A Geometrical Refinement of Shape Calculus Enabling Direct Simulation

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Abstract: The Shape Calculus is a bio-inspired timed and spatial calculus for describing 3D geometrical shapes moving in a space. Its purpose is twofold: i) modelling and formally verifying (not only) biological systems, and ii) simulating the models for validation and hypothesis testing. The original geometric primitives of the calculus are highly abstract: the associated simulator needs to attach a lot of code to the model specification in order to perform an effective simulation. In this work we propose a calculus refinement in which a detailed 3D characterization of the geometric primitives is injected into the syntax of the calculus. In this way, models written with the new syntax can be directly simulated.

1 INTRODUCTION

Systems Biology (Kitano, 2002) could affect quite deeply our everyday life in the next few years. Modelling and computer simulation are rapidly changing the way in which biological phenomena and processes are studied. Contrasted to *in vivo* and *in vitro* experimentations, *in silico* (i.e. simulation) experimentation is cheaper, faster and much less expensive.

In silico experimentation is increasingly used, from the prediction of pathological phenomena (Grupe et al., 2001) to the tailoring of medical treatments based on the characteristics of an individual patient (Manos et al., 2008; Taylor et al., 1999) to the application of nanotechnologies for the diagnosis, prevention and treatment purely from a preventative state (Lim, 2004; Kumar, 2007; Torchilin, 2006). The final aim is to identify and stop potential sources of disease/illness, such as cancer, *before* they even get started (Ferrari, 2005; Kawasaki and Player, 2005).

In the context of this important challenge raised by Systems Biology, computer scientists have started to contribute by adapting (computational) models and languages, originally thought for the design and the analysis of hardware/software systems, to biological systems. This adaptation process has revealed that some of the languages, although general-purpose, needed to be expanded with concepts and characteristics typical of biological modelling. One of these features is surely *space*, considered both in a topological and a geometrical way. It is indeed well-known that space and physical concepts like *space occupancy*, *space subdivision*, *crowding* and *co-localization* play a fundamental role in determining bio-interactions, for instance at the cellular level (Takahashi et al., 2005). Crowding, in particular, may lead to significant alterations of biochemical or biological recognition processes at the molecular level (Minton, 1998) and affects folding and refolding of proteins, i.e. the process by which a protein structure assumes its functional shape or conformation (van den Berg et al., 1999).

Despite this, most of the modelling and the simulation approaches available today tend to assume a homogeneous distribution of entities in space and to abstract away specific spatial information. The Shape Calculus (SC) (Bartocci et al., 2010a; Bartocci et al., 2010b) has been proposed as a process calculus with a rich set of primitives to describe mainly, but not only, biological phenomena. The main characteristics of this calculus are that it is spatial — with a 3D geometric notion of space — and it is shape-based, i.e. entities have geometric simple or complex shapes that affect the possible interactions with other entities.

Formal SC models, i.e. process specifications, are currently used as a stub code for the associated simulation environment BioShape (Buti et al., 2010a; Buti et al., 2011b). However, the original SC 3D characterization of shapes and spatial channels is highly abstract and its bond with the actual geometrical data structures and code libraries used in BioShape is quite loose.

In this work we provide a different, more detailed and simulation-oriented syntax of the calculus. The

Table 1: A comparative table containing the Shape Calculus original syntax (left) with highlighted abstract geometric primitives and the new, simulation-oriented, syntax (right).

Basic Shapes	$\sigma = \langle \textcircled{H}, m, \mathbf{p}, \mathbf{v} \rangle$	$\sigma = \langle W, m, \mathbf{v}, \omega, s, T \rangle$
Shapes	$S ::= \sigma \mid S \langle \textcircled{X} \rangle S$	$S ::= \sigma \mid S \langle \{\varphi_1, \varphi_2\} \rangle S$
Behaviours	$B ::= \mathsf{nil} \mid \langle \alpha, \textcircled{X} \rangle.B \mid$ $\omega(a, \textcircled{X}).B \mid$ $\rho(\textcircled{L}^{*}).B \mid$ $\varepsilon(t).B \mid B + B \mid K$	$B ::= \mathsf{nil} \mid \langle \alpha, \{\varphi_1, \ldots, \varphi_n\} \rangle.B \mid$ $\omega(a, \{\varphi_1, \ldots, \varphi_n\}).B \mid$ $\rho(L^{**}).B \mid$ $\varepsilon(t).B \mid B + B \mid K$
3D Processes	$P ::= S[B] \mid P \langle a, \textcircled{X} \rangle P$	$P ::= S[B] \mid P \langle a, \{\varphi_1, \varphi_2\} \rangle P$
3D Networks	$N ::= \mathsf{Nil} \mid P \mid N \| N$	$N ::= \mathsf{Nil} \mid P \mid N \| N$

*where $L = \{\langle a, \textcircled{X} \rangle \mid \langle a, \textcircled{X} \rangle$ is a channel$\}$
**where $L = \{\langle a, \{\varphi_1, \ldots, \varphi_n\} \rangle \mid \langle a, \{\varphi_1, \ldots, \varphi_n\} \rangle$ is a channel$\}$

final aim is to produce a refinement of the language that syntactically incorporates a *finitary*, complete description of the geometry involved. This will make the bond between the specification language and the simulating code more tight, thus allowing the direct simulation of the models. It is worth noting that the resulting refined language does not loose the necessary abstraction needed to perform formal verification. In Table 1 we show, on left, the original grammar of SC where the abstract geometrical representations are highlighted. Throughout the paper we briefly explain and then revisit all the syntax categories and for each of them we introduce a finitary geometrical representation, summarized on the right.

The rest of the paper is structured as follows: Section 2 summarizes some basic concepts about the calculus, highlighting its limitations w.r.t. a computational simulation setting, Section 3 briefly introduces the simulation tool BioShape, Section 4 defines the new 3D representation of shapes, Section 5 describes the new syntax to define the behaviours associated to shapes, Section 6 provides some insight about the implementation of the new syntax in the simulation environment. Finally, Section 7 traces ongoing and future work.

2 THE SHAPE CALCULUS

The general idea of the SC is to consider a 3D space in which shapes move and interact. Shapes can be simple 3D generic geometric primitives (cubes, cylinders, etc.) or complex (even non convex) compositions of simpler shapes. While time flows, shapes move according to their velocity vectors that can change over time due to a general motion law (e.g. for an electromagnetic field), Brownian motion or collisions occurring between shapes.

Let us now briefly and informally summarize the semantics of the language passing through all the syntax categories (always refer to Table 1); the full formal semantics can be found in (Bartocci et al., 2010a; Bartocci et al., 2010b). Basic shapes are represented as tuples containing a set $\textcircled{H}$ of 3D points defining the shape (with a non-specified finitary representation), a mass $m \in \mathbb{R}^{+}$, a point p in 3D representing the centre of mass and a velocity $\mathbf{v}$. Composed shapes ($S \langle \textcircled{X} \rangle S$) are generated by glueing together basic or composed shapes on touching common surfaces ($\langle \textcircled{X} \rangle$, again with a non-specified finitary representation).

A shape (S) together with a behaviour (B) defines a *3D process* ($S[B]$), the basic building block of a SC model. 3D processes can also be composed processes ($P \langle a, \textcircled{X} \rangle P$) that are such that their original shapes are glued together on a certain *bound* ($\langle a, \textcircled{X} \rangle$) and their original behaviours operate in parallel (in Figure 1 we show an example of two 3D processes interacting). Action prefixing in behaviours ($\langle \alpha, \textcircled{X} \rangle.B$) represents an open channel ($\langle \alpha, \textcircled{X} \rangle$) associated to a shape.

Channels are derived from classical CCS (Milner, 1982) channels, where α is the channel name, intended as a type for binding certain species, and X is a certain region on the surface of the associated 3D shape in which the channel is “active”. Channels determine how a process responds to a collision. One of the first motivations of the calculus comes from the dynamics of molecules inside a cell, thus behaviours mimic what it is known to happen in biochemical reactions[1]. Like molecules, which can bind on a particular portion of their physical shape, 3D processes can bind if they collide on *compatible* surfaces.

A collision happening on *compatible channels*, i.e. having a corresponding CCS name/co-name and such that the intersection between their active surfaces is not empty, results in an *inelastic* response; the colliding processes bind and become a compound new process moving in a different way and having a different behaviour. Collisions on non-compatible channels

[1]However the calculus has then been demonstrated to be general enough to be applied to a lot of scenarios, at different scales, in different fields.

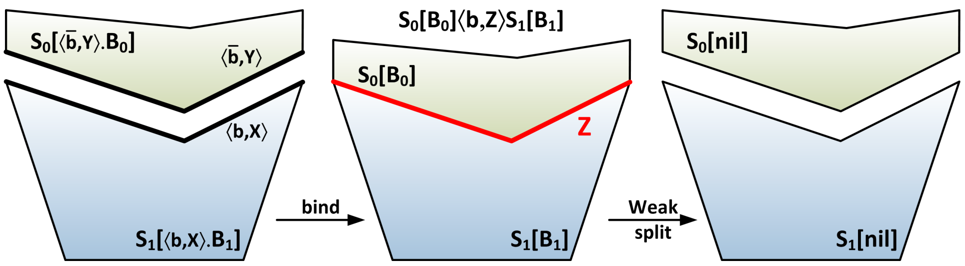

$S_0[\langle \bar{b},Y\rangle.B_0]$
$\langle \bar{b},Y\rangle$
$\langle b,X\rangle$
$S_1[\langle b,X\rangle.B_1]$
bind
$S_0[B_0]\langle b,Z\rangle S_1[B_1]$
$S_0[B_0]$
Z
$S_1[B_1]$
Weak split
$S_0[nil]$
$S_1[nil]$

Figure 1: Two 3D processes get near after an interval t (left) and then clash on compatible surfaces X and Y. Hence, an inelastic collision occurs and a binding is generated on surface $Z = X \cap Y$ (centre). After some other time, the compound shape weakly split and the components move away (right).

result in an *elastic* response, i.e. they bounce away. Compound processes can split weakly ($\omega(a, \textcircled{X}).B$) by non-deterministically releasing a previously established bond, or "react" (operator $\rho(\textcircled{L}).B$), by splitting in as many pieces as the products of the reaction are (i.e. the bonds in $\textcircled{L}$). Non-determinism in behaviours ($B + B$) permits the opening of several channels and the enabling of different splitting behaviours at the same time. The timed operator $\varepsilon(t).B$ waits t time units before proceeding with the continuation B. Finally, the process variable K is needed to specify recursive behaviours. A complete SC model corresponds to a 3D Network, i.e. the parallel composition of several 3D processes that are intended to evolve in the same space.

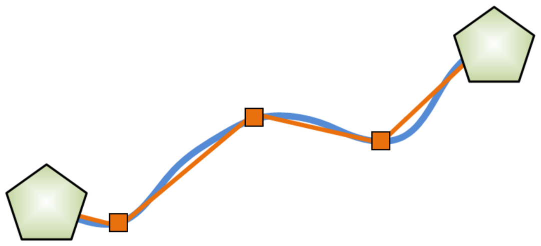


Figure 2: A continuous trajectory (blue) approximated via a polygonal chain (orange).

Time evolves discretely by timesteps of duration Δ, also called *movement time step*. At the beginning of each timestep the velocity of the shapes is updated by means of a so called steer function and remains constant until the subsequent timestep update. Both velocity update and evolution of shapes are represented as an update of the shape tuple(s). The resulting polygonal chain describing the movement of the shape approximates a corresponding continuous trajectory of the shape (see Figure 2). This approach is computationally cheaper than modelling continuous trajectories (Ericson, 2005) and quite faithful for reasonably small Δ. If a collision occurs, the timestep is shortened to the *instant* before the shapes start to interpenetrate (so called *first time of contact* or Ftoc) and the collision is resolved, according to what stated above for elastic and inelastic collisions. After the resolution a new timestep begins. The calculus does not embed a specific algorithm for Ftoc calculation and resolution so that any desirable collision detection/collision resolution system can be adopted.

3 BIOSHAPE: SHAPE CALCULUS MODELS AT WORK

BioShape (Buti et al., 2010a; Buti et al., 2010b; Buti et al., 2011a; Buti et al., 2011b) is a modelling and simulation environment that has been engineered in the perspective of being *uniform*, *particle-based*, *3D space-* and *3D geometry-oriented*. A shape in BioShape, being the concept inherited from the SC, can be either a basic one (a convex closed polyhedron) or a correctly composed one (a generic polyhedron). Note that differently from SC, here only the specific class of polyhedra is used for shapes. The basic element of a simulation is the *entity*, corresponding to a SC *3D process*. In other terms, an entity owns a particular 3D shape and a specific behaviour along with an associated physical motion law (the latter represented by an instance of the so called *Driver* class). The behaviour of every entity, i.e. the way in which it interacts with other entities and with the environment, is defined partially through the SC behaviour, and partially through Java programming. Hence, the SC acts as a sort of *stub code* for the simulation, but there is not a tight bond between the specification language and the implementation.

In the SC, shapes are defined w.r.t. a global 3D coordinate system that we call *world space*, whereas binding sites are always defined w.r.t. a system local to the shape. This approach poses a performance issue: the same redundant geometry structure is maintained for each instance of a 3D process whereas it would be sufficient to manage the *position* and the *orientation* of each process referring to a unique instance of the geometry structure. The simulator solves this problem by following a classical approach of rigid body simulations (Baraff, 1997). The shapes are defined in terms of a fixed and unchanging space called *body space*. A suitable *affine transformation* must be applied to move (i.e. translate and rotate) the shape points from the body-space description into the world space description. An affine transformation T is any transformation that preserves collinearity (i.e. all points lying on a line initially still lie on a line after transformation) and ratios of distances (e.g. the midpoint of a line segment remains the midpoint after transformation) and can be used to describe both rotations and translations, along with other transformations. Affine transformations are finitely represented by a 4x4 matrix. Thus, using this approach, the geometry is defined only once and acts as a sort of *template* which is then instanced to real shapes by defining different affine transformations. Figure 3 shows a shape template that is defined at the origin and then two shape instances, σ_0 and σ_1, with different positions and orientations, generated applying suitable transformations T_0 and T_1. Obviously, both instances will refer to the same, unique, shape template.

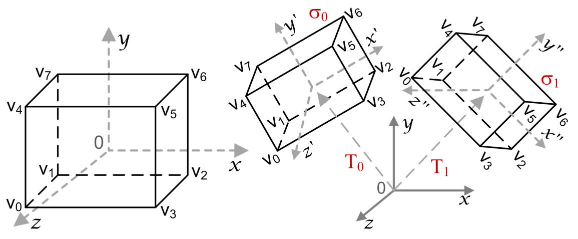


Figure 3: The declaration of a shape template (left) and its instantiation into two shapes (right), σ_0 and σ_1 with different positions and orientations due to their transformations T_0 and T_1.

Note that the description of the shape in body space is required to be such that the centre of mass of the body lies at the origin. Despite not being a strict requirement, this choice simplifies operations over the shapes and their transformations.

Whereas in the SC no specific collision detection algorithm is defined, in BioShape a two-phase algorithm based on V-Clip algorithm (Mirtich, 1998) is adopted in order to establish whether shapes collide and when (Ftoc).

To handle the computational cost of simulating 3D shapes moving in an environment, BioShape has been engineered to support both the *cluster* and the *distributed* computational approaches. BioShape is based on the agent-based Java framework Hermes[2], a middleware supporting distributed applications and mobile computing — see (Corradini and Merelli, 2005) for further information. Such framework enables BioShape to split the simulated space into *portions* which are assigned to different communicating computational nodes.

For other features of the modelling and simulation environment BioShape see (Buti et al., 2010a; Buti et al., 2010b; Buti et al., 2011a; Buti et al., 2011b).

4 NEW SHAPES

The usage of the calculus in a simulation setting requires that the boundary of a shape is correctly described and binding sites are unambiguously identified. However, as explained in the introduction, the calculus poses some limitations to its direct usage in a simulation setting: the *geometrical* representation of a shape is, in fact, unspecified and the identification of common touching surfaces is vague. These limits call for a different, more detailed, representation of the shapes in which all the geometric elements composing them can be finitely embedded into the syntax and unequivocally identified.

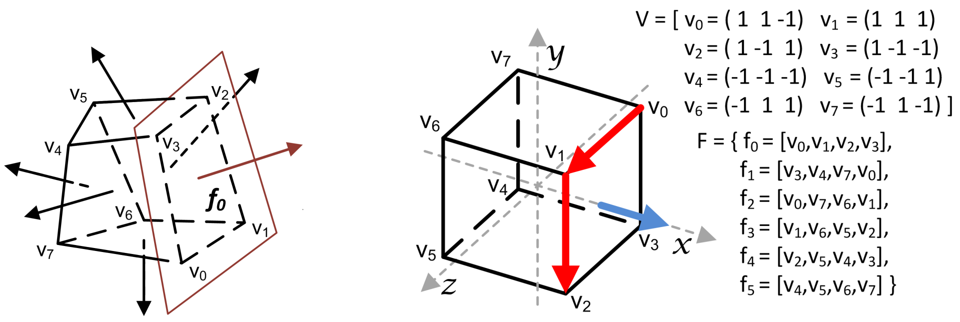
Since interactions occur on compatible shape *surfaces*, we are interested in characterizing a shape in terms of its *boundary* more than in terms of *all* its constituent points, as done in the original syntax. To this purpose, as a first step, we discard the generic primitives mentioned in Section 2, to focus solely on polyhedral shapes.

Polyhedra (or polyhedrons) are one of the most widely used geometric solids in computer-modelling applications (Ericson, 2005). In particular, they are used to model real-world objects in computer graphics and obstacles in robotic systems. Given a polyhedron W in 3D, it is a set of points whose boundary consists of planar pieces called *facets* (*faces* in 3D). The faces of W meet along straight line segments, called *edges* while its edges meet at *vertices*. Faces, edges and vertices of a polyhedron are called its **features** — see (Hoffmann, 1989; Mäntylä, 1988) for a deeper introduction on polyhedra. We are particularly interested in polyhedra which are *convex* and *closed* because these will be the new basic shapes.

4.1 Basic Shapes

A *convex* polyhedron is a solid for which the entire figure lies on one side of the plane of each constituent polygon. Equivalently, we can say that a polyhedron is convex iff it contains the entire segment between any pair of its points. Since a convex polyhedron lies

[2]HermesV2 official site: `http://hermes.cs.unicam.it`


v5
v2
v4
v3
f0
v6
v1
v7
v0
V = [v0 = (1 1 -1) v1 = (1 1 1)
v2 = (1 -1 1) v3 = (1 -1 -1)
v4 = (-1 -1 -1) v5 = (-1 -1 1)
v6 = (-1 1 1) v7 = (-1 1 -1)]
F = { f0 = [v0,v1,v2,v3],
f1 = [v3,v4,v7,v0],
f2 = [v0,v7,v6,v1],
f3 = [v1,v6,v5,v2],
f4 = [v2,v5,v4,v3],
f5 = [v4,v5,v6,v7] }
y
x
z
v7
v6
v1
v4
v0
v5
v3
v2

(a) (b)

Figure 4: A convex polyhedron **(a)** with the faces outward normals. A cube description **(b)** in terms of an IFS; note the example normal (blue) automatically calculated by cross product of the first two edges (red) of the corresponding face.

on one side of the plane of each of its faces, it is easy to show that at most *two* faces meet at any edge and that any interior point of one face cannot belong to another face. A convex polyhedron is *closed* if all its edges belong to exactly two faces.

In a convex polyhedron the planes of all its faces are *support planes*. A support plane is a plane having at least one point in common with the figure and such that the entire figure lies in one of the two half-spaces bounded by the plane[3]. In particular, the direction of a support plane is always the direction of its outward normal. Thus, the direction of a face of a polyhedron is the direction of the same outward normal vector, i.e. the direction pointing away from the face. In Figure 4(a) a convex polyhedron is shown, along with the support plane for the face $[v_0, v_1, v_2, v_3]$ and the outward normal; normals for other faces are also represented. Looking at the picture, we can intuitively identify an important property captured by the following theorem — see (Aleksandrov, 2005) for the proof:

Theorem 4.1 (Polyhedron and support planes)**.** *Every convex closed polyhedron is determined by the planes of its faces and their outward normals.*

Hence, we can correctly define a convex, closed polyhedron in terms of its faces, which in turn can be defined in terms of the composing vertices and the normal.

For the purpose of this paper, we adopt the approach of *indexed face set* (IFS), a general data structure often used in computer graphics (Hartman and Wernecke, 1996; Murray and VanRyper, 1996). However, since we want to use *names* in the syntax, we slightly adapt this approach as described below.

In an IFS representation, a sequence of points is followed by the definition of a sequence of faces. Each face is a list of indices referring to the sequence of vertices. The latter are stored in a **counter-clockwise** (ccw) order by default, making explicit declaration of normals unnecessary. Indeed, the vector normal is automatically calculated via the cross product of two vectors connecting the first vertex of the face to the second, and the second to the third. Edges must be derived implicitly from adjacent vertices in the enumeration of the vertices of a face. Picture 4(b) shows an example of IFS for a cube of side two. The cube is generated with its centre at the origin (as suggest in Section 3) so that its vertices are positioned at a maximal distance of one in all of the three coordinates. Note also the normal calculated as described above (i.e. $(v_3 - v_2) \times (v_0 - v_3)$). A clockwise order of the vertices would have generated negated vectors and thus a negated normal, i.e. with *opposite* direction, and the resulting polyhedron would have *not* been closed.

Let us formalize all these concepts into the SC setting. We are interested in correctly identifying all the features of a polyhedron. Hence, we enrich the notation of the IFS by adding a name to each vertex and by defining faces as tuples over these names.

Let $\mathbb{P} = \mathbb{R}^3$ be the sets of positions. Let NamesV be an infinite numerable set of names $\{u, v, w, \ldots\}$ that will be used to denote positions. Vertices denotes the set of all tuples of length one composed by names in NamesV. These tuples will be used to represent vertex features. For instance, face f_0 in Figure 4(a) has the following four vertices: $[v_0], [v_1], [v_2]$ and $[v_3]$. We will range over both elements of NamesV and Vertices by $u, v, w, \ldots$ since the denoted element can be always understood by the context. Edges, ranged over by $e, e', e_1, \ldots$ denotes the set of all tuples of names in NamesV with length two. These will represent the edge features. For instance, face f_0 in Figure 4 has the following four edges: $[v_0, v_1]$, $[v_1, v_2]$, $[v_2, v_3]$ and $[v_3, v_4]$. Faces, ranged over by $f, f', f_1, \ldots$

[3]Following the definition, it is possible to define support planes also for vertices and edges. However they are of no interest in this work.

denotes the set of all tuples of names in NamesV, with length greater than or equal to three[4], representing face features of our shapes. For instance, face f_0 of Figure 4(a) can be represented by $[v_0, v_1, v_2, v_3]$.

Note that, each type of feature can be characterised by its *dimension*, which can be defined informally as the minimum number of coordinates needed to specify any point within it. Hence, vertices have dimension *zero*, edges have dimension *one* and faces have dimension *two*.

Note also that, as we explained above, the order of the names in the tuples matter. However, since a face is basically a sequence of its vertices (listed in the tuple), there are multiple tuples denoting the same face, one for each composing vertex. This naturally leads to the definition of an equivalence relation in Faces.

Definition 4.1 (Rotation equivalence)**.** *Given a face representation as a tuple $f = [v_1, \dots, v_n]$, then the tuple $f' = [v_n, v_1, \dots, v_{n-1}]$ is an equivalent representation of f. We will write $f \equiv f'$.*

For instance, the face of the polyhedron of Figure 4(a) can be equivalently represented by $[v_0, v_1, v_2, v_3]$, $[v_3, v_0, v_1, v_2]$, $[v_2, v_3, v_0, v_1]$ and $[v_1, v_2, v_3, v_0]$.

Finally, we define the set Features of all features, ranged over by $\varphi, \varphi', \varphi_1, \dots$ as the union Vertices $\cup$ Edges $\cup$ Faces. Now we need to introduce some functions that will be useful in the following.

Definition 4.2 (Downgrade and Closure functions)**.** *Given $e \in$ Edges, $f \in$ Faces and given $V \subset$ Vertices, $E \subset$ Edges and $F \subset$ Faces, we define downgrade functions $\mathbf{dg}(e) \triangleq \{[v] \mid e = [v_1, v_2] \wedge v \in \{v_1, v_2\}\}$ and $\mathbf{dg}(f) \triangleq \{[v_i, v_j] \mid f = [v_0, \dots, v_{n-1}] \wedge i \in \{0, \dots, n-1\} \wedge j = i + 1 \mod n\}$. We also lift the functions $\mathbf{dg}$ on sets: $\mathbf{dg}(E) \triangleq \bigcup_{e \in E} \mathbf{dg}(e)$ and $\mathbf{dg}(F) \triangleq \bigcup_{f \in F} \mathbf{dg}(f)$. Finally, we define a closure operator on a set of Features Φ:*

$$\mathbf{closure}(\Phi) \triangleq \begin{array}{l} \{v \mid v \in \Phi \wedge v \in \text{Vertices}\} \cup \\ \{e \mid e \in \Phi \wedge e \in \text{Edges}\} \cup \\ \{f \mid f \in \Phi \wedge f \in \text{Faces}\} \cup \\ \mathbf{dg}(\{e \mid e \in \Phi \wedge e \in \text{Edges}\}) \cup \\ \mathbf{dg}(\{f \mid f \in \Phi \wedge f \in \text{Faces}\}) \cup \\ \bigcup_{e \in \mathbf{dg}(\{f \mid f \in \Phi \wedge f \in \text{Faces}\})} \mathbf{dg}(e) \end{array}$$

Downgrade functions are used to obtain a set of features of lower dimension from features of higher one. For instance, the application of the downgrade function to face $f_0 = [v_0, v_1, v_2, v_3]$ of polyhedron of Figure4(a) returns the composing edges: $\mathbf{dg}(f_0) = \{[v_0, v_1], [v_1, v_2], [v_2, v_3], [v_3, v_0]\}$. The same applies to the edges, e.g. for $e_0 = [v_0, v_1]$ in f_0 we have that $\mathbf{dg}(e_0) = \{[v_0], [v_1]\}$. The closure operator is used to add to any given set of features all missing features of lower dimensions that compose them. For instance, consider the set $\Phi = \{f_0, [v_1]\}$, then $\mathbf{closure}(\Phi) = \{f_0, [v_0, v_1], [v_1, v_2], [v_2, v_3], [v_3, v_0], [v_0], [v_1], [v_2], [v_3]\}$.

We are now ready to introduce formally a convex polyhedron described as an IFS.

Definition 4.3 (Convex closed polyhedron)**.** *Let $V \subset$ Vertices be a finite set of vertices and let $F \subset$ Faces be a finite set of faces. The set $W = V \cup F$ represents a convex closed polyhedron iff all of the following conditions hold:*

1. *$|V| \geq 4$ and $|F| \geq 4$[5];*
2. *each tuple $f \in F$ is composed only of vertices in V;*
3. *V is not a collinear set, i.e. the positions of the vertices do not lie on a single line;*
4. *$\forall f \in F, f$ is a convex polygon;*
5. *$\forall f_i, f_j \in F$, it holds that $f_i \not\equiv f_j$, according to Definition 4.1;*
6. *angles between any two edges in $\mathbf{dg}(F)$ are convex, i.e. less than 180 degrees;*
7. *the Euler characteristic, i.e. $\chi = |V| - |\mathbf{dg}(F)| + |F|$ must be equal to 2.*

The first condition is necessary, since the simplest polyhedron which can be defined is a tetrahedron, having exactly four vertices and four triangular faces. Second condition ensures that the generated IFS contains only faces whose vertices are available in the set itself. Conditions 3-7 are sanity checks, needed to guarantee that a generated IFS correctly describes a convex closed polyhedron — see again (Aleksandrov, 2005) for deeper geometrical details.

Apart from tetrahedrons, other basic figures can be defined according to the definition above, such as cubes, parallelepipeds and generic convex *prismatoids*, i.e. prisms, antiprisms, pyramids, cupolas, frustums and wedges. Other primitives, i.e. cones, cylinders and spheres cannot be used directly but can be approximated to corresponding polyhedral representations.

We are now ready to introduce the new basic shapes of our calculus, following the previous definitions. Similarly to the approach described in Section 3, we will use a convex closed polyhedron, as defined in Definition 4.3, as a *template*, i.e. only one data structure for one kind of W is created. Then, any *instance* of the template can be obtained by applying an affine transformation that will move the shape into

[4]Indeed, a face must be at least a triangle.

[5]By $|\cdot|$ we denote the cardinality of a set.

the world space. Moreover, we add a name for basic shapes that will create a *namespace* to give unique names to the feature of each instance. For example, if in the template W there is a face $f_0 = [v_1, v_2, v_3, v_4]$, then in an instance s_0 the corresponding face will be denoted by $s_0.f_0 = [s_0.v_1, s_0.v_2, s_0.v_3, s_0.v_4]$, where s_0 is the name of the instance.

Definition 4.4 (New Basic Shapes)**.** *A basic shape σ is a tuple $\langle W, m, \mathbf{v}, \omega, s, T\rangle$ where $W = V \cup F$ is an IFS representing a convex closed polyhedron as described in Definition 4.3, $m \in^+$ is the mass*[6]*, $\mathbf{v}$ is the translation velocity, ω is the angular velocity, s is the name of the basic shape taken from an infinite numerable set of names* NamesB *and T is a transformation matrix that moves the template W from the body space to the world space of the model. We denote by $T(W)$ the IFS moved to the world space. All possible basic shapes are ranged over by $\sigma, \sigma', \sigma_1 \ldots$.*

Differently from the original definitions, now shapes have also an associated angular velocity, i.e. they can also rotate in addition to translate. While time flows the position of each shape will be updated by changing its affine transformation according to the associated translation and rotation velocities.

Consider a cube whose geometry $W_0 = V \cup F$ where V and F are the ones provided in Figure 4(b). A correctly instanced cube σ is a tuple such as the following: $\sigma = \langle W_0, m = 3, \mathbf{v} = (2,1,1), \omega = (0,0,0), s_0, T\rangle$ where T is such that the shape does not rotate and translate of a vector $(2,3,1)$. The current position of the cube can be derived by its transformation T and its position in the body space. Since the geometry is defined in a body space with the centre of mass in the origin, $(2,3,1)$ corresponds also to the current position of σ. Moreover, since the instance has no angular velocity, it is only going to translate by the amount specified by $\mathbf{v}$.

4.2 Compound Shapes

Basic shapes can be glued together to form more complex shapes, also non-convex ones. Intuitively, two shapes can be attached if they do not interpenetrate and at least one of their features *touch* in the world space. Note that more than one feature from both shapes may be touching, e.g. when two shapes are involved in a perfect face-face collision such that also edges and vertices are in contact. However, just one feature of each shape may be involved, e.g. when the shapes collide in a face-vertex case.

It is sufficient for our purposes to syntactically specify just *one* feature from each of the composing shapes, but with the requirement that it is with the highest possible dimension.

Definition 4.5 (New 3D Shapes)**.** *The set of the* new 3D shapes*, ranged over by $S, S', S_1 \ldots$, is generated by the grammar: $S ::= \sigma \mid S\langle\{\varphi_1, \varphi_2\}\rangle S$ where σ is a new basic shape and φ_1, φ_2 are two features, one from each of the two glued shapes, such that they touch without interpenetrating and they are of the highest possible dimension.*

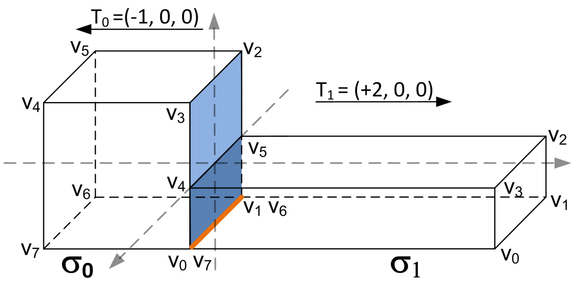


Figure 5: A compound shape S_0, obtained by glueing together two basic shapes, σ_0 and σ_1.

For example, with this definition, we can generate a concave compound shape, as the one represented in Figure 5. This shape is formed by an instance of the cube template of Figure 4(b) and an instance of a parallelepiped template W_1. For the sake of brevity we do not present the IFS defining the parallelepiped but we assume that, like the cube, it has been defined with the centre of mass in the origin and also that it has sides of size $4, 1, 2$, i.e. it is double the length of the cube, half its height and has the same depth.

The final compound shape of Figure 5 is obtained by generating the two instances and by moving them on the x-axis according to the vectors depicted in figure. The two instances are represented by tuples: $\sigma_0 = \langle W_0, m_0 = 3, \mathbf{v}_0 = (2,1,0), \omega_0 = (0,0,0), s_0, T_0\rangle$ and $\sigma_1 = \langle W_1, m_1 = 3, \mathbf{v}_1 = (2,1,1), \omega_1 = (0,0,0), s_1, T_1\rangle$[7]. The glueing features is the set of two faces touching at the origin, (blue features in Figure 5) even if the two shapes touch only on a portion of such features (dark blue section in Figure 5). The features are called $s_0.f_0 = [s_0.v_0, s_0.v_1, s_0.v_2, s_0.v_3,]$ and $s_1.f_1 = [s_1.v_4, s_1.v_5, s_1.v_6, s_1.v_7,]$. Hence, the final shape is defined as $S_0 = \sigma_0\langle\{s_0.f_0, s_1.f_1\}\rangle\sigma_1$. Note that, in this case, it is not possible to select another set of features. For instance, if we select edges $s_0.e_0 = [s_0.v_0, s_0.v_1]$ and $s_1.e_1 = [s_1.v_6, s_1.v_7]$ (coloured orange in the picture) we would not satisfy the requirement of the highest dimension.

[6]We will always consider solid bodies with uniform mass density.

[7]The velocity vectors of the two shapes are the same, this ensure that while moving they would not eventually interpenetrate or move apart.

5 NEW CHANNELS AND 3D PROCESSES

Channels in SC represent active sites on the surfaces of shapes on which a possible collision-driven interaction can occur. In the original syntax they are of the form $\langle \alpha, X \rangle$ where α is the channel name and X is a surface of contact that must belong to the surface of the shape in which the channel is opened. The name α belongs to NamesC, ranged over by $\alpha, \beta, \ldots$, defined as $\Lambda \cup \bar{\Lambda}$ where Λ is an infinite numerable set of names $a, b, c, \ldots$ and $\bar{\Lambda} = \{\bar{a} \mid a \in \Lambda\}$. The set X must be substituted by a finitary representation. The natural candidate is a finite set of features belonging to the shape in which the channel is embedded. To avoid writing a long list of features one can use the closure operator of Definition 4.2.

5.1 Channels in Behaviours

Channels are part of behaviours. They can occur in action prefix ($\langle \alpha, X \rangle$) as well as in weak- and strong split operators ($\omega(\langle a, X \rangle)$ and $\rho(L)$ respectively).

Definition 5.1 (New Behaviours)**.** *The set of* new Behaviours*, ranged over by $B, B', B_1 \ldots$, is generated by the grammar:*
$B ::= \mathsf{nil} \mid \langle \alpha, \{\varphi_1, \ldots, \varphi_n\} \rangle . B \mid \omega(a, \{\varphi_1, \ldots, \varphi_n\}) . B \mid \rho(L) . B \mid \varepsilon(t) . B \mid B + B \mid K$
where $\varphi_1, \ldots, \varphi_n$ are feature representations and $L = \{\langle a, \{\varphi_1, \ldots, \varphi_n\} \rangle \mid \langle a, \{\varphi_1, \ldots, \varphi_n\} \rangle$ is a channel$\}$. For any channel $\langle \alpha, \{\varphi_1, \ldots, \varphi_n\} \rangle$, its surfaces of contact will always be intended as the union of all features in **closure**$(\{\varphi_1, \ldots, \varphi_n\})$*. It is also required that the features of the channel with the highest dimensions are listed in $\{\varphi_1, \ldots, \varphi_n\}$.*

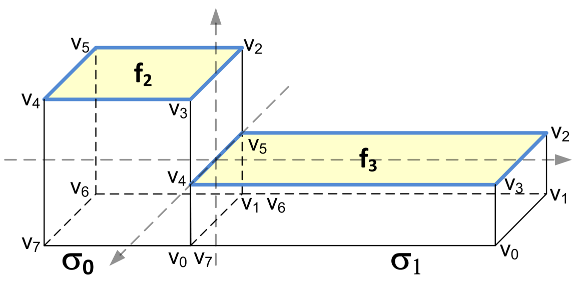


Figure 6: A channel α (yellow) defined over two faces, f_2 and f_3, of the compound shape S_0. The features generated by the closure function are also represented (blue).

Consider the compound shape of Figure 5. We would like to define a communication channel named α on the face $f_2 = [v_3, v_2, v_5, v_4]$ and the face $f_3 = [v_3, v_2, v_5, v_4]$ (highlighted in Figure 6). Thanks to the closure function we do not need to enumerate all the involved features but just the ones at higher dimensions. Hence, we can define a channel $\langle \alpha, \{s_0.f_2, s_1.f_3\} \rangle$. The closure function will correctly generate all the edge/vertex features of both f_2 and f_3.

Note that the features declaration in a channel *always* requires that shapes names are prepended to the features names. However, when the channel is declared on a basic shape, the naming can be dropped since the features are unambiguously identified by their names. In any case, when two shapes are glued together, the shape naming must be used to avoid features name clashing, e.g. when two instances of the same shape template bind together.

5.2 3D Processes

A 3D process is the composition of a shape S with a behaviour B ($S[B]$). In the new setting, name correspondence is a crucial constraint to be satisfied: all the channels in B must syntactically be consistent with the names of features belonging to S. Recall that these features are named using the namespace created by each basic shape.

When a collision-driven interaction occurs, we have that two 3D processes are colliding on compatible channels and the result is that they bind on the surfaces of contact and become a new compound 3D process. We syntactically represent the bound in the same way we used for compound shapes. In this case, however, also the name of the channel must be retained.

Definition 5.2 (New 3D Processes)**.** *The set of* new 3D processes*, ranged over by $P, P', P_1 \ldots$, is generated by the grammar: $P ::= S[B] \mid P \langle a, \{\varphi_1, \varphi_2\} \rangle P$ where a is the name of the channel and φ_1, φ_2 are features belonging to the shapes associated with the compound 3D processes.*

Consider a 3D process with a shape as in Figure 5 and with an active communication channel α as in Figure 6, i.e. a 3D process $P_0 = S_0[\langle \alpha, \{s_0.f_2, s_1.f_3\} \rangle . B_0]$. Then, assume that a second 3D process $P_1 = \sigma_2[\langle \bar{\alpha}, \{s_2.f_4\} \rangle . B_1]$ with $\sigma_2 = \langle W_2, m_2 = 3, \mathbf{v}_2, \omega_2, s_2, T_2 \rangle$ clashes[8] with P_0, as shown in Figure 7. Since the collision happens on compatible features the processes can bind. This is a particular case since the processes have *more than one* contact point. It is solved simply by choosing non-deterministically one of the two. Suppose that

[8]Again we do not present W_2, i.e. the IFS defining the shape. Moreover, we assume that the transformation T_2 applied to P_1 not only translated it but also applied a rotation which resulted in the particular position assumed in the picture.

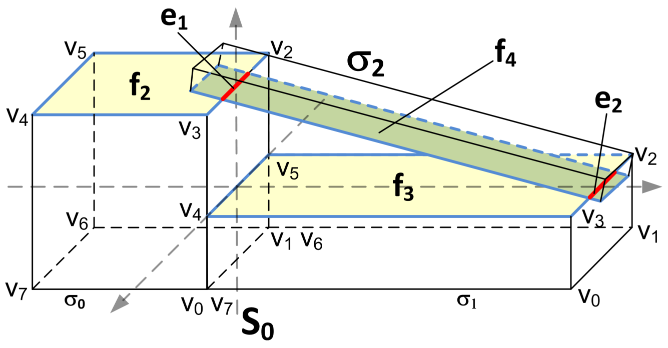


Figure 7: A compound 3D process, generated by glueing together a process with a compound shape (S_0) and a process with a simple shape (σ_2), clashing on compatible channels. Supposed α the name of the channel, two possible bounds can be created: $\langle a, \{s_0.e_1, s_2.f_4\}\rangle$ and $\langle a, \{s_1.e_2, s_2.f_4\}\rangle$ with s_0 and s_1 names of the basic shapes σ_0 and σ_1 components of shape S_0. With more than one contact point available (red), one is chosen non-deterministically as the binding surface.

the processes are going to bind on the edge $s_0.e_1 = [s_0.v_2,\ s_0.v_3]$ of σ_0, then the new compound 3D process has the form: $S_0[B_0]\langle a, s_0.e_1,\ s_2.f_4\rangle\sigma_2[B_1]$ where B_0 and B_1 are the behaviours after the binding occurred.

6 IMPLEMENTATION

The current implementation of BioShape takes as input an XML file containing the specification of the shapes, the behaviours associated and other simulation-related information. The related XML Schema provides the right means to declare vertices and faces according to the IFS representation described in Section 4.

It can be argued that such representation is quite tedious to be defined by hand and also difficult to understand at first glance (cfr. Figure 4(b)), discouraging a potential user. However, in the 3D simulation field, several different approaches have been proposed to alleviate this issue simply by making the generation of the actual coordinate points and faces transparent to the user. Among others, the *inflatable icons* approach (Repenning, 2005) seems the most suitable to be implemented in BioShape (Buti et al., 2011a).

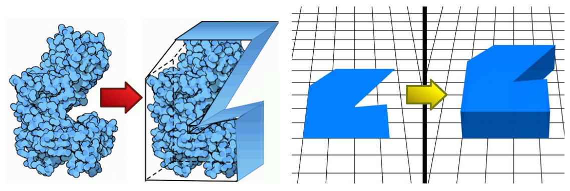


Figure 8: An hexokinase enzyme can be approximated to a concave polyhedral shape **(a)**. The same polyhedral shape can be generated through inflation **(b)**.

In the inflatable icons technique the user draws a simple 2D form of the final shape and then *inflates* it in order to create a 3D form (see Figure 8 for an example). Inflation can be applied with different strengths to different portions of the 2D/3D entity, to create particularly complex (still polyhedral) shapes. Note that the user can generate even non-convex shapes, such as the approximated hexokinase enzyme in Figure 8. Suitable algorithms can be applied to calculate automatically a convex decomposition of the shape, either on the 2D representation — see (Keil, 2000) for several approaches — or on the final 3D one — see (Belov, 2002).

7 CONCLUSIONS

The Shape Calculus provides a power syntax and semantics to model (not only) biological processes with particular regard to the spatial aspects. In this paper we refined the language to provide a more detailed, finitary, geometric representation of shapes and their communication channels. The resulting language maintains the same characteristics of the original one, adding a simple, yet powerful, way to define and manage geometry. Differently from the original characterization the newer syntax permits to directly embed a Shape Calculus model into a simulation in BioShape and still verification techniques can be applied. To give more evidence on this, the refinement proposed in this work can be re-formulated in the Abstract Interpretation (Cousot and Cousot, 1977) framework. We leave this as future work.

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