transformations and on the definition of the Householder transformation, introduces the formula that generates the orthogonal basis, deduces the Householder expression and proves the collinear and orthogonal relationships between the participating vectors. Section 6 introduces a set of non-linear differential operators for calculating the normal, tangent, and binormal vector fields of an implicit surface and also the relation of this transformation with the principal curvature directions. Section 7 presents a numerical evaluation where the Householder formula is compared to other vector orthogonalization techniques in terms of numerical robustness and computational efficiency. Numerical examples and a contact mechanics demonstrative application are given in Section 8. The remaining sections are dedicated to the discussion, to present some conclusions and future prospects.

2. CAD/CAM and vector orthogonalization

The importance of vector orthogonalization within CAD and CAM can be summarized to its intrinsic geometric purpose which consists of establishing an orthogonal reference system given a vector at a spatial point. This point may lie on a geometric object such as a curve, surface, or mesh, while the associated vector is normal or tangent to the geometric object. In order to be useful for CAD applications, this orthogonal reference system must contain numerical and graphical information related to geometric, visualization, and product manufacturing attributes.

There are several concrete CAD applications which benefit directly from vector orthogonalization techniques. Regarding geometric and topological methods for shape and solid modeling, vector orthogonalization techniques are used for computing skeleton edges of free-form solid models [36] and also for modeling generalized cylinders (with applications in hair design [37,38], muscle design [39,40], and other tube-like structures, e.g., ropes, ribbons, strands, braids, knots). In the latter application, reference frames are calculated based on the tangent vector to the drawn 3-D curve [26], and should have minimal twist [27].

Also in CAM processes, vector orthogonalization plays an important role as its tangent vectors are intimately related to differential properties of surfaces, namely, curvature attributes (see Section 6). This is of interest for shape interrogation purposes which is extremely relevant for CAM systems. For instance, shape information is used in manufacturing for calculating cutting path sequences for numerically controlled milling machines, where principal curvature calculations must be performed with the greatest precision to avoid gouging problems and to improve the fairing process [22]. In addition, shape interrogation is required to check if a product satisfies functionality and aesthetic shape requirements [23].

3. Contact mechanics and vector orthogonalization

Within contact mechanics, tracking the continuous evolution of the contact point location, relative velocities, normal and tangential velocities are of utmost importance for appraising the contact forces. Therefore, any valuable vector orthogonalization procedure for contact mechanics applications must not only contribute for accurate and efficient contact detection procedures but also to ensure that the normal force evaluation and the tangential (creep and friction) forces are properly monitored.

Regarding contact detection, the following concept is worth mentioning: the points where two C^1 continuous surfaces make contact or, alternatively, have minimum distance, present normal vectors that share a common direction [3]. Such a geometrical feature is called the common normal concept and it consists of a set of geometric conditions defined as confinement to geometric *loci*, and as collinear and orthogonal vector relationships between the minimum distance vectors jointly with the normal, tangent, and binormal vectors [2,12], namely: collinearity between the distance vector that unites surface points P and Q, $\mathbf{d}_{PQ}$, with the surface normals, $\mathbf{n}_{OP}$ and $\mathbf{n}_{OQ}$ or, equivalently, orthogonal conditions involving surface normal vectors and the tangent vectors $\mathbf{t}_{OP}$ and $\mathbf{t}_{OQ}$. Fig. 1 illustrates the common normal concept for a pair of convex surfaces.

Hence, the common normal concept is crucial for the formulation of contact detection procedures [2,41] as the minimum distance between surfaces is determined by the localization of the surface points that satisfy the common normal conditions. Consequently, the common normal concept is strictly related to vector orthogonalization since the minimum distance between two surfaces requires, for each time instant, the definition of orthogonal reference systems composed by the normal, tangent and binormal surface vectors.

Vector orthogonalization operations are particularly relevant for contact detection procedures that deal with implicit surface representations, since only the normal vector is directly available by taking the gradient of the surface function [3,14]. Contrary to the parametric surface representation, where tangent vector formulae are well-known both in the classical and contemporary literature on Differential Geometry [32] and on Geometric Modeling [42],

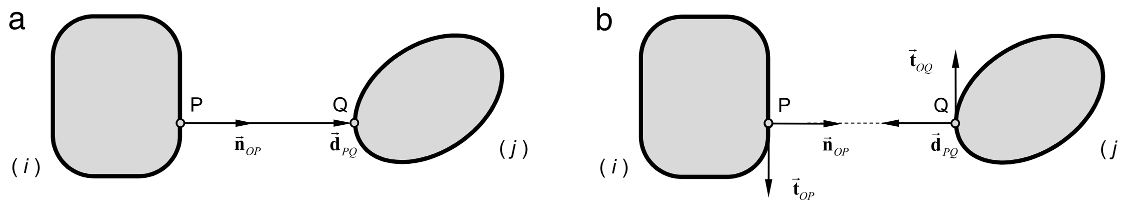

Fig. 1. Orthogonal and collinear vector relationships of the common normal concept established between (a) normal and minimum distance vectors and (b) normal and tangent vectors.

tangent vector formulae for implicitly defined surfaces are not well developed, being harder to find and more scattered throughout the literature in comparison to parametric surfaces. While, for parametric surfaces, tangent and binormal vectors are all obtained by straightforward differential and vector calculus, deriving such vectors recurring to differential operators is not as trivial for the implicit surface case (see Section 6). Thus, defining the explicit formulae of such a geometric attribute for implicit surfaces is valuable for computational geometry, computer graphics and related communities, namely, the computational mechanics community.

The vector orthogonalization procedure must also be accurate since the tangent vectors enter directly in the contact detection formulation. Accuracy is here considered as the value of the inner product between the given normal vector and the computed tangent vectors which must be virtually zero. Any small error in calculating orthogonal vectors may affect the contact points calculation and the contact forces and, ultimately, affect the results obtained from solving the equations of motion.

Regarding force models, one of the continuous approaches to solve contact-impact problems relies on continuous contact and friction force models. These models represent the forces arising from body interactions, assuming that local deformations and, consequently, the forces vary in a continuous manner (i.e., are considered as continuous functions) [4–6]. These forces are then introduced into the equations of motion of the mechanical system as external generalized forces, leading to continuous velocities and accelerations. This promotes a stable numerical integration of the equation of motion and discontinuous disturbances for control are diminished or even nonexistent [43]. The correct knowledge of these forces during the contact process is crucial for the design and analysis of multibody systems. Thus, the geometric information computed by a vector orthogonalization technique (i.e., an orthogonal reference system composed by the normal, tangent and binormal surface vectors) is necessary to efficiently and accurately calculate the contact forces established between two interacting bodies for each contact point, as the normal reaction direction coincides with the surface normals and the friction force direction are written in order to the tangential vector basis vectors [4], as well as other relevant contact quantities. Since reaction and friction forces are time dependent, this referential must be calculated and updated with maximum efficiency, especially for real-time applications [41]. For mechanical systems with bodies in contact describing motions such as sliding or rolling, the contact methodologies must provide a continuous control of the normal and tangential vectors which, consequently, will guarantee continuous force and moment loading due to tangential friction forces.

4. 2-D vector orthogonalization

Finding a perpendicular vector in 2-D Euclidean space has a well-known rule of thumb in computer geometry: just swap the

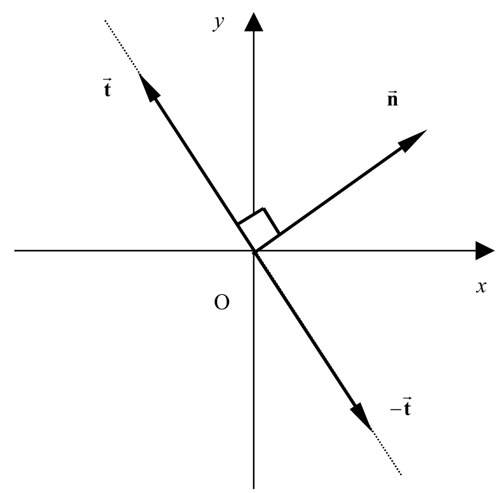

Fig. 2. 2-D vector orthogonalization.

vector components and invert the sign of one of the entries (Fig. 2). More specifically, given an arbitrary, non-null and real valued vector $\mathbf{n} \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$, the orthogonal vectors, $\mathbf{t}$ and $-\mathbf{t}$, with $\mathbf{t} \in \mathbb{R}^2 \setminus \{\mathbf{0}\}$, are obtained by premultiplying $\mathbf{n}$ by one of the following 2×2 real valued generalized permutation matrices, $\mathbf{P}^+$ and $\mathbf{P}^-$:

$$\mathbf{P}^+\mathbf{n} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} n_x \\ n_y \end{bmatrix} = \begin{bmatrix} -n_y \\ n_x \end{bmatrix} = \mathbf{t} \tag{1}$$

$$\mathbf{P}^-\mathbf{n} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} n_x \\ n_y \end{bmatrix} = \begin{bmatrix} n_y \\ -n_x \end{bmatrix} = -\mathbf{t}. \tag{2}$$

The generalized permutation matrices $\mathbf{P}^+$ and $\mathbf{P}^-$ are in fact reflection matrices in which the reflecting line segment (i.e., the 2-D (hyper)plane) makes an angle of $\pm 45°$ with the given vector $\mathbf{n}$. Since the permutation matrix is valid for the 2-D case, it is legitimate to question if there exists a similar or an equivalent transformation to perform vector orthogonalization in 3-D. If such a transformation exists, does it represent a reflection, a rotation, or another type of orthogonal transformation?

Within linear algebra and numerical analysis, the Householder transformation represents the generalization of reflection matrices. To assume that the Householder transformation encloses a highly efficient, accurate and robust solution towards the vector orthogonalization problem, that is capable of satisfying real-time applications, becomes quite a natural hypothesis. Therefore, the purpose is to exploit a formula that is both a non-trivial and elegant way to obtain a vector basis that is orthogonal to an arbitrary vector.

5. 3-D vector orthogonalization

5.1. Orthogonal matrices

Let K be the field of real numbers, and let E be a real vector space over K defined as the three-dimensional Euclidean space $\mathbb{R}^3$. The elements of K are called scalars and the elements of E are called vectors. A vector space E is a set that is closed under finite vector addition and scalar multiplication. In 3-D space, a vector basis is any set of three linearly independent vectors capable of generating the vector space of E and is defined as a subset of vectors $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ in E that are linearly independent and span E.

Central to the problem in question are the definitions of orthogonality for vectors and matrices. Two vectors, $\mathbf{u} \in \mathbb{R}^3$ and $\mathbf{v} \in \mathbb{R}^3$, are said to be orthogonal if they meet at a right angle, i.e., $\mathbf{u}^T\mathbf{v} = 0$. A matrix $\mathbf{Q} \in \mathbb{R}^{3\times 3}$ is orthogonal if its inverse is its transpose. An equivalent characterization of an orthogonal matrix is that its columns form an orthonormal set of vectors $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3 \in \mathbb{R}^3$. Therefore, a matrix is said to be orthogonal if its columns are linearly independent, hence, forming a basis. Orthogonal matrices have several key properties. For instance, by multiplying a vector by an orthogonal matrix the norm of a vector remains invariant, hence, orthogonal matrices preserve Euclidean length. It follows that all eigenvalues of an orthogonal matrix $\mathbf{Q}$ have unit magnitude and, consequently, $|\det(\mathbf{Q})| = 1$.

Geometrically, multiplying a vector by an orthogonal matrix reflects the vector about a plane or rotates it along an axis. In 2-D, these transformations have simple geometric interpretations: reflection matrices reflect an arbitrary vector $\mathbf{n} \in \mathbb{R}^2$ across a rectilinear curve; rotation matrices by premultiplying an arbitrary vector $\mathbf{n} \in \mathbb{R}^2$ produce a vector $\mathbf{Qn}$ that lies at an angle θ to $\mathbf{n}$.

5.2. Householder reflection

The Householder transformation consists of a linear transformation that describes a reflection about a (hyper)plane that contains the origin and sends a chosen axis vector, $\mathbf{h}$, to its negative and reflects all other vectors through the (hyper)plane perpendicular to $\mathbf{h}$. This transformation has the following definition (Fig. 3).

Definition. A mapping $\mathbb{R}^N \to \mathbb{R}^N$, $\mathbf{n} \to \mathbf{Hn}$, for a matrix $\mathbf{H} \in \mathbb{R}^{NxN}$ of the form $\mathbf{H} = \mathbf{I} - 2\mathbf{hh}^T/\mathbf{h}^T\mathbf{h}$, with $\mathbf{h} \in \mathbb{R}^N$, is called a Householder transformation.

Thus, the matricial expression for the 3-D Householder matrix is

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{hh}^T}{\mathbf{h}^T\mathbf{h}} = \begin{bmatrix} 1 - 2\dfrac{h_1^2}{h^2} & -2\dfrac{h_1h_2}{h^2} & -2\dfrac{h_1h_3}{h^2} \\ -2\dfrac{h_1h_2}{h^2} & 1 - 2\dfrac{h_2^2}{h^2} & -2\dfrac{h_2h_3}{h^2} \\ -2\dfrac{h_1h_3}{h^2} & -2\dfrac{h_2h_3}{h^2} & 1 - 2\dfrac{h_3^2}{h^2} \end{bmatrix} \tag{3}$$

where $\mathbf{h} = \begin{bmatrix} h_1 & h_2 & h_3 \end{bmatrix}^T$ and $h = \|\mathbf{h}\|_2$ is the Euclidean norm of vector $\mathbf{h}$.

Note that the Householder matrix results from the sum of two orthogonal matrices: the identity matrix and the projection matrix of $\mathbf{h}$ upon itself. Depending on the coordinate type considered, Eq. (3) can be expressed in either Cartesian or curvilinear coordinates (e.g., polar coordinates).

Table 1 lists the orthogonal matrix properties of the Householder reflection along with the corresponding geometric meaning.

A Householder transformation is geometrically defined as a reflection of $\mathbf{n}$ about the (hyper)plane $H = \{\mathbf{x} \in \mathbb{R}^N : \mathbf{x}^T\mathbf{h} = 0\}$,

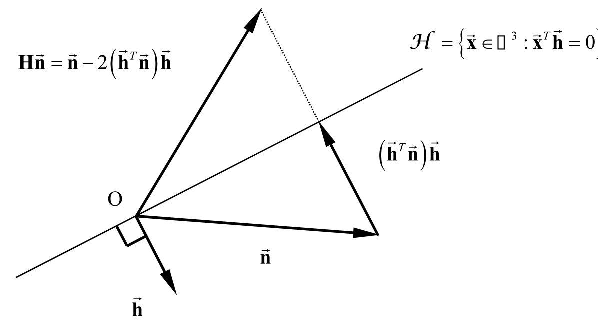

Fig. 3. Householder reflection illustrated on the plane that contains $\mathbf{n}$, $\mathbf{h}$, and $\mathbf{Hn}$. $\mathcal{H}$ defines a mirror (hyper)plane reflecting any vector to the other half (hyper)space.

where $\mathbf{h}$ is the vector whose components define the (hyper)plane. This follows from the vectorial identity obtained by applying the parallelogram law that decomposes the vector $\mathbf{n}$ into a component in the direction $\mathbf{h}$ and into an orthogonal component: $\mathbf{n} - 2(\mathbf{h}^T\mathbf{n})\mathbf{h} = \mathbf{n} - (\mathbf{h}^T\mathbf{n})\mathbf{h} - (\mathbf{h}^T\mathbf{n})\mathbf{h}$ (see Fig. 3). Note that the vectors $\mathbf{n}$, $\mathbf{h}$, and $\mathbf{Hn}$ are coplanar. In particular, if $\mathbf{n} \in \mathbb{R}^N$ and $\mathbf{h}^T\mathbf{n} = 0$, then $\mathbf{Hn} = \mathbf{n}$. If the angle between $\mathbf{n}$ and $\mathbf{h}$ is denoted by φ, then the angle between $\mathbf{h}$ and $\mathbf{Hn}$ is equal to $\varphi + \pi$. From these observations, the vector $\mathbf{Hn}$ is the reflection of $\mathbf{n}$ in the (hyper)plane $\mathcal{H}$.

5.2.1. 3-D Householder vector orthogonalization formula

Within the 3-D vector Euclidean space E, the objective is to obtain a subspace B that spans $E = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, where $\mathbf{e}_i$ are the columns of the identity matrix. Therefore, the solution of the vector orthogonalization problem consists of a base, $B = \{\mathbf{n}, \mathbf{t}, \mathbf{b}\}$, where $\mathbf{n}$ is the explicitly given vector and $\mathbf{t}$ and $\mathbf{b}$ are the desired orthogonal vectors with $\mathbf{n}, \mathbf{t}, \mathbf{b} \in \mathbb{R}^3 \setminus \{\mathbf{0}\}$. In the face of the typical nomenclature used in contact mechanics, vectors, $\mathbf{n}, \mathbf{t}, \mathbf{b}$ are referred to as the normal, tangent, and binormal vectors respectively. Ideally, the base B should have an analytical expression that depends solely on the normal vector, i.e., $B = \{\mathbf{n}, \mathbf{t}, \mathbf{b}\} \Leftrightarrow B(\mathbf{n}) = \{\mathbf{n}, \mathbf{t}(\mathbf{n}), \mathbf{b}(\mathbf{n})\}$, where both tangent and binormal vectors depend on the coordinates of $\mathbf{n}$.

Regarding the case of $\mathbf{n}$ being a 3-D normal vector to a surface, the Householder transformation that sets the normal vector to be collinear with the first column thus discloses an explicit geometric meaning for the second and third columns (or lines) as they provide the formulae for calculating a tangent vector basis to the given 3-D normal vector. This geometric meaning is extremely relevant for contact detection formulations [2] since the system of equations $\mathbf{Hn} = \lambda\mathbf{e}_1$ consists of a set of collinear and orthogonal conditions formulated by the common normal concept [4]. Hence, what remains is to determine the auxiliary vector $\mathbf{h}$ that produces a matrix $\mathbf{H}$ whose rows satisfy the following collinear and orthogonal conditions:

$$\mathbf{n} \parallel \mathbf{h}_1, \qquad \mathbf{n} \perp \mathbf{h}_2 \perp \mathbf{h}_3 \tag{4}$$

where $\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3$ are the columns of the Householder matrix, i.e.,

$$\mathbf{H} = \begin{bmatrix} \mathbf{h}_1 & \mathbf{h}_2 & \mathbf{h}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{h}_1^T \\ \mathbf{h}_2^T \\ \mathbf{h}_3^T \end{bmatrix}. \tag{5}$$

Given the Householder matrix (Eq. (3)) a construction proof of vector orthogonalization is provided hereafter. The analytical formula consists of a matrix whose rows or columns form an orthogonal basis. The overall strategy relies on applying the Householder transformation to zero the $3 - 1$ elements below the first element of a given column vector. Thus, the geometric conditions of collinearity and orthogonality of Eq. (4), written as

Table 1
Orthogonal matrix properties of the Householder reflection matrix. Vectors $\mathbf{u}, \mathbf{v} \in \mathbb{R}^N$ and $\|\cdot\|_2$ represents the Euclidean norm.

Property	Equation	Geometric meaning
H is orthogonal	$\mathbf{H}^T\mathbf{H} = \mathbf{I}$, $(\mathbf{Hu})^T\mathbf{Hv} = \mathbf{u}^T\mathbf{v}$	**H** preserves norms and angles
H is symmetric	$\mathbf{H}^T = \mathbf{H}$, $(\mathbf{Hu})^T\mathbf{v} = \mathbf{u}^T(\mathbf{Hv})$	**H** preserves norms and angles
H is involuntary	$\mathbf{H}^2 = \mathbf{I}$	**H** reflects **u** to its mirror image, a second application of **H** sends it back again
Unitary determinant	$\det(\mathbf{H}) = -1$	**H** turns the unit cube inside out along one axis
Unitary matrix norm	$\|\mathbf{H}\|_2 = 1$	**H** preserves norms

a system of three equations in order to 3 unknowns (i.e., the coordinates of vector $\mathbf{h}$), can be expressed in the matrix form as:

$$\begin{cases}\mathbf{n} \parallel \mathbf{h}_1\\ \mathbf{n}\perp\mathbf{h}_2\\ \mathbf{n}\perp\mathbf{h}_3\end{cases} \Leftrightarrow \begin{cases}\mathbf{h}_1^T\mathbf{n} = \lambda\,\|\mathbf{n}\|_2\\ \mathbf{h}_2^T\mathbf{n} = 0\\ \mathbf{h}_3^T\mathbf{n} = 0\end{cases}$$
$$\Leftrightarrow \begin{bmatrix}\mathbf{h}_1^T\\ \mathbf{h}_2^T\\ \mathbf{h}_3^T\end{bmatrix}\begin{bmatrix}\mathbf{n}\end{bmatrix} = \begin{bmatrix}h_{1x} & h_{1y} & h_{1z}\\ h_{2x} & h_{2y} & h_{2z}\\ h_{3x} & h_{3y} & h_{3z}\end{bmatrix}\begin{bmatrix}n_x\\ n_y\\ n_z\end{bmatrix}$$
$$= \begin{bmatrix}\lambda\,\|\mathbf{n}\|_2\\ 0\\ 0\end{bmatrix} \tag{6}$$

with $\lambda \in \mathbb{R}\setminus\{0\}$ and where $\mathbf{h}$ is the unknown vector for which an analytical expression is desired. Note that, by Eq. (3), $\mathbf{H}$ is not uniquely defined by a single vector $\mathbf{h}$, thus, any non-null multiple of $\mathbf{h}$ defines the same Householder matrix. Therefore, a proper vector $\mathbf{h}$ that defines the desirable Householder matrix $\mathbf{H}$ must be such that $\mathbf{Hn}$ is a nonzero multiple of $\mathbf{e}_1$ and Eq. (6) can be presented in a more compact form as:

$$\mathbf{Hn} = \lambda\,\|\mathbf{n}\|_2\,\mathbf{e}_1. \tag{7}$$

Note that Eq. (7) is essentially the first stage of a QR decomposition using Householder reflections [1,30,35] with $\mathbf{H}$ playing the role of $\mathbf{Q}$ and λ playing the role of $\mathbf{R}$.

Vector $\mathbf{h}$ is chosen so that an arbitrary and non-null (but fixed) vector $\mathbf{n}$ is mapped by $\mathbf{H}$ onto a multiple of the axis vector $\mathbf{e}_1$. The deduction of the associated vector $\mathbf{h}$ that defines the Householder matrix of Eq. (3) has the following two steps: (i) determination of the magnitude and sense of vector $\mathbf{h}$; and (ii) determination of the direction of vector $\mathbf{h}$. The former step is done considering that orthogonal matrices preserve the lengths of vectors, $\|\mathbf{Hn}\|_2 = \|\mathbf{n}\|_2$, thus, there are only two possibilities for λ:

$$\mathbf{Hn} = \|\mathbf{n}\|_2\,\mathbf{e}_1 \vee \mathbf{Hn} = -\|\mathbf{n}\|_2\,\mathbf{e}_1 \;\Rightarrow\; \lambda = \pm 1. \tag{8}$$

The latter step is done recalling that any non-null multiple of $\mathbf{h}$ (e.g., $\tau\mathbf{h}$, with $\tau \in \mathbb{R}\setminus\{0\}$) has the same Householder matrix which is an important result to symbolically determine $\mathbf{h}$:

$$\mathbf{Hn} = \pm\|\mathbf{n}\|_2\,\mathbf{e}_1 \Leftrightarrow \left(I - 2\frac{\mathbf{h}\mathbf{h}^T}{\mathbf{h}^T\mathbf{h}}\right)\mathbf{n} = \pm\|\mathbf{n}\|_2\,\mathbf{e}_1$$
$$\Leftrightarrow \mathbf{n} - 2\frac{\mathbf{h}\mathbf{h}^T}{\mathbf{h}^T\mathbf{h}}\mathbf{n} = \pm\|\mathbf{n}\|_2\,\mathbf{e}_1$$
$$\Leftrightarrow \mathbf{n} - \tau\mathbf{h} = \pm\|\mathbf{n}\|_2\,\mathbf{e}_1$$
$$\Leftrightarrow \tau\mathbf{h} = \mathbf{n} \mp \|\mathbf{n}\|_2\,\mathbf{e}_1 \;\Rightarrow\; \mathbf{h} = \mathbf{n} \mp \|\mathbf{n}\|_2\,\mathbf{e}_1 \tag{9}$$

with

$$\tau = 2\frac{\mathbf{h}^T\mathbf{n}}{\mathbf{h}^T\mathbf{h}}. \tag{10}$$

To ensure that the first component of $\mathbf{h}$ is always non-null for any n_x, the first component of $\mathbf{h}$ must be chosen as the maximal value of the following set:

$$\mu = \max\left(\{n_x - \|\mathbf{n}\|_2\,,\, n_x + \|\mathbf{n}\|_2\}\right) \tag{11}$$

with $n_x \in \mathbb{R}$.

It is also necessary to demonstrate, by symbolic calculus, that the lines (or columns) of the $\mathbf{H}$ matrix form an orthogonal basis in which the first column is collinear to $\mathbf{n}$. If the given vector is written as

$$\mathbf{n} = \begin{bmatrix}n_x & n_y & n_z\end{bmatrix}^T \tag{12}$$

and without loss of generality, by assuming that the norm of vector $\mathbf{n}$ is unitary, $\|\mathbf{n}\|_2 = 1$, and considering vector $\mathbf{h}$ to be

$$\mathbf{h} = \mathbf{n} + \|\mathbf{n}\|_2\,\mathbf{e}_1 = \begin{bmatrix}n_x + \|\mathbf{n}\|_2 & n_y & n_z\end{bmatrix}^T \tag{13}$$

in which the first element of $\mathbf{h}$ is considered as $\mu = n_x + \|\mathbf{n}\|_2$, thus, $h = (2(n_x+1))^{1/2}$, then the first column of $\mathbf{H}$, $\mathbf{h}_1$, is expressed as

$$\mathbf{h} = \mathbf{n} + \|\mathbf{n}\|_2\,\mathbf{e}_1 \Rightarrow \mathbf{h}_1 = \begin{bmatrix}1 - 2\dfrac{h_1^2}{h^2}\\ -2\dfrac{h_1h_2}{h^2}\\ -2\dfrac{h_1h_3}{h^2}\end{bmatrix}$$
$$= \begin{bmatrix}1 - 2\dfrac{(n_x+n)^2}{h^2}\\ -2\dfrac{(n_x+n)\,n_y}{h^2}\\ -2\dfrac{(n_x+n)\,n_z}{h^2}\end{bmatrix} \tag{14}$$

The normal vector and the first column vector are collinear if and only if their cross-product outputs a null vector:

$$\mathbf{n}\times\mathbf{h}_1 = \begin{bmatrix}n_y\left(-2\dfrac{(n_x+n)\,n_z}{h^2}\right) - n_z\left(-2\dfrac{(n_x+n)\,n_y}{h^2}\right)\\ n_z\left(1 - 2\dfrac{(n_x+n)^2}{h^2}\right) - n_x\left(-2\dfrac{(n_x+n)\,n_z}{h^2}\right)\\ n_x\left(-2\dfrac{(n_x+n)\,n_y}{h^2}\right) - n_y\left(1 - 2\dfrac{(n_x+n)^2}{h^2}\right)\end{bmatrix}$$
$$= \begin{bmatrix}n_y\left(-2\dfrac{(n_x+1)\,n_z}{2\,(n_x+1)}\right) - n_z\left(-2\dfrac{(n_x+1)\,n_y}{2\,(n_x+1)}\right)\\ n_z\left(1 - 2\dfrac{(n_x+1)^2}{2\,(n_x+1)}\right) - n_x\left(-2\dfrac{(n_x+1)\,n_z}{2\,(n_x+1)}\right)\\ n_x\left(-2\dfrac{(n_x+1)\,n_y}{2\,(n_x+1)}\right) - n_y\left(1 - 2\dfrac{(n_x+1)^2}{2\,(n_x+1)}\right)\end{bmatrix}$$
$$= \begin{bmatrix}n_y\,(-n_z) - n_z\,(-n_y)\\ n_z\,(-n_x) - n_x\,(-n_z)\\ n_x\,(-n_y) - n_y\,(-n_x)\end{bmatrix} = \begin{bmatrix}0\\0\\0\end{bmatrix} \tag{15}$$

with

$$h = \|\mathbf{h}\|_2 = \sqrt{2(n_x+1)}. \tag{16}$$

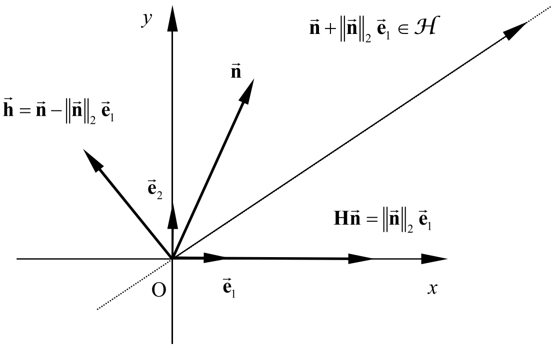

Fig. 4. The desired Householder matrix transforms $\mathbf{n}$ into a multiple of $\mathbf{e}_1$.

Since $\mathbf{h}_1$ is collinear to $\mathbf{n}$ then, by the property of matrix orthogonality, the second and third columns of $\mathbf{H}$, $\mathbf{h}_2$ and $\mathbf{h}_3$, are also perpendicular to $\mathbf{n}$. Consequently, the tangent and binormal vectors can be considered as the second and third columns of $\mathbf{H}$, respectively.

In geometrical terms, as represented in Fig. 4, this result can be rephrased by stating that for any vector $\mathbf{n}$ there exists a $(3-1)$-dimensional (hyper)plane $\mathcal{H}$ passing through the origin in $\mathbb{R}^3$ such that the reflection $\mathbf{Hn}$ of $\mathbf{n}$ in $\mathcal{H}$ is equal to a nonzero multiple of $\mathbf{e}_1$. To find H it suffices to identify a vector $\mathbf{h} \in \mathbb{R}^3$ normal to $\mathcal{H}$. Since $\mathbf{H}$ is unaffected by rescaling $\mathbf{h}$, the length of $\mathbf{h}$ is immaterial. As mentioned previously, the vectors $\mathbf{Hn}$, $\mathbf{n}$ and $\mathbf{h}$ are coplanar. Therefore, $\mathbf{h}$ is a suitable linear combination of $\mathbf{n}$ and $\mathbf{e}_1$.

It has been shown that the process of vector orthogonalization may consist in transforming a vector by applying an operation of reflection, but the same result could be obtained from a rotation. Recall that the product of two reflections gives a rotation matrix as stated by the theorem of Cartan [32,33]: every orthogonal transformation in $\mathbb{R}^N$ can be expressed as a product of at most N simple reflections by (hyper)plane. Determining such rotation matrices is outside the scope of this paper.

5.3. Algorithm for 3-D vector orthogonalization

Table 2 presents the pseudo-code to calculate the Householder matrix for vector orthogonalization in 3-D Euclidean space. The only input is the non-null, fixed, and real valued vector $\mathbf{n} = [n_x\ n_y\ n_z]^T$. Note that step 1.2 of the algorithm (Table 2) ensures that the first component of $\mathbf{h}$ is always non-null.

Table 2
Pseudo-code for 3-D Householder vector orthogonalization.

1. Determine vector $\mathbf{h}$:
   1.1 Calculate the Euclidean norm of the given vector, $n = \|\mathbf{n}\|_2$;
   1.2 Determine the first component of $\mathbf{h}$: $h_1 = \max(\{n_x - n, n_x + n\})$;
   1.3 Define $h_2 = n_y$ and $h_3 = n_z$;
2. Determine matrix $\mathbf{H} = [\mathbf{h}_1\ \mathbf{h}_2\ \mathbf{h}_3]$:
   2.1 Calculate the Euclidean norm of $\mathbf{h}$, $h = \|\mathbf{h}\|_2$;
   2.2 Use the analytical expression of $\mathbf{H}$ to calculate the matrix:

$$\mathbf{H} = \mathbf{I} - 2\frac{\mathbf{h}\mathbf{h}^T}{\mathbf{h}^T\mathbf{h}} = \begin{bmatrix} 1 - 2\dfrac{h_1^2}{h^2} & -2\dfrac{h_1 h_2}{h^2} & -2\dfrac{h_1 h_3}{h^2} \\ -2\dfrac{h_1 h_2}{h^2} & 1 - 2\dfrac{h_2^2}{h^2} & -2\dfrac{h_2 h_3}{h^2} \\ -2\dfrac{h_1 h_3}{h^2} & -2\dfrac{h_2 h_3}{h^2} & 1 - 2\dfrac{h_3^2}{h^2} \end{bmatrix}.$$

3. Set the tangent, $\mathbf{t}$, and binormal, $\mathbf{b}$, vectors as the 2nd and 3rd column of $\mathbf{H}$, respectively: $\mathbf{t} = \mathbf{h}_2$ and $\mathbf{b} = \mathbf{h}_3$.

6. Differential operators for calculating normal, tangent, and binormal vector fields of implicit surfaces

Several areas of mathematics and engineering make use of the implicit object definition to represent the geometric *loci* of curves and surfaces [3,14,44]. Implicit geometric objects are defined by a scalar functional $\mathsf{F}(x)$, $\mathsf{F} : \mathbf{x} \in \mathbb{R}^3 \to \mathbb{R}$ (either a Euclidean or non-Euclidean spatial metric), and the curve or surface is the set of points, $\mathbf{x}$, that satisfy a level-set equation, e.g., $\mathsf{F}(\mathbf{x}) = 0$. In vector calculus, for an implicitly defined surface, the normal vectors are obtained by differentiation of the surface function in order to the spatial coordinates. When considering Cartesian coordinates, the normal vectors are, by definition, the variation of the surface functional in the x, y, and z directions. These first order spatial variations are gathered together forming the gradient operator. This opens the way to apply the Householder vector orthogonalization formula (see Eqs. (3) and (9)) to the surface gradient vector leading to the deduction, by symbolic calculus, of a set of non-linear differential operators that provide tangential vector fields to an implicit surface. These non-linear differential operators are directly obtained by symbolic substitution of the gradient vector components into the Householder formula. In this manner, the operators are expressed in order to the first order differential terms along x, y, and z, i.e., $\partial/\partial x$, $\partial/\partial y$, and $\partial/\partial z$ (see Example 4 in Section 8). Therefore, the Householder transformation provides, in an explicit fashion, an analytic formula of geometric attributes related to tangential vectors of an implicit surface. Obviously, these operators are only valid for implicit objects that are at least C^1 continuous.

Since differential operators are available to compute tangent vector fields to an implicit surface, an immediate application consists of determining the curvature at a point. The link between the tangential vectors and the curvature is given by the following expression:

$$k_{\mathbf{w}} = -\frac{\mathbf{w}^T \nabla\nabla F \mathbf{w}}{\|\mathbf{n}\|_2} \tag{17}$$

where $\mathbf{w} \in \mathbb{R}^3$ is a unit vector that belongs to the tangent plane at the surface point, $\nabla\nabla\mathsf{F} \in \mathbb{R}^{3\times3}$ is the Hessian matrix of the implicit function, and $\mathbf{n}$ is the normal vector or gradient of the implicit function at the surface point [36]. An interesting topic that naturally arises consists of determining if the tangent vectors computed with the Householder formula are or are not principal curvature directions. Vector $\mathbf{w}$ can be expressed as a linear combination of the orthonormal basis defined by the Householder formula,

$$\mathbf{w}(\theta) = \cos(\theta)\,\mathbf{t} + \sin(\theta)\,\mathbf{b} \tag{18}$$

where $\theta \in [0, 2\pi[$ is the angular deviation of $\mathbf{w}$ from the tangent base vectors. If θ is a principal curvature direction then it must zero the derivative of $k_{\mathbf{w}}$ in order to θ, i.e., the maxima and minima of $k_{\mathbf{w}}$ are given by

$$\frac{dk_{\mathbf{w}}}{d\theta} = 0 \Leftrightarrow \tan(2\theta) = \frac{2\mathbf{t}^T \nabla\nabla\mathsf{F}\,\mathbf{b}}{\mathbf{t}^T\nabla\nabla\mathsf{F}\,\mathbf{t} - \mathbf{b}^T\nabla\nabla\mathsf{F}\,\mathbf{b}} = M$$
$$\Leftrightarrow \left(\theta = \theta_1 = \frac{\arctan M}{2}\right) \vee \left(\theta = \theta_1 + \frac{\pi}{2}\right). \tag{19}$$

Assuming that $\mathbf{t}$ and $\mathbf{b}$ are principal curvature directions, then the angular deviation is equal to zero. This assumption implies that

$$\arctan M = 0 \Leftrightarrow \mathbf{t}^T\nabla\nabla\mathsf{F}\,\mathbf{b} = 0 \Leftrightarrow \mathbf{t}^T\mathbf{q} = 0 \tag{20}$$

with $\mathbf{q} = \nabla\nabla\mathsf{F}\,\mathbf{b}$. Since $\mathbf{t}$ and $\mathbf{b}$ are orthogonal, in order to $\mathbf{q}$ to maintain vector orthogonality with $\mathbf{t}$, the Hessian matrix must be a full scalar matrix, i.e.,$\nabla\nabla\mathsf{F} = \lambda\mathbf{I}$ with $\lambda \in \mathbb{R}$, or a scalar matrix with some diagonal entries equal to zero. The plane, sphere and cylinders (e.g., spherical, parabolic, and hyperbolic cylinders) are examples of such surfaces. However, in general, the Householder vectors do not correspond to the principal curvature directions

Table 3
Speedup ratios between the considered vector orthogonalization techniques, taking HH as the baseline. The CPU time variance of the considered vector orthogonalization techniques is also shown. (IQM—interquartile range).

	Householder	Eberly	Square plate	Projection matrix
Speedup	–	1.017	2.795	7.527
IQM	3.49×10^{-7}	3.48×10^{-7}	1.05×10^{-6}	2.79×10^{-6}

since Eq. (20) does not hold for the vast majority of Hessian matrices, thus, the orthonormal basis defined by the Householder formula presents an angular deviation that varies throughout the surface.

7. Numerical evaluation of vector orthogonalization techniques

A series of numerical tests was carried out to compare, in terms of computational efficiency, numerical accuracy and numerical robustness, the Householder formula with other vector orthogonalization techniques. For practical purposes, the considered techniques, which have been briefly described in the introduction, are here called as Householder (HH), Eberly (EB) [28], Square Plate (SP) [2], and Projection Matrix (PM) [29]. The numerical tests consisted of calculating real-valued tangent and binormal vectors for a set of 10^5 unitary vectors in $\mathbb{R}^3$. The input vectors were randomly calculated with a uniformly distributed pseudorandom number generator. CPU execution times to compute both tangent and binormal vectors were then measured. Whenever possible, symbolic calculations were performed upon the vector orthogonalization expressions in order to find a simplified expression with the minimum number of floating-point operations per second (FLOPS) (see the Appendix). Each expression was further simplified having in consideration that the input vectors were unitary. By direct examination of the analytical and numerical expressions, the considered vector orthogonalization techniques revealed to be numerically robust since no type of indetermination occurs (e.g., $1/0, 0/0, 0\times\infty, \pm\infty, \sqrt{-1}$). A statistical analysis was performed upon the measured CPU times and relative speedups. Finally, the accuracy (i.e., the value of the inner product between the given normal vector and the computed tangent vectors) of each technique was also calculated to verify how close the products $\mathbf{n}^T\mathbf{t}$, $\mathbf{n}^T\mathbf{b}$ and $\mathbf{t}^T\mathbf{b}$ are to zero. Table 3 lists the speedups (defined as the ratio between the 10% trimmed mean execution time of the EB, SP, PM and HH) and the interquartile ranges of each vector orthogonalization technique. These measures are robust to outliers, and thus, are statistically representative of the time data. Table 4 lists the average and variance accuracy measures for the considered battery of unit vector sets. The vector orthogonalization code was developed in MATLAB® R2009b and ran on a PC with an Intel® Core™i7 CPU 870 @ 2.93 GHz processor with 8 GB of RAM. All the calculations and CPU time measures were performed with double precision. As a special remark, the same numerical test was performed using MATLAB®'s qr (·) command [45], which computes the **Q** and **R** matrices using Householder reflectors generating a full form QR decomposition, presenting a speedup value of approximately 2.20 and similar accuracy statistics in the order of 10^{-18}.

8. Examples

Four examples of the use of the Householder reflection formula for vector orthogonalization (Eqs. (3) and (9)) and an example in contact mechanics are presented in this section. The first example illustrates the orthogonalization of an arbitrary vector. The second example consists of a vector contained within the *xOy* plane giving rise to a permuted vector (Eq. (2)) and the *z* canonical base vector (for a Euclidean space), while the third example contemplates the application of the formula to a canonical base vector which gives rise to an orthonormal basis. The fourth example can be regarded as the application of the derived differential operators to a generic implicit surface that is C^n continuous, with $n > 1$. This example is supplemented with Fig. 5 that illustrates the normal, tangent and binormal surface vector fields (or superficial direction fields) for some members of the quadric surface family. The final example consists of a demonstrative application representing a ball rolling inside a spherical bowl (i.e., two spheres in a conformal contact configuration). The objective of this example is to emphasize the points mentioned above in Section 3 regarding the applicability of the Householder transformation in contact mechanics and its merits to realistically simulate the motion of a mechanical system.

Table 4
Accuracy statistics of the considered vector orthogonalization techniques. (TM—10% trimmed mean; IQM—interquartile range).

		Householder	Eberly	Square plate	Projection matrix
TM	$\mathbf{n}^T\mathbf{t}$	1.69×10^{-19}	-1.71×10^{-20}	-1.95×10^{-18}	-3.51×10^{-18}
	$\mathbf{n}^T\mathbf{b}$	1.15×10^{-19}	-2.91×10^{-19}	1.83×10^{-18}	2.36×10^{-19}
	$\mathbf{t}^T\mathbf{b}$	-5.92×10^{-20}	1.62×10^{-20}	-2.41×10^{-19}	7.86×10^{-19}
IQM	$\mathbf{n}^T\mathbf{t}$	8.33×10^{-17}	0	3.47×10^{-18}	1.11×10^{-16}
	$\mathbf{n}^T\mathbf{b}$	1.11×10^{-16}	5.55×10^{-17}	2.47×10^{-19}	1.11×10^{-16}
	$\mathbf{t}^T\mathbf{b}$	2.78×10^{-17}	0	1.39×10^{-18}	1.11×10^{-16}

Example 1. Consider the non-null vector $\mathbf{n} = [-2.500, 10.02, 3.960]^T$. The auxiliary vector is equal to $\mathbf{h} = [8.560, 10.020, 3.960]^T$ and the corresponding Householder matrix is given by

$$\mathbf{H} = \begin{bmatrix} 0.226 & -0.906 & -0.358 \\ -0.906 & -0.060 & -0.419 \\ -0.358 & -0.419 & 0.834 \end{bmatrix}.$$

Example 2. Consider the non-null vector $\mathbf{n} = [1.500, -0.200, 0.000]^T$. The auxiliary vector is equal to $\mathbf{h} = [3.013, -0.200, 0.000]^T$ and the corresponding Householder matrix is given by

$$\mathbf{H} = \begin{bmatrix} -0.991 & 0.132 & 0.000 \\ 0.132 & 0.991 & 0.000 \\ 0.000 & 0.000 & 1.000 \end{bmatrix}.$$

Example 3. Consider the versor $\mathbf{n} = [0.000, 1.000, 0.000]^T$. The auxiliary vector is equal to $\mathbf{h} = [1.000, 1.000, 0.000]^T$ and the corresponding Householder matrix is given by

$$\mathbf{H} = \begin{bmatrix} 0.000 & -1.000 & 0.000 \\ -1.000 & 0.000 & 0.000 \\ 0.000 & 0.000 & 1.000 \end{bmatrix}.$$

Example 4. Consider the normal of a $C^n, n > 1$, continuous surface implicitly defined. Given the functional expression of the implicit surface, $\mathsf{F}(\mathbf{x}) : \mathbb{R}^3 \to \mathbb{R}$, whose zero-level defines a set of surface points $\partial\Omega = \left\{\mathbf{x} = \begin{bmatrix} x & y & z \end{bmatrix}^T \in \mathbb{R}^3 : \mathsf{F}(\mathbf{x}) = 0\right\}$, the normal vector is derived as

$$\mathbf{n} = \nabla \mathsf{F}(x, y, z) = \begin{bmatrix} \mathsf{F}_x & \mathsf{F}_y & \mathsf{F}_z \end{bmatrix}^T.$$

The auxiliary vector comes as

$$\mathbf{h} = \begin{bmatrix} \mu & \mathsf{F}_y & \mathsf{F}_z \end{bmatrix}^T,$$

with

$$\mu = \max\left(\left\{\mathsf{F}_x - \|\nabla\mathsf{F}\|_2, \mathsf{F}_x + \|\nabla\mathsf{F}\|_2\right\}\right).$$

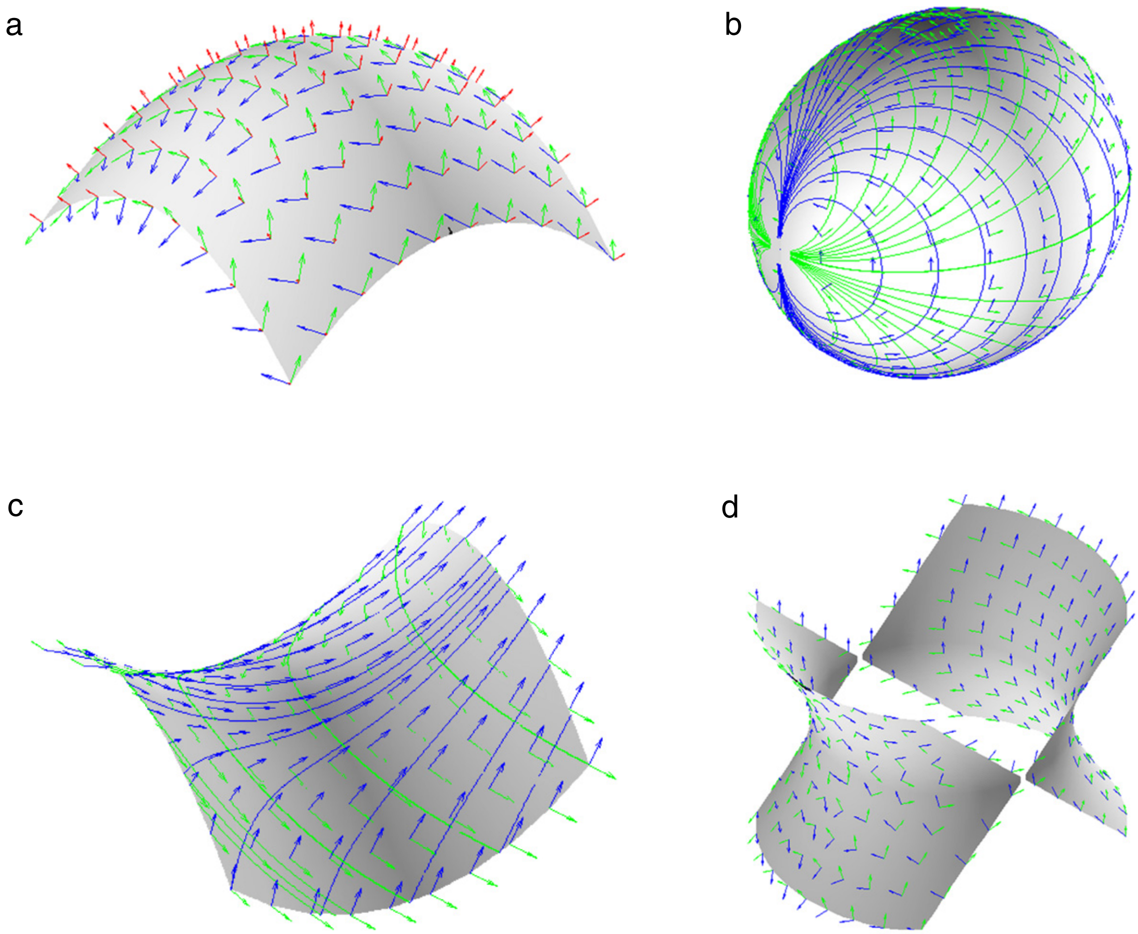

Fig. 5. Superficial direction fields defined by the normal (red), tangent (green), and binormal (blue) vectors. (a) Elliptic paraboloid (radii: 1.0, 1.0); (b) ellipsoid with tangent and binormal streamlines (radii: 0.5, 0.4, 0.45); (c) hyperbolic paraboloid with tangent and binormal streamlines (radii: 1.0, 1.0); (d) one sheet hyperboloid (radii: 1.0, 1.0, 1.0). Radii are listed for the *x*, *y*, and *z* directions of the canonical quadric representation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Consequently, the Householder's analytical expression is written as

$$\mathbf{H} = \begin{bmatrix} 1-2\dfrac{\mu^2}{h^2} & -2\dfrac{\mu \mathsf{F}_y}{h^2} & -2\dfrac{\mu \mathsf{F}_z}{h^2} \\ -2\dfrac{\mu \mathsf{F}_y}{h^2} & 1-2\dfrac{\mathsf{F}_y^2}{h^2} & -2\dfrac{\mathsf{F}_y \mathsf{F}_z}{h^2} \\ -2\dfrac{\mu \mathsf{F}_z}{h^2} & -2\dfrac{\mathsf{F}_y \mathsf{F}_z}{h^2} & 1-2\dfrac{\mathsf{F}_z^2}{h^2} \end{bmatrix},$$

with

$$h = \sqrt{\mu^2 + \mathsf{F}_y^2 + \mathsf{F}_z^2}$$

where the first, second and third columns can be assigned as $D_{\mathbf{n}}(\mathsf{F}(\mathbf{x}))$, $D_{\mathbf{t}}(\mathsf{F}(\mathbf{x}))$, and $D_{\mathbf{b}}(\mathsf{F}(\mathbf{x}))$, respectively. Hence, given the implicit surface function F and a specific level-set, it is possible to visualize the set of orthogonal vector fields defined by $D_{\mathbf{n}}(\mathsf{F}(\mathbf{x}))$ and corresponding tangential vectors $D_{\mathbf{t}}(\mathsf{F}(\mathbf{x}))$ and $D_{\mathbf{b}}(\mathsf{F}(\mathbf{x}))$. Fig. 5 illustrates the vector fields of the surface's gradient orthogonal basis for an elliptic paraboloid, ellipsoid, hyperbolic paraboloid and a one sheet hyperboloid. As expected, both tangent and binormal vector fields define tangential direction fields upon the surfaces which, by numerical integration, draw surface curves defined as streamlines [18] that are orthogonal trajectories, as shown in Fig. 5(b)–(c). Note that, at each point throughout the surface, the basis vectors are everywhere orthogonal but are rotated along the normal vector direction. Although vector orthogonalization is performed locally, the tangent and binormal vector fields are globally consistent. This vectorial aspect is related to the angular deviation of the Householder tangent vectors from the principal curvature directions as discussed in Section 6.

Example 5. The demonstrative application considered is a simple contact system which consists of a small ball rolling inside a spherical bowl (see Fig. 6). The bowl is made of PTE, has a radius of 1.0 m and is assumed to have infinite mass, thus, is considered rigid and stationary. The ball is a homogeneous sphere made of PTFE, with a mass of 1.0 kg, a radius of 0.1 m, a moment of inertia equal to 0.01 kgm^2, an equivalent stiffness equal to 140×10^6 N/m$^{3/2}$, a coefficient of restitution equal to 0.9, and a Coulomb friction of 0.01. The ball is released from a point on the equator of the bowl with an initial *y*-angle and *y*-angular velocity of 10.0 rad and 9.0 rad/s, respectively, and rolls under the action of gravity, which acts in the negative *z* direction, and contact forces which are modeled based on the Hunt and Crossley contact [6] and Coulomb friction [4] models. Therefore, the ball rolls (and eventually slides) throughout the bowl in a descending spiral path until it lands on the lowest point of the bowl, where it then slightly bounces until losing all its mechanical energy due to damping and frictional energy dissipation. This example clearly benefits from the continuity of the tangential and binormal vector fields ensured by the Householder method, since rolling (and sliding) demands

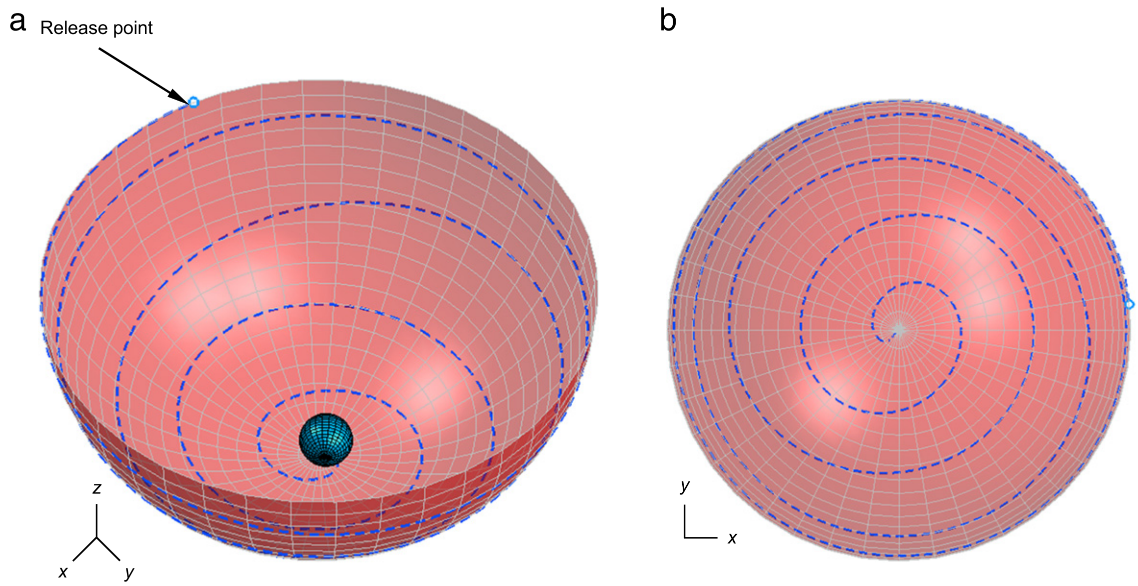

Fig. 6. The rolling ball inside a bowl example. (a) When the ball is released with an initial angular velocity it describes a descending spiral path. (b) Top view of the bowl where the spiral form of the ball's path is more evident.

a continuous evaluation of the tangential (creep and friction) forces.

9. Discussion

The generalized 2-D permutation matrix serves as a motto for the assumption that orthogonal transformations may offer a potential solution for the vector orthogonalization problem. In this paper, it is shown how the orthogonal transformation defined by Householder [33] holds as an efficient, accurate and elegant analytical expression that solves this problem for a diverse range of applications. One of the motivations of this work is to explicitize an expression that calculates the tangent and binormal vectors from a given normal at a surface point, and that must be a computationally efficient and robust expression for contact detection and normal and tangential force calculations in applications with implicit surfaces.

The numerical tests (Table 3) indicate that every vector orthogonalization technique has small interquartile range values, thus, the measured times do not fluctuate much around their mean value making it reliable to compare speedups among the different techniques. More importantly, the results indicate that, on average, the Householder formula is the most efficient from all considered vector orthogonalization techniques. Although both HH and EB techniques show similar computational performance and are both simple algorithms, the former technique achieves speedups that are close to 1.017 times better (Table 3). This slight difference (1.7%) can be significant when translated to time savings for mechanical systems with thousands or even millions of contact pairs that happen in a single time instant of a dynamic simulation [11,12]. The 1.7% speedup is intimately related to the number and type of floating-point operations involved: while HH presents an additional 2 summations and 2 multiplications EB has 1 division more, 2 moduli, and, detrimentally, 1 square root which justifies the higher computational time as such a flop consists of a costly operation. Note that HH is more efficient when considering a unit vector as input but not as efficient for an arbitrary vector. In this case, EB presents lesser FLOPS (e.g., compare HH formula in Table 2 with the following EB tangent vector expressions (assuming $|n_x| \geq |n_y|$): $\mathbf{t} = [-n_z, 0, n_x]^T$ and $\mathbf{b} = [n_y n_x, -n_z^2 - n_x^2, n_y n_z]^T$). The drawback is that EB applied to arbitrary vectors does not guarantee that the output vectors are unitary, while for HH the computed tangents are always unit vectors which is an advantageous feature since it is not necessary to normalize them afterwards. Regarding the SP and PM techniques, these are less efficient as they require a greater number of FLOPS. Contrary to the SP and MP techniques, the Householder formula does not consist of an intricate geometric process involving vector testing. Note that the same numerical evaluation but with increased number of inputs were also run, showing that independently of the number of vectors tested the observed speedups remained greater than 1.0 with respect to HH (results not presented). As for MATLAB®'s qr $(\cdot)$ command performance, although the software uses compiled LAPACK routines for its basic linear algebra computations, the code is not fully optimized for 3×1 input matrices, hence, the large speedup comparative to the implemented HH. Relative to vector orthogonalization accuracy, all methods revealed to be very accurate with inner product values virtually equal to zero (10^{-20}–10^{-18}).

One of the culminating points of the Householder formula is that its analyticity offers a useful symbolic expression to deduce a set of differential operators to calculate tangential vector fields to a surface. From the standpoint of implicit surfaces, the Householder transformation provides explicitly analytic formulae for other geometric attributes defined with tangential vectors, namely, principal curvature directions and associated curvatures. These attributes are extremely important geometric quantities for CAD/CAM processes ranging from the elaboration of rough solid models to the precise geometric description of a product, such as shape interrogation [22,23], and minimizing reference frame computation [26,27], which may benefit from using the Householder vector orthogonalization approach. The tangential differential operators are of great interest for linear algebra, vector calculus, differential geometry or multivariate calculus, and can come in handy in different physical areas that are mathematically formulated based on field theory, such as electromagnetism and continuum mechanics. Apparently the practicality and applicability of the Householder reflection in computer graphics, geometry design and CAM is yet to be explored and expanded to other geometric and algebraic problems. Note that the theoretical results here presented are extendible for $\mathbb{R}^P$, $P > 3$.

As future works, it would be interesting to instigate about the following matters: (i) to determine the Householder matrices that, when premultiplying the normal vector, give raise to tangent vectors; (ii) to better understand the tangential streamlines that are traced upon a surface given by the tangent vector fields of an implicit surface; (iii) to explore other orthogonal transformations such as the exponential matrix which generalizes every orthogonal transformation; (iv) to determine the rotation matrices that are equivalent to the reflection matrix; (v) to explore similar theoretical and numerical results for the EB formula; and (vi) to perform more in-depth analysis regarding differential geometry applications of the Householder formula.

10. Conclusion

This paper presents interesting results, application framework and extensions of the Householder reflection matrix with the explicitation of the associated formula to calculate tangent and binormal vectors given a normal vector. To the authors' knowledge, this explicit description of the use of the Householder transformation to orthogonalize 3-D vectors and its application to contact mechanics does not appear to be elsewhere. The formula is simple, efficient, and numerically robust for geometric and linear algebraic problems. The applicability of the Householder formula as an efficient geometric tool in contact mechanics with implicit surfaces is emphasized and demonstrated, as it provides the orthonormal set of tangential vectors that enters the minimum distance calculations and a continuous control of the tangential force functions. Although computing orthogonal vectors is a quite basic operation, the advantages of the Householder technique are highlighted by introducing benchmark results in which a numerical evaluation is performed in order to compare the Householder method with other alternative vector orthogonalization techniques, based on numerical robustness, accuracy and computer efficiency. The analytical expressions of the considered techniques reveal that they are all numerically robust and accurate, but the Householder technique is shown to be the most efficient compared to the other standard methods. In addition, it is possible to directly apply the Householder formula to deduce, analytically, differential operators to compute tangent vectors to an implicit surface, hence, also surface streamlines that are orthogonal to each other. In addition, these tangent vector fields can be used to calculate the principal curvature directions of implicitly defined surfaces. Such a vector operation may find other applications in mesh generation, surface streamline calculation, surface fitting with implicit surfaces, surface analysis or shape interrogation.

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Appendix

This section presents the vector orthogonalization techniques in an algorithmic form when considering unit vectors as inputs (Tables A.1–A.4). In particular, the HH and EB vector orthogonalization techniques are written with the minimum number of FLOPS. As for the SP and PM, no simplified expressions were deduced due to the intricate complexity of the involved vector and matrix operations. Note that the input unit vector is given by $\mathbf{n} = [n_x, n_y, n_z]^T$, and each method outputs normalized tangent and binormal vectors. In addition, the amount of FLOPS is compared for the HH and EB techniques (Table A.5).

Table A.1
Pseudo-code for unit vector HH orthogonalization.

1. Evaluate the sign of the unit's vector first component, i.e., $\mathrm{sign}(n_x)$;
2. Determine the tangent vector with the following simplified expression:

$$\mathbf{t} = \begin{cases} \begin{bmatrix} -n_y & 1 - \dfrac{n_y^2}{n_x+1} & -\dfrac{n_y n_z}{n_x+1} \end{bmatrix}^T, & n_x \geq 0 \\ \begin{bmatrix} n_y & 1 + \dfrac{n_y^2}{n_x-1} & \dfrac{n_y n_z}{n_x-1} \end{bmatrix}^T, & n_x < 0. \end{cases}$$

3. Determine the binormal vector with the following simplified expression:

$$\mathbf{b} = \begin{cases} \begin{bmatrix} -n_z & -\dfrac{n_y n_z}{n_x+1} & 1 - \dfrac{n_z^2}{n_x+1} \end{bmatrix}^T, & n_x \geq 0 \\ \begin{bmatrix} n_z & \dfrac{n_y n_z}{n_x-1} & 1 + \dfrac{n_z^2}{n_x-1} \end{bmatrix}^T, & n_x < 0. \end{cases}$$

Table A.2
Pseudo-code for unit vector EB orthogonalization.

1. Determine the non-collinear vector **v** by choosing the identity matrix column whose unit component value corresponds to the entry of the given vector with the least magnitude:
   if $|n_x| \geq |n_y|$
   $\mathbf{v} = [0, 1, 0]^T$
   else
   $\mathbf{v} = [1, 0, 0]^T$
2. Determine the tangent vector by taking the cross-product between **n** and **v**, i.e., $\mathbf{t} = \mathbf{n} \times \mathbf{v}$;

$$\mathbf{t} = \begin{cases} \begin{bmatrix} \dfrac{-n_z}{\sqrt{n_x^2+n_z^2}} & 0.0 & \dfrac{n_x}{\sqrt{n_x^2+n_z^2}} \end{bmatrix}^T, & |n_x| \geq |n_y| \\ \begin{bmatrix} 0.0 & \dfrac{n_z}{\sqrt{n_y^2+n_z^2}} & \dfrac{-n_y}{\sqrt{n_y^2+n_z^2}} \end{bmatrix}^T, & |n_x| < |n_y|. \end{cases}$$

3. Determine the binormal vector by taking the cross-product between **n** and **t**, i.e., $\mathbf{b} = \mathbf{n} \times \mathbf{t}$;

$$\mathbf{b} = \begin{cases} \begin{bmatrix} \dfrac{n_x n_y}{\sqrt{n_x^2+n_z^2}} & -\sqrt{n_x^2+n_z^2} & \dfrac{n_y n_z}{\sqrt{n_x^2+n_z^2}} \end{bmatrix}^T, & |n_x| \geq |n_y| \\ \begin{bmatrix} -\sqrt{n_y^2+n_z^2} & \dfrac{n_x n_y}{\sqrt{n_y^2+n_z^2}} & \dfrac{n_x n_z}{\sqrt{n_y^2+n_z^2}} \end{bmatrix}^T, & |n_x| < |n_y|. \end{cases}$$

Table A.3
Pseudo-code for SP vector orthogonalization.

1. Determine the non-collinear vector **v**:
   if $|n_x|, |n_y| \geq 0$ or $|n_x|, |n_y| \leq 0$
   $\mathbf{v} = [n_x + 1, n_y - 1, n_z]^T$
   else
   $\mathbf{v} = [n_x - 1, n_y - 1, n_z]^T$
2. Determine the tangent vector:
   2.1 take the cross-product between **n** and **v**, i.e., $\mathbf{t} = \mathbf{n} \times \mathbf{v}$;
   2.2 normalize vector **t**.
3. Determine the binormal vector:
   3.1 take the cross-product between **n** and **t**, i.e., $\mathbf{b} = \mathbf{n} \times \mathbf{t}$;
   3.2 normalize vector **b**.

Table A.4
Pseudo-code for PM vector orthogonalization.

1. Determine the projection matrix $\mathbf{nn}^T = [\mathbf{n}_1\ \mathbf{n}_2\ \mathbf{n}_3]$;
2. Normalize vectors $\mathbf{n}_1$, $\mathbf{n}_2$, and $\mathbf{n}_3$;
3. Determine the column vector $\mathbf{n}_k$ that makes the second greatest angle, θ, with the given vector **n**;
4. Determine the axis of rotation as the cross-product between **n** and $\mathbf{n}_k$, i.e., $\mathbf{u} = \mathbf{n} \times \mathbf{n}_k$;
5. Calculate the rotation matrix with the Rodrigues' formula, $\mathbf{R} = \mathbf{R}(\mathbf{u}, \theta)$;
6. Premultiply the remaining projection matrix columns with the rotation matrix **R** to obtain vectors **t** and **b**.

Table A.5
Number of FLOPS of the HH and EB techniques given a unit vector. For the HH case, the values in parentheses correspond to $n_x < 0$.

HH		EB	
Common factor: $(n_x \pm 1)^{-1}$	1 order operation 1 summation/subtraction 1 division	Common factor: $(n_x^2 + n_z^2)^{-1/2}$	1 order operation 1 summation/subtraction 2 multiplications 1 division 2 moduli 1 square root
Vector **t**	1 summation/subtraction 6 (5) multiplications	Vector **t**	3 multiplications
Vector **b**	1 summation/subtraction 6 (5) multiplications	Vector **b**	5 multiplications 1 division
Total	1 order operation 3 summations/subtractions 12 (10) multiplications 1 division	Total	1 order operation 1 summation 10 multiplications 2 division 2 moduli 1 square root

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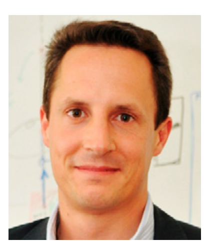

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