CERTIFIED FUNCTIONS FOR MESH GENERATION

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ABSTRACT

Formal methods allow for building correct-by-construction software with provable guarantees. The formal development presented here resulted in certified executable functions for mesh generation. The term certified means that their correctness is established via an artifact, or certificate, which is a statement of these functions in a formal language along with the proofs of their correctness. The term is meaningful only when qualified by a specific set of properties that are proven. This manuscript elaborates on the precise statements of the properties being proven and their role in an implementation of a version of the Isosurface Stuffing algorithm by Labelle and Shewchuk. This work makes use of the Calculus of Inductive Constructions for defining executable functions, stating their properties, and proving these properties via a direct examination of these functions (the property of liveness). The certificate is made available for inspection and execution using the Coq proof assistant.

Keywords: guaranteed quality mesh generation, formal methods, correct-by-construction, certified software

1. INTRODUCTION

Formal methods have undergone a rapid development in recent years. There are a number of reasons for this phenomenon. First, as algorithms and their software implementations are becoming increasingly sophisticated, they require a corresponding increase in the efforts to argue about the properties of the results they produce. For a number of complex algorithms, like unstructured guaranteed quality mesh generation, the complexity of stating and proving their specifications necessitates multiple manuscripts and pushes the limits of the traditional paper-and-pencil approach. Second, parallel algorithms, which have been developed for virtually all areas of computing, often bear another order-of-magnitude intricacy factor over the corresponding sequential algorithms due to numerous ways a parallel system can process and move data. Third, as automated systems are becoming increasingly integrated, a failure of one component has ramifications for the whole software-hardware system and can lead to costly and/or dangerous consequences. A number of major organizations, including Amazon [1], Microsoft [2], Twitter [3], Intel [4], MIT [5][6], and Inria [7][8], have made progress in the development and the use of formal methods and functional programming towards managing software correctness and maintainability.

This work is the second formal verification in the area of mesh generation, to the best of the author’s knowledge, that exhibits the property of liveness [9], i.e., being connected to the implementation via machine-checked proofs. The property of liveness increases the level of confidence in the correctness, as the proofs make use of the properties of the actual operations used in the code, not just abstracted models of those operations. The first work was published by Chernikov and Xu [10] on the correctness of a version of a Marching Cubes algorithm [11]. The present work proves certain correctness properties of the Isosurface Stuffing algorithm [12], and also differs from the previous [10] in two major aspects. The first one is that it works with tetrahedra, not just triangular faces. The second difference is in the proof approach. The previous work [10] used proofs via computation, i.e., the properties being proven were embedded in the functions computed as part of the proof. The present work sep-
The development presented herein resulted in certified executable functions for mesh generation. The term certified means that their correctness is established via an artifact, or certificate, which is a statement of these functions in a formal language along with the proofs of their correctness. The term is meaningful only when qualified by a specific set of properties that are proven. The functions whose properties are being proven and the precise formal statements of their certified properties are elaborated further down in this manuscript. The certificate in the form of an accompanying Coq script is made available [14]. As can be seen from the Venn diagram in Figure 1, only a subset of the entire implementation is involved in the proof of the properties stated below. A certificate with a formal proof of another set of properties may involve a different subset of functions.

**Figure 1:** A Venn diagram for the components of certified executable software. The parts described here are in yellow.

Published in 2007 by Labelle and Shewchuk [12], the Isosurface Stuffing (IS) algorithm solved a longstanding problem in tetrahedral meshing of geometrically complex shapes, that of achieving practically significant guaranteed dihedral angle bounds. Among other favorable properties of this algorithm are its fast execution, mesh gradation, placement of mesh boundary vertices exactly (to within a tolerance) onto the domain boundaries, as well as certain fidelity guarantees. Conceptually, the IS algorithm is similar to the well-known Marching Cubes (MC) algorithm [11]. Both algorithms employ a regular cubical grid to cover the region of interest. The IS algorithm uses a body centered cubic (BCC) lattice that is tessellated into a structured tetrahedral grid. Both the MC and the IS algorithms evaluate each vertex of the corresponding grid using a given cut function, which returns one of three values, corresponding to the vertex being inside, outside, or on the surface of the shape defined by this function. Depending on the local combination of these values in the vertices of a cube, the MC algorithm outputs one of the predefined stencils, which is a set of triangles that approximates the surface inside this cube. The IS algorithm evaluates the cut function in the vertices of a structured tetrahedron and outputs one of predefined sets of stencil tetrahedra (referred to as unstructured below). Both algorithms also make use of approximated locations of zero values of the cut function along the edges of the respective cubes or tetrahedra.

What distinguishes the IS algorithm from the MC and its variations is the presence of proofs that guarantee a priori, i.e., before the execution, that the dihedral and certain other angles will be bounded by known constant values. Due to a large number of cases to examine and, most importantly, to the unknown locations of the zero values within respective edges, these proofs would be next to impossible to construct manually. Instead, the IS authors implemented and described a computer-assisted approach where the computation of the angle bounds is done in software with the use of interval arithmetic and of recursive bisection of the parameter space. What was not described, however, is an a priori proof of correct connectivity between the adjacent tetrahedral stencils. Such a proof is important as a precedent is known with the original MC algorithm, wherein symmetry was incorrectly used to reduce the number of stencils, thus causing topological holes in the approximated surface [10]. The present work offers a formal statement of the connectivity properties of the IS stencils along with the proofs that these properties hold.

Figure 2 shows two example meshes obtained with the certified implementation discussed here. The implementation uses the same stencils in the uniformly refined area next to the domain boundary as the original IS algorithm. However, unlike the IS algorithm, it does not implement the octree optimization with additional stencils that allow for fewer tetrahedra in the interior of the domain by omitting the creation of certain octree leaves. These additional octree stencils are left for future work.

The number of IS connectivity cases to be verified, when unfolded, grows rapidly. Every two adjacent structured tetrahedra that share a triangular face in-
involves 5 vertices (see Figure 3) and, since each vertex can evaluate the cut function to one of 3 values, the number of 5-vertex sign assignments is $3^5 = 243$. If a higher confidence in the stencils is aimed at, as is the case in the proofs that follow, each of the four faces of a structured tetrahedron needs to be examined separately, which leads to a multiplier of 4: $243 \cdot 4 = 972$. Also, if formulas for each case of a translation and a rotation of a structured tetrahedron differ, these formulas need to be looked at separately as well. In this development, 12 variations of a formula are used, which raises the number of cases to $972 \cdot 12 = 11,664$. Moreover, each case involves several (0 to 3 on each side of the shared face) unstructured tetrahedra that subdivide either of the adjacent structured tetrahedra, and every edge of each of these unstructured tetrahedra needs to be examined with respect to the subdivision of the shared face from the other side. A manual enumeration and examination of all such cases becomes highly time-consuming and error-prone. Another important consideration is the ability to modify and extend this algorithm without the need for a repeated manual analysis. Once an automatic (i.e., not depending on the stencils) verification procedure is developed, it can be trivially applied to another set of stencils.

As an example, Figure 3 shows two structured tetrahedra, $(f_1, f_2, f_3, p)$ and $(f_1, f_2, f_3, q)$, that share face $(f_1, f_2, f_3)$. The symbols in vertex positions show the signs of the cut function: “+” symbolizing the vertex being inside the domain, “−” being outside, and “0” lying on the boundary. The signs of vertices $f_1$, $f_2$, $f_3$, $p$, and $q$ are computed by direct evaluation of the cut function. The positions of vertices $u$, $v$, and $w$ are computed by iterative bisection of the edges $(q, f_1)$, $(f_3, f_1)$, and $(f_2, f_1)$, respectively, in order to find (to within a tolerance) the zero values of the cut function, i.e., the intersections of these edges with the domain boundary. Applying the corresponding stencils [12] to subdivide the structured tetrahedron $(f_1, f_2, f_3, p)$, one obtains three unstructured tetrahedra: $(f_1, p, w, v)$, $(f_3, p, w, v)$, and $(w, f_3, f_2, p)$. Similarly, for the structured tetrahedron $(f_1, f_2, f_3, q)$, one obtains four unstructured tetrahedra: $(f_1, u, v, w)$, $(f_3, u, v, w)$, $(w, f_2, u, f_3)$, and $(q, f_2, u, f_3)$. Tetrahedra $(f_1, p, w, v)$ and $(f_1, u, v, w)$ are classified as located outside the domain, and are not considered in this work. The remaining unstructured tetrahedra, three on one side of the shared face and two on the other side, are classified as lying within the domain and are considered further.

Figure 2: Top: the surface and a cross-section of a mesh of a torus defined by an analytical function (61,528 tetrahedra, 20.2° minimum output dihedral angle). Bottom: a cross-section of a mesh of a human brain atlas [15] defined by an image (9,788,808 tetrahedra, 30° minimum output dihedral angle).

Figure 3: An example of two face-adjacent structured tetrahedra, $(f_1, f_2, f_3, p)$ and $(f_1, f_2, f_3, q)$ shown with black lines, a sign assignment to their vertices, and a subdivision into unstructured tetrahedra shown with purple lines. The shared face $(f_1, f_2, f_3)$ is shaded.

Via an examination of all edges of the unstructured tetrahedra classified as lying inside the domain, it can be concluded that the two sets of edges created inside the two respective structured tetrahedra are consistent.
within the shared face. In the rest of this work, formal conditions for such a verification are developed and proven.

Section 2 introduces the methodology used in this work. Section 3 describes the executable functions whose properties are certified. Section 4 presents the formally stated properties of the function that constructs structured tetrahedra and the proof of these properties. Section 5 certifies the function that constructs unstructured tetrahedra, considered separately, in a similar progression. In Section 6, the properties of both functions are proven together, which is necessary since unstructured tetrahedra are constructed out of the structured ones. Section 7 concludes the exposition with the summary of the presented work and expected extensions.

2. METHODOLOGY

The Curry-Howard correspondence is a fundamental concept in proof theory that considers proving to be a kind of programming. Indeed, while a computer program is a sequence of transformations of input data to output data, a proof is a sequence of transformations that takes the input proposition (premise) and converts it to the output proposition (conclusion). In this sense, implementing an algorithm as a function is similar to proving a theorem.

Computer-assisted proving involves a human user who guides the process through formulating intermediate steps and choosing proof techniques. The user interacts with a software program that manages the state of the proof, verifies the validity of the typed commands, and executes those commands.

Proof automation allows for finding proofs in special cases by invoking predefined proof search strategies. Once the user identifies that at a certain stage in the proving process a particular proof goal is suitable for some predefined automatic procedure, that procedure can be invoked in order to reduce the number of manually guided steps.

Purely functional programming is a programming methodology that views the subroutines to be similar to mathematical functions, whose return value depends only on the values of the parameters, and that produce no side effects. This methodology, when enforced in a ‘pure’ language, often translates to restricting the programming constructs so that there is no memory aliasing via pointers, parameters to functions are passed and returned ‘by value’, and mutable global values are not allowed. Eliminating side effects and aliasing makes it much easier to argue about the return value of a function, and therefore a pure functional programming language is a suitable choice for a proof assistant. Functional programming is contrasted to imperative programming that changes state with commands, such as, for example, an assignment.

Extraction is a methodology that separates the executable part of a program’s specification from its logical part and saves it in a language that supports compilation and deployment.

The Coq formal proof management system 8 was chosen for this development. Coq combines a purely functional programming language called Gallina, which is based on a formal language Calculus of Inductive Constructions, and a vernacular language of commands that allow for stating software specifications and proving mathematical theorems. Some of the Coq’s salient features that are relevant to the current exposition are briefly reviewed below. A thorough treatment can be found in relevant texts [7,16,17].

Coq’s Calculus of Inductive Constructions is a general theory that defines a typed programming language that can serve as constructive foundation of mathematics. Inductive definitions are in the core of Coq’s language. For example, a basic number type used in this development, binary integer numbers (Z), are defined inductively in Coq’s standard library as follows.

\[
\text{Inductive } \text{positive} : \text{Set} := \\
\text{zI} : \text{positive } \rightarrow \text{positive} \\
\text{zO} : \text{positive } \rightarrow \text{positive} \\
\text{zH} : \text{positive}.
\]

\[
\text{Inductive } \text{Z} : \text{Set} := \\
\text{Z0} : \text{Z} \\
\text{Zpos} : \text{positive } \rightarrow \text{Z} \\
\text{Zneg} : \text{positive } \rightarrow \text{Z}.
\]

Type Z can be thought of as a wrapper around the positive type, with its constructors corresponding to number 0, some positive number, or some negated positive number, respectively. The positive number type is defined via constructor zH, representing binary digit 1 in the most significant position, and two constructors, zO and zI, that add a least significant digit, 0 or 1 respectively, to a given positive number. For example, Zneg (zO (zI zH)) represents −6. The arrow operator → is a special case of a universal quantifier and is used in a variety of contexts, including listing function and constructor arguments, as well as logical implication.

Polymorphism is a concept in programming that stands for providing a single interface to elements of different types. Polymorphism is fully supported in Coq by declaring undefined types as variables. In the current development, for example, the concrete representation of the Vertex data structure is irrelevant to the proof of unstructured stencil correctness. As a result, in the Coq script it was abstracted as an unspecified type:
Variable Vertex : Type.

The unstructured tetrahedron data structure is then defined as four Vertex data elements appearing as parameters to the tetrahedron constructor UT:

Inductive UnstructuredTet :=
  UT : Vertex → Vertex →
  Vertex → Vertex → UnstructuredTet.

Closure of a function is a function that carries bindings to all the data structures referenced within it [15]. Along with polymorphism, functional closure allows for abstracting implementation details that are not needed for the proof part. One example of closure used in this development is the cut function named GetSign, which is bound to the definition of the domain to be meshed in the executable part of the implementation. However, the proof part only needs to know that this function takes a parameter of type Vertex and returns its Sign:

Variable GetSign : Vertex → Sign.

Tactics are predefined commands that are executed in the current proof environment to transform and eventually discharge the proof goal. Coq offers a collection of tactics that can accomplish a variety of logical transformations, such as applying a previously proven theorem (apply), proof by case enumeration (destruct), substitution of previously defined expressions (unfold), and many more. Some tactics exhibit a high degree of automation to ease the development effort on the part of the user. For example, one of the tactics used hereby, eauto, combines a Prolog-like resolution procedure auto with deferred instantiation of existential variables.

Tactical language in Coq is called Ltac. It contains a number of high-level commands that allow for applying tactics in various arrangements, including sequences, loops, and branches. The current development makes use of some of the features of this language, such as repeated application of tactics, catching exceptions, defining automated reusable proof procedures, and matching the shape of the current goal against a given pattern.

3. CERTIFIED EXECUTABLE FUNCTIONS

3.1 Function for Constructing Structured Tetrahedra

The IS algorithm uses structured tetrahedra to fill in the region of space to be meshed in the proximity of the domain boundary. The data structure for structured tetrahedra contains not only their vertex information, but also a sufficient amount of data to query all four of its neighbors adjacent via the faces, along with the vertices of the neighbors that correspond to the vertices of the given tetrahedron.

Inductive StructuredTet :=
  ST : Coord3 → Coord3 → Coord3 → Coord3 →
  StructuredTetId x VertexOrder →
  StructuredTetId x VertexOrder →
  StructuredTetId x VertexOrder →
  StructuredTetId x VertexOrder →
  StructuredTet.

Here the Coord3 parameters to the constructor ST are the three-dimensional coordinates of its vertices. The Coord3 data type simply combines three Z values corresponding to each of the Euclidean dimensions.

Inductive Coord3 :=
  C3 : Z → Z → Z → Coord3.

As mentioned above, the data structure for unstructured tetrahedra uses a variable, i.e., unspecified, type Vertex. When it is necessary to make the vertex types used in the proofs match, the Coord3 type is passed as a parameter that instantiates the Vertex type.

The type StructuredTetId is defined as follows.

Inductive StructuredTetId :=
  STId : Coord3 → StructuredTetCase →
  StructuredTetId.

The Coord3 parameter to the constructor STId is the three-dimensional coordinate of the reference, or anchor, that defines the position of the tetrahedron.

The type StructuredTetCase defines one of 12 possible orientations that are enumerated as constructors of this type:

Inductive StructuredTetCase :=
  Tet_I1 | Tet_I2 | Tet_I3 | Tet_I4 |
  Tet_J1 | Tet_J2 | Tet_J3 | Tet_J4 |
  Tet_K1 | Tet_K2 | Tet_K3 | Tet_K4.

The VertexOrder parameters to the ST constructor specify the ordering of the vertices of each neighbor tetrahedron, so that the corresponding vertices can be known (see Section 6). It is a function that returns a permutation of four vertices:

Definition VertexOrder : Type :=
  Coord3 → Coord3 → Coord3 → Coord3 →
  (Coord3 × Coord3 × Coord3 × Coord3).

Figure illustrates some of these data elements. The cube drawn with black lines has even-coordinate corners, and the one drawn with blue lines has odd-coordinate corners. The corner marked ijk is the reference. The other corner labels indicate the offset from the reference coordinate. The red lines show the edges that are added to form four tetrahedra shown: (220, 222, 311, 331), (220, 222, 311, 111),
(220, 222, 131, 331), (220, 222, 131, 111). These tetrahedra correspond to cases Tet_K1, Tet_K2, Tet_K3, and Tet_K4, respectively. Another set of four tetrahedra (not shown) is constructed around edge (202, 222). The third set of four tetrahedra (also not shown) is constructed around edge (022, 222). Twelve tetrahedra correspond to each reference coordinate ijk. The executable function GetStructuredTet returns one of these tetrahedra, depending on the case requested.

![Figure 4: The vertices used by the function that constructs structured tetrahedra.](image)

The structured tetrahedra can be defined by a simple formula that returns their connectivity with respect to the vertices of the BCC grid. This formula will translate and rotate a reference tetrahedron to define all other similar tetrahedra. Such a formula was encoded into an executable function named GetStructuredTet.

**Definition** GetStructuredTet (tid : StructuredTetId) : StructuredTet := [omitted]

### 3.2 Function for Constructing Unstructured Tetrahedra

The executable function GetUnstructuredTets returns a list of tetrahedra that subdivide a given structured tetrahedron. The parameters to this function v1, v2, v3, v4 are vertices of the given structured tetrahedron. This function enumerates all of the 81 possible combinations of values GetSign v1, GetSign v2, GetSign v3, and GetSign v4, and returns a corresponding predefined list of unstructured tetrahedral stencils adopted from the original publication [12].

**Definition** GetUnstructuredTets (v1 v2 v3 v4 : Vertex) : list UnstructuredTet := [omitted]

### 4. Certificate for Structured Tetrahedra

#### 4.1 Specification

The specification for the correctness of the structured tetrahedron returned by function GetStructuredTet states the following requirement. Let v1, v2, v3, v4 be the vertices of this tetrahedron, and nei_tid and nei_order be the identifier and the order of vertices of its i-th neighbor (i = 1, 2, 3, 4). A convention is used that the i-th neighbor is the one that is across from the i-th vertex. Then, if the same function GetStructuredTet is called for nei_tid, and the returned vertices u1, u2, u3, u4 are permuted by function nei_order, then the vertices with the corresponding positions are equal, except for the vertices in position i that are not equal. The Section mechanism of Coq allows for moving the frequently used parameters of the constructs defined within this section to its Variables clause, thus improving readability.

**Section** GetStructuredTet_Spec.

**Variables** (v1 v2 v3 v4 : Coord3) (nei_tid : StructuredTetId) (nei_order : VertexOrder).

**Definition** U :=

match GetStructuredTet nei_tid with
ST u1 u2 u3 u4 _ _ _ _ ⇒
nei_order u1 u2 u3 u4
end.

**Definition** Face1Correct :=

match U with (u1, u2, u3, u4) ⇒
(v1 = u1) ∧ (v2 = u2) ∧
(u3 = u3) ∧ (v4 = u4)
end.

**Definition** Face2Correct :=

match U with (u1, u2, u3, u4) ⇒
(v1 = u1) ∧ (v2 = u2) ∧
(u3 = u3) ∧ (v4 = u4)
end.

[omitted]

**End** GetStructuredTet_Spec.

#### 4.2 Proof

The following theorem proves the specification above.

**Theorem** FacesCorrect :

∀ tid : StructuredTetId,
match GetStructuredTet tid with
ST v1 v2 v3 v4 (tid1, o1) (tid2, o2) (tid3, o3) (tid4, o4) ⇒
(Face1Correct v1 v2 v3 v4 tid1 o1) ∧
(Face2Correct v1 v2 v3 v4 tid2 o2) ∧
(Face3Correct v1 v2 v3 v4 tid3 o3) ∧
Let \( v \in \mathbb{R}^3 \), given as triples of coordinates. For some point \( u \in \mathbb{R}^3 \), the real numbers \( a_1, a_2, a_3 \), not all equal to zero, such that

\[
(a_1 + \cdots + a_n)u = a_1v_1 + \cdots + a_nv_n,
\]

are called barycentric coordinates of \( u \) with respect to the simplex with vertices \( v_1, \ldots, v_n \). Barycentric coordinates with \( a_1 + \cdots + a_n = 1 \) will be used below. For the proofs presented, only three values of a barycentric coordinate are relevant: zero, some unknown value strictly between zero and one, and one. These are defined symbolically by the following respective constructors of type \( \text{BCoord} \):

Inductive \( \text{BCoord} := \text{Zero} \mid \text{Interior} \mid \text{One} \).

5. CERTIFICATE FOR UNSTRUCTURED TETRAHEDRA

5.1 Specification

Given two edges, each belonging to the stencil edges, these edges are considered compatible if they do not intersect in their interiors. A set of conditions is developed below that allow for verifying this requirement.

5.1.1 Barycentric Coordinate System

Let \( v_1, \ldots, v_n \) be the vertices of a simplex in Euclidean space \( \mathbb{R}^3 \), given as triples of coordinates. For the present exposition, the relevant values of \( n \) are 3 and 4, corresponding to a triangle or a tetrahedron, respectively. For some point \( u \in \mathbb{R}^3 \), the real numbers \( a_1, a_2, a_3 \), not all equal to zero, such that

\[
(a_1 + \cdots + a_n)u = a_1v_1 + \cdots + a_nv_n,
\]

are called barycentric coordinates of \( u \) with respect to the simplex with vertices \( v_1, \ldots, v_n \). Barycentric coordinates with \( a_1 + \cdots + a_n = 1 \) will be used below. For the proofs presented, only three values of a barycentric coordinate are relevant: zero, some unknown value strictly between zero and one, and one. These are defined symbolically by the following respective constructors of type \( \text{BCoord} \):

Inductive \( \text{BCoord} := \text{Zero} \mid \text{Interior} \mid \text{One} \).

5.1.2 Barycentric Coordinates Within a Triangle

Consider the barycentric coordinate system defined by the shared face \( (f_1, f_2, f_3) \). Then the following proposition \( \text{FCoord} \) lists the barycentric coordinates of vertices \( f_1, f_2, f_3 \), as well as of the vertices computed on the edges of this face by function \( \text{GetIntersection} \):

Variables \( f_1 f_2 f_3 p q : \text{Vertex} \).

Inductive \( \text{FCoord} : \text{Vertex} \to \text{BCoord} \to \text{BCoord} \to \text{BCoord} \to \text{Prop} :=
\)

\[
\begin{align*}
| \text{FC}_1 : \text{FCoord} f_1 \text{One Zero Zero} \\
| \text{FC}_2 : \text{FCoord} f_2 \text{Zero One Zero} \\
| \text{FC}_3 : \text{FCoord} f_3 \text{Zero Zero One} \\
| \text{FC}_4 : \text{FCoord} (\text{GetIntersection} f_1 f_2) \\
\text{Interior Zero Zero} \\
| \text{FC}_5 : \text{FCoord} (\text{GetIntersection} f_2 f_3) \\
\text{Interior Zero Zero} \\
| \text{FC}_6 : \text{FCoord} (\text{GetIntersection} f_1 f_3) \\
\text{Interior Zero Interior} \\
| \text{FC}_7 : \text{FCoord} (\text{GetIntersection} f_3 f_2) \\
\text{Zero Interior Interior}. \\
\end{align*}
\]

5.1.3 Barycentric Coordinates Within a Tetrahedron

For the tetrahedron \( (f_1, f_2, f_3, p) \), the barycentric coordinate system is defined similarly. For the proof that follows, however, the full coordinates of the vertices are not needed. The only needed piece of information is which vertices lie off the shared face \( (f_1, f_2, f_3) \), as evidenced by their non-zero last barycentric coordinate (i.e., the one corresponding to vertex \( p \)). The proposition below makes this information available.

Inductive \( \text{PCoord} : \text{Vertex} \to \text{Prop} :=
\)

\[
\begin{align*}
| \text{PC}_1 : \text{PCoord} p \\
| \text{PC}_2 : \text{PCoord} (\text{GetIntersection} p f_1) \\
| \text{PC}_3 : \text{PCoord} (\text{GetIntersection} f_1 p) \\
| \text{PC}_4 : \text{PCoord} (\text{GetIntersection} p f_2) \\
| \text{PC}_5 : \text{PCoord} (\text{GetIntersection} f_2 p) \\
| \text{PC}_6 : \text{PCoord} (\text{GetIntersection} p f_3) \\
| \text{PC}_7 : \text{PCoord} (\text{GetIntersection} f_3 p). \\
\end{align*}
\]

The predicate \( \text{QCoord} \) is defined similarly to \( \text{PCoord} \), only with respect to vertex \( q \) of tetrahedron \( (f_1, f_2, f_3, q) \).

5.1.4 Barycentric Non-Intersection in the Shared Face

Given a point \( p \) and a segment \( (q_1, q_2) \), both lying in face \( (f_1, f_2, f_3) \), a proposition can be stated that guarantees \( p \) not being in the interior of \( (q_1, q_2) \). Let the barycentric coordinates of points \( q_1, q_2 \) with respect to vertex \( f_1 \) be \( a, b, c \), respectively, see Figure 5. Then, if \( c \) is above or below \( a \) and \( b \), as specified precisely by the propositions that follow, this requirement can be formalized.

Proposition \( \text{Below} \) enumerates the cases (i.e., combinations of values of its parameters) that assure the required property of segment-point non-intersection, where the first parameter is the coordinate of the point, while the second and the third parameters are the coordinates of the segment’s vertices. Care is taken not to make conclusions based on comparing two \( \text{Interior} \) coordinates, since their specific values are unknown before they are computed.

Inductive \( \text{Below} : \text{BCoord} \to \text{BCoord} \to \text{BCoord} \to \text{Prop} :=
\)

\[
\begin{align*}
| \text{B}_1 : \text{Below Zero Interior} \\
| \text{B}_2 : \text{Below Zero One} \\
| \text{B}_3 : \text{Below Zero Interior}. \\
\end{align*}
\]
Not Intersecting Not Segment
2D
Above Intersecting 3D
Not 3D
2 Symm Segment 1D
1 Not Intersecting 2 Segment 1D
1 Intersecting Point
Intersecting Above 3D
Not 3D
2 Symm
Intersecting
d
Not 1D Point
Point 1D
Intersecting

f1

Figure 5: Point p with barycentric f1-coordinate c not lying in the interior of segment \((q1, q2)\) whose vertices have barycentric f1-coordinates a and b.

\[
| B_{-4} : \text{Below Zero Interior One.} |
\]

Proposition Above is stated similarly.

**Inductive Above :** BCoord \(\rightarrow\) BCoord \(\rightarrow\) BCoord \(\rightarrow\) Prop

- **A_1** : Above One Zero Interior
- **A_2** : Above One Zero One
- **A_3** : Above One Interior Interior
- **A_4** : Above One Interior One

In order to allow the vertices of the segment to appear in an arbitrary order, symmetric versions of propositions Below and Above are defined. They simply refer to these propositions with both orderings of parameters.

**Section Below_Above_Symm.**

Variables c a b : BCoord.

**Inductive Below_Symm :** Prop :=

- **BS_1** : Below c a b \(\rightarrow\) Below_Symm
- **BS_2** : Below c b a \(\rightarrow\) Below_Symm.

**Inductive Above_Symm :** Prop :=

- **AS_1** : Above c a b \(\rightarrow\) Above_Symm
- **AS_2** : Above c b a \(\rightarrow\) Above_Symm.

End Below_Above_Symm.

The proposition SPNI1D below states that BCoord value c is either above or below values a and b (regardless of the ordering of a and b), which guarantees that a point with coordinate c does not lie in the interior of the segment whose vertices have corresponding coordinates a and b.

**Section Segment_Point_Not_Intersecting_1D.**

Variables c a b : BCoord.

**Inductive SPNI1D :** Prop :=

- **SPNI1D_1** : Below_Symm c a b \(\rightarrow\) SPNI1D
- **SPNI1D_2** : Above_Symm c a b \(\rightarrow\) SPNI1D.

End Segment_Point_Not_Intersecting_1D.

If the non-intersection condition SPNI1D holds with respect to at least one barycentric coordinate, then the vertex with barycentric coordinates \((c_1, c_2, c_3)\) does not intersect the interior of the segment whose vertices have coordinates \((a_1, a_2, a_3)\) and \((b_1, b_2, b_3)\):

**Section Segment_Point_Not_Intersecting_3D.**

Variables a1 a2 a3 b1 b2 b3 c1 c2 c3 : BCoord.

**Inductive SPNI3D :** Prop :=

- **SPNI3D_1** : SPNI1D c1 a1 b1 \(\rightarrow\) SPNI3D
- **SPNI3D_2** : SPNI1D c2 a2 b2 \(\rightarrow\) SPNI3D
- **SPNI3D_3** : SPNI1D c3 a3 b3 \(\rightarrow\) SPNI3D.

End Segment_Point_Not_Intersecting_3D.

A similar approach is used in the case of two segments lying in face \((f1, f2, f3)\), see Figure 6.

First, a proposition is stated that establishes a one-dimensional barycentric condition of their non-intersection in the interiors. Given that the coordinates of the first segment’s vertices are a and b, and the coordinates of the second segment’s vertices are c and d, the condition requires that either both vertices of the first segment are below the vertices of the second segment or vice versa:

**Section Segment_Segment_Not_Intersecting_1D.**

Variables a b c d : BCoord.

**Inductive SSNI1D :** Prop :=

- **SSNI1D_1** : Below_Symm a c d \(\rightarrow\) Below_Symm b c d \(\rightarrow\) SSNI1D
- **SSNI1D_2** : Below_Symm a d b \(\rightarrow\) Below_Symm b d a \(\rightarrow\) SSNI1D.

End Segment_Segment_Not_Intersecting_1D.

Then a proposition is stated requiring that the one-dimensional condition holds with respect to at least one of three barycentric dimensions.

**Section Segment_Segment_Not_Intersecting_3D.**

Variables a1 a2 a3 b1 b2 b3 c1 c2 c3 d1 d2 d3 : BCoord.

**Inductive SSNI3D :** Prop :=

- **SSNI3D_1** : SSNI1D a1 b1 c1 d1 \(\rightarrow\) SSNI3D

Figure 6: Segment \((p1, p2)\) whose vertices have barycentric f1-coordinates c and d and segment \((q1, q2)\) whose vertices have barycentric f1-coordinates a and b not intersecting in their interiors.
In Intersecting Edges

Vertex \( p_1 \) is in a special position (proposition \( \text{SpecialVertex} \) described further below) with respect to edge \( (q_1, q_2) \) and vertex \( p_2 \) is not in the interior of edge \( (q_1, q_2) \) (proposition \( \text{NotIn} \) described further below).

The condition above holds if vertices \( p_1 \) and \( p_2 \) are interchanged.

The two conditions above hold if edges \( (p_1, p_2) \) and \( (q_1, q_2) \) are interchanged.

If both edges \( (p_1, p_2) \) and \( (q_1, q_2) \) lie in the shared face \( \{f_1, f_2, f_3\} \), then they do not intersect in their interiors as defined by proposition \( \text{SSNI3D} \) above.

**5.1.5 Barycentric Non-Intersection Within Adjacent Tetrahedra**

In this section, a condition is established that formally defines a sufficient condition for two edges, each incident on the irregular tetrahedra on either side of the shared face, to be compatible, i.e., not intersecting in their interiors. This condition is given by the proposition \( \text{TwoEdgesCompatible} \) stated below. Two edges, \( (p_1, p_2) \) and \( (q_1, q_2) \), are considered compatible if at least one of the following conditions is satisfied:

- Vertex \( p_1 \) is in a special position (proposition \( \text{SpecialVertex} \) described further below) with respect to edge \( (q_1, q_2) \) and vertex \( p_2 \) is not in the interior of edge \( (q_1, q_2) \) (proposition \( \text{NotIn} \) described further below).
- The condition above holds if vertices \( p_1 \) and \( p_2 \) are interchanged.
- The two conditions above hold if edges \( (p_1, p_2) \) and \( (q_1, q_2) \) are interchanged.
- If both edges \( (p_1, p_2) \) and \( (q_1, q_2) \) lie in the shared face \( \{f_1, f_2, f_3\} \), then they do not intersect in their interiors as defined by proposition \( \text{SSNI3D} \) above.

**Section Two_Edges_COMPATIBLE.**

**Variables** \( p_1 \ p_2 \ q_1 \ q_2 \) : \( \text{Vertex} \).

**Inductive** \( \text{TwoEdgesCompatible} \) : \( \text{Prop} \) :=

- \( \text{EC}_1 \) : \( \text{SpecialVertex} \ p_1 \ q_1 \ q_2 \ PCoord \rightarrow \text{NotIn} \ p_2 \ q_1 \ q_2 \ PCoord \ QCoord \rightarrow \text{TwoEdgesCompatible} \)
- \( \text{EC}_2 \) : \( \text{SpecialVertex} \ p_2 \ q_1 \ q_2 \ PCoord \rightarrow \text{NotIn} \ p_1 \ q_1 \ q_2 \ PCoord \ QCoord \rightarrow \text{TwoEdgesCompatible} \)
- \( \text{EC}_3 \) : \( \text{SpecialVertex} \ q_1 \ p_1 \ p_2 \ QCoord \rightarrow \text{NotIn} \ q_2 \ p_1 \ p_2 \ QCoord \ QCoord \rightarrow \text{TwoEdgesCompatible} \)
- \( \text{EC}_4 \) : \( \text{SpecialVertex} \ q_2 \ p_1 \ p_2 \ QCoord \rightarrow \text{NotIn} \ q_1 \ p_1 \ p_2 \ QCoord \ QCoord \rightarrow \text{TwoEdgesCompatible} \)
- \( \text{EC}_5 \) : \( \forall \ a_1 \ a_2 \ a_3 \ b_1 \ b_2 \ b_3 \ c_1 \ c_2 \ c_3 \ d_1 \ d_2 \ d_3 : \text{BCoord}, \ PCoord \ p_1 \ a_1 \ a_2 \ a_3 \rightarrow \ PCoord \ p_2 \ b_1 \ b_2 \ b_3 \rightarrow \ PCoord \ q_1 \ c_1 \ c_2 \ c_3 \rightarrow \ PCoord \ q_2 \ d_1 \ d_2 \ d_3 \rightarrow \text{SSNI3D} \ a_1 \ a_2 \ a_3 \ b_1 \ b_2 \ b_3 \ c_1 \ c_2 \ c_3 \ d_1 \ d_2 \ d_3 \rightarrow \text{TwoEdgesCompatible} \)

End \( \text{Two_Edges_COMPATIBLE} \).

The special status of vertex \( v \) with respect to edge \( (u_1, u_2) \) here means that \( v \) is equal to one of the vertices \( u_1 \) or \( u_2 \), or it is off the shared face as defined by the corresponding parameter proposition \( \text{V} \) (equal to \( PCoord \) or \( QCoord \) depending on the branch of \( \text{TwoEdgesCompatible} \)).

**Section Special_Vertex.**

**Variables** \( v \ u_1 \ u_2 : \text{Vertex} \)

- \( \text{Inductive} \ \text{SpecialVertex} \) : \( \text{Prop} := \)
- \( \text{SV}_1 \) : \( v = u_1 \rightarrow \text{SpecialVertex} \)
- \( \text{SV}_2 \) : \( v = u_2 \rightarrow \text{SpecialVertex} \)
- \( \text{SV}_3 \) : \( v \rightarrow \text{SpecialVertex} \).

End \( \text{Special_Vertex} \).

Vertex \( v \) being \( \text{NotIn} \) edge \( (u_1, u_2) \) holds if at least one of the following conditions is satisfied:

- \( v \) is a special vertex with respect to \( u_1, u_2 \) as defined above.
- At least one of \( u_1, u_2 \) is off the shared face as defined by the appropriate proposition \( PCoord \) or \( QCoord \).
- All three vertices \( v, u_1, u_2 \) lie in the shared face and \( v \) is not in the interior of edge \( u_1, u_2 \) as defined by proposition \( \text{SPNI3D} \).

**Section NotIn.**

**Variables** \( v \ u_1 \ u_2 : \text{Vertex} \)

- \( \text{Inductive} \ \text{NotIn} \) : \( \text{Prop} := \)
- \( \text{NL}_1 \) : \( \text{SpecialVertex} \ v \ u_1 \ u_2 \ V \rightarrow \text{NotIn} \)
- \( \text{NL}_2 \) : \( u_1 \rightarrow \text{NotIn} \)
- \( \text{NL}_3 \) : \( u_2 \rightarrow \text{NotIn} \)
- \( \text{NL}_4 \) : \( \forall \ a_1 \ a_2 \ a_3 \ b_1 \ b_2 \ b_3 \ c_1 \ c_2 \ c_3 : \text{BCoord}, \ PCoord \ u_1 \ a_1 \ a_2 \ a_3 \rightarrow \ PCoord \ u_2 \ b_1 \ b_2 \ b_3 \rightarrow \ PCoord \ v \ c_1 \ c_2 \ c_3 \rightarrow \text{SPNI3D} \ a_1 \ a_2 \ a_3 \ b_1 \ b_2 \ b_3 \ c_1 \ c_2 \ c_3 \rightarrow \text{NotIn} \).

End \( \text{NotIn} \).

Proposition \( \text{AllEdgesCompatible} \) below makes use of \( \text{TwoEdgesCompatible} \) by passing to it every pair of edges, each pair consisting of edges from both sides of the shared face.

**Definition** \( \text{AllEdgesCompatible} \)

- \( (u_1 \ u_2 \ v_1 \ v_2 : \text{Vertex}) \)

End \( \text{Two_Edges_COMPATIBLE} \).
Forall EdgePairCompatible
  (list_prod (Edges t1) (Edges t2)).

Given two regular tetrahedra, one defined by vertices
u1, u2, u3, u4, and the other by v1, v2, v3, v4, function
GetUnstructuredTets is called for each of these
tetrahedra. This function returns a list of irregular
tetrahedra for each regular tetrahedron. Let t1 be an
arbitrary tetrahedron in the list returned for u1, u2,
w3, u4. Let t2 be an arbitrary tetrahedron in the list
returned for v1, v2, v3, v4. Six edges of t1 and six
edges of t2 are collected into two respective lists using
function Edges below:

Definition Edges (t : UnstructuredTet Vertex) :
  list Edge :=
  match t with
    | UT u v w r =>
      [(u, v); (u, w); (u, r); (v, w); (v, r); (w, r)]
  end.

The standard library function list_prod returns a
cartesian product of two lists, which are Edges t1 and
Edges t2 in this development. Finally, the standard
library proposition Forall asserts that a proposition
supplied as its first parameter (EdgePairCompatible)
holds for all elements of the list supplied as
its second parameter. EdgePairCompatible simply un-
packs the vertices of both edges and passes them to
TwoEdgesCompatible:

Definition EdgePairCompatible ee :=
  let '((p1, p2), (q1, q2)) := ee in
  TwoEdgesCompatible p1 p2 q1 q2.

5.2 Proof

The following lemma proves that the proposition
AllEdgesCompatible holds for six arrangements of five
vertices f1, f2, f3, p, q that define two tetrahedra with
shared face (f1, f2, f3).

Lemma CompatibilityOrders :
  \forall Vertex GetSign GetIntersection f1 f2 f3 p q,
  let P := AllEdgesCompatible Vertex GetSign
    GetIntersection f1 f2 f3 p q in
    P p f1 f2 f3 f1 q f2 f3 ∧
    P p f1 f2 f3 f1 q f3 f2 ∧
    P f1 p f2 f3 f1 q f2 f3 ∧
    P f1 p f2 f3 f1 q f2 f3 ∧
    P f1 f2 p f3 f1 f2 q f3 ∧
    P f1 f2 p f3 f1 f2 q f3 ∧
  Proof. [omitted] Qed.

6. CERTIFICATE FOR STRUCTURED
   AND UNSTRUCTURED
   TETRAHEDRA

In this section, the correctness of the two functions,
one returning structured and the other returning un-
structured tetrahedra, is proven when they are used
together. Function GetStructuredTet returns a struct-
ured tetrahedron which is then passed to GetUnstruc-
turedTets.

Theorem Face1Compatible :
  \forall GetSign GetIntersection tid,
  match GetStructuredTet tid with
    | ST v1 v2 v3 v4 (tid1, order1) _ _ _ =>
      match GetStructuredTet tid1 with
        | ST u1 u2 u3 u4 _ _ _ =>
          let \'(w1, w2, w3, w4) :=
            order1 u1 u2 u3 u4 in
          AllEdgesCompatible Coord3 GetSign
            GetIntersection w2 w3 w4 v1 w1
            v1 v2 v3 v4 u1 u2 u3 u4
        end
      end
    end.
    Proof. [omitted] Qed.

The statement of this theorem is somewhat similar to
that of theorem FacesCorrect. Both theorems exam-
ine the result of two calls to function GetStructuredTet
with respect to the face shared by the two returned
structured tetrahedra. Theorem FacesCorrect proves
that the shared face is identified correctly. Theorem
Face1Compatible, on the other hand, proves that two
sets of unstructured tetrahedra, each computed via
function GetUnstructuredTets within the definition of
proposition AllEdgesCompatible, satisfy this propo-
sition. The proof of theorem Face1Compatible makes
use of lemma CompatibilityOrders that requires one of
six specific orderings of vertices of the two structured
tetrahedra. The orderings of vertices returned by the
calls to GetStructuredTet satisfy this requirement.
Another three theorems are proven, Face2Compatible,
Face3Compatible and Face4Compatible, that are identi-
cal to Face1Compatible except for the faces that are
examined.

7. DISCUSSION AND CONCLUSIONS

Currently, major software projects consist of millions
of lines of code, multiple subsystems, and are man-
aged by large teams of developers (who tend to move
between positions). With this level of complexity, for-
mulating and maintaining the specifications of such
systems, and ensuring that the implementation meets
these specifications become a major challenge. The
traditional approach to software specifications consists
in writing textual descriptions in English (or other nat-
ural language) with a mix of mathematical statements,
and maintaining them as code comments and/or as
separate documents. There are two problem with such
specifications. The first is that they tend to be high-
level and not necessarily reflective of the rich set of
behaviors the code can exhibit. The second problem is
that they are disconnected from the code, in the sense
that updates to the code and to these specifications may be performed separately and not necessarily consistently with each other. The certified software development process illustrated in this paper solves both of these problems by virtue of the specifications referring to the actual implementation. It solves the first problem by using specifications stated in a precise logical language, and having these statements automatically checked for exhaustive coverage of all possible cases. It solves the second problem by having the specification directly reference the implementation. Appel et al. [9] coined the term deep specification to refer to specifications that are simultaneously rich (sufficiently detailed), two-sided (both implementable and useful), formal (stated in a formal language which supports automated tools), and live (connected to implementation). A number of model checking and design specification approaches based on formal languages like Alloy [5], AADL [19], VDM [20], and Z [21], operate on a high level of abstraction that is not connected with the implementation. An approach of annotating the routines with pre- and post-conditions, such as Design by Contract [22], relies on the developer's current understanding of these conditions and is also not live.

In addition to providing live specifications of software, the presented certification approach also guarantees that the proven properties hold for all input parameters that can be passed to the routines. In other words, it by design eliminates the need to test the resulting software for these properties. The caveat, however, is that the formally stated specifications have to correctly represent the expected properties.

Mesh generation is one of the application domains that is likely to benefit from the use of formal methods in general and of certified software development in particular. One reason behind this expectation is the complexity of mesh generation algorithms that need to balance multiple, often contradictory, requirements of element shape, boundary fidelity, mesh grading, number of elements, software running time and memory use, and others. These requirements can be thought of as a multidimensional design space, where each requirement represents one dimension of this space. Being able to a priori formally guarantee, or certify, certain properties of an algorithm's implementation allows for the reduction of the dimensionality of the remaining design space. An example of this phenomenon from the current work is the unfolding of the tetrahedral stencils: because the unfolded stencils have been automatically checked for consistency during a single certification event, the Parity Rule [12] does not need to be enforced at runtime during every execution of the software. Another reason behind the expectation of the usefulness of formal methods in mesh generation is the combinatorial nature of mesh stencils, or elements, which is suitable for automated enumeration and analysis of their possible arrangements.

The efficiency of the proof execution does not influence the performance of the final software product. Indeed, the proof is run at design time and then separated from the executable part by the process of extraction. This executable part, on the other hand, is the component which gets deployed and whose performance contributes to the efficiency of the resulting product. The main requirement on the proof efficiency is that it does not unreasonably slow down the design effort. The experience of the author of this work suggests that the proof design effort is dominated by the time spent on elucidating the properties that need to be proven, formalizing them, and discovering the appropriate proof strategies. The proof execution part appeared minor relative to these time investments. It was also noticed that the same result can be proven with different strategies that sometimes vary significantly in performance. The accompanying certificate [14] was run on a MacBook Pro equipped with an 8-core Intel Core i9 @ 2.4 GHz processor and 32 GB of RAM memory. In the serial mode the proof completed in 46 minutes. Virtually all of this time was taken by the proof of lemma CompatibilityOrders. Experimentation with Coq's parallel proof modes revealed that this time can be reduced to 31 minutes with two proof threads. Increasing the number of proof threads to six, which is the number of independent proof goals in this lemma, did not yield further speedup.

The present work lays out a methodological foundation and a case study for developing certified mesh generation software. It demonstrates the use of the Calculus of Inductive Constructions for defining executable functions, stating their properties, and proving these properties via a direct examination of these functions (the property of liveness). These functions were extracted into OCaml code, supplemented with other OCaml functions needed for a working computer program, compiled, and executed. The evaluation of the performance of this program, as well as of the choices of the data structures, is out of the scope of this exposition and will be presented elsewhere.

It is anticipated that this work will be extended in the following directions. The first direction is the live proofs of the angle bounds reported in the original IS presentation [12]. The second direction is the addition of other shapes of structured tetrahedra that allow for more flexibility in filling in the octree leaves, leading to fewer resulting tetrahedra, as also originally reported [12]. The third direction is the study of stencils for multi-material interfaces, which can potentially be informed by previous work [23].
References


