Shape Calculus
A spatial calculus for 3D colliding shapes

Ezio Bartocci, Flavio Corradini, Maria Rita Di Berardini,
Emanuela Merelli, Luca Tesei

Shape Calculus
A spatial calculus for 3D colliding shapes

Ezio Bartocci   Flavio Corradini   Maria Rita Di Berardini

Emanuela Merelli   Luca Tesei

School of Sciences and Technology, University of Camerino
Via Madonna delle Carceri 9, 62032, Camerino (MC), Italy.
Email: `name.surname@unicam.it`

Abstract

We present a bio-inspired calculus for describing 3D shapes moving in a space. A shape forms a 3D process when combined with a behaviour. Behaviours are specified with a timed CCS-like process algebra using a notion of channel that models naturally binding sites on the surface of shapes. Processes can represent molecules or other mobile objects. The calculus embeds collision detection and response, binding of compatible 3D processes and splitting of previously established bonds.

1 Introduction

The inspiration for this work mainly originates from the potential that moving objects, 3D-shaped colliding in a space, may have in modelling the real dynamics of the cell, or of a biological system in general, towards a personalised virtual physiological human. In a near future, systems biology will profoundly affect healthcare and medical science. The aim is to design and test "in-silico" drugs giving rise to individualised medicines that will take into account physiology and genetic profiles [11]. The advantages of performing in-silico experiments by simulating a model, instead of arranging expensive in-vivo or in-vitro experiments, are evident. But of course the models should be as faithful as possible to the *real system*. Takahashi et al. underline, in [18], the importance of considering space when modelling cellular phenomena and in particular biochemical signal cascades. They also highlight that macromolecular crowding in a limited space can also deeply affect biochemical reactions in the cell. Since physical concepts like space occupancy, intra-cellular movement, contacts (collisions) and shape transformation determine biomolecular interactions and therefore cell life, there is the need to provide physical characteristics (shape, mass, size, position) to entities. Then, we can collocate them in the continuum space, allow them to autonomously move and to interact with their spatial neighbour/colliding entities, reacting accordingly to their specified behaviour in order to reproduce the *emerging behaviour* observable in in-vivo and in-vitro experiments.

Many process algebras have been proposed in systems biology for modelling biological systems [16, 17, 7, 4, 9], accomplishing different kinds of abstractions. The common assumption in these calculi is that the systems are always well-stirred, which means that the positions become randomly uniform over a contained volume. This distribution is often generated by several simulation methods [12] based on the theory of stochastic chemical kinetics. When systems are not well-stirred, the ideal way to simulate the time evolution of a chemical system would be to use molecular dynamics, in which the exact positions and velocities of all the molecules in the systems are tracked. In these cases the concepts of space and time play a fundamental role, and only recently they have been taken into account in process calculi for systems biology. BioAmbients [17]
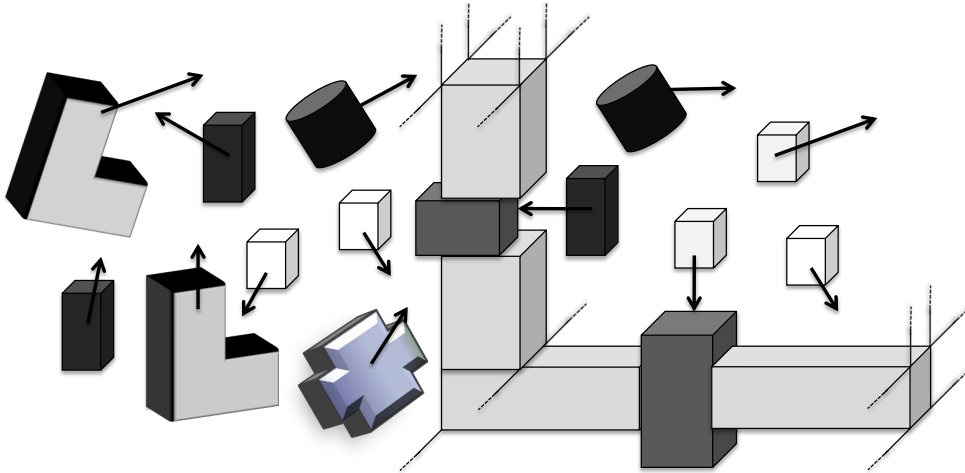
Figure 1: An example of a network of 3D processes.

considers space as a set of communicating compartments, while in Spatial CLS [2] and SpacePI [14] the entities involved are modeled as spheres situated in space. SpacePI [14] proposes an extension of the π calculus equipped with time and space. In this algebra processes can communicate if they are sufficiently close, but no shapes are considered. However, in biochemistry, the shape of an enzyme plays a very important role in biochemical interactions. The behaviour or the function of an enzyme is mostly determined by its 3D structure (shape).

The paradigm of our calculus goes towards this direction defining 3D processes as entities composed of a 3D shape and a dynamic behaviour. Processes are situated in a space, move accordingly to specific motion laws (as, for instance, acceleration in a gravitational field or Brownian motion), collide and possibly bind with others processes becoming compound 3D processes. The binding depends on channels $\langle a, X \rangle$, derived from classical CCS [15] channels, where a is the channel name, intended as a type for binding certain species, and X is a certain region on the surface of the 3D process in which the channel is "active". The binding corresponds to communication on these channels. It occurs if and only if the surface of collision of two 3D processes belongs to active channels of both processes and the names of the channels are co-names à la CCS. Compound processes can split weakly, by non-deterministically releasing a previously established bond, or "react", by splitting urgently in as many pieces as the products of the reaction are. If communication (i.e. binding) does not occur, the collision of two 3D processes is considered elastic, i.e. the shapes bounce and proceed independently.

In this paper we mainly focus on the definition of the calculus and its semantics proving a basic correctness property of dynamic well-formedness conservation. The contribution of this work is twofold. On the theoretical side it is one of the first steps, within concurrency theory, that starts modelling and reasoning about combined complex aspects such as space, shapes, movement and collisions (an ongoing work in the framework of π calculus is available in [8]). On the practical side, it is a fundamental step of formalisation in a design process, on which we have been working for a few years, of a spatiotemporal simulator [5, 6] that is intended to become the computational engine of a workbench within which biologists can define, run, monitor, stop, modify and re-run in-silico experiments. In this (future) scenario the Shape Calculus has to be considered the low-level executable language of the simulator on which more complex high-level-specified simulations are mapped. This is because the calculus embeds the minimum set of primitives that are needed to treat this kind of problems, that is to say it represents a kernel language on which high-level languages for biological specifications can be built.

The paper is organised as follows. Section 2 gives an overview of the calculus combining graphical
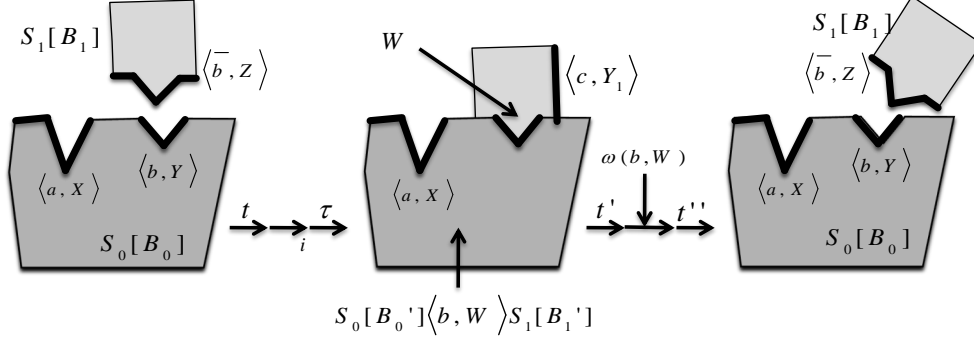
Figure 2: An example of binding and subsequent weak-splitting of two 3D processes.

intuition with sample pieces of processes in order to understand the basic operators of the calculus and the reasons behind their introduction. Section 3 introduces more formally 3D shapes, shape composition, movement, collision detection and collision response. Section 4 defines behaviours and 3D processes giving them full semantics. Section 5 puts all the pieces together and specifies precisely networks of 3D processes and a general result of dynamic well-formedness is proven. Finally, Section 6 concludes with ongoing and future work directions. For the sake of readability the proofs of all the propositions and theorems are placed in Appendices A, B and C.

A short preliminary version of this paper appeared in [3].

2 Overview of the Calculus

In this section we give some intuitions about the objects of the calculus and their possible behaviours. The general idea of the Shape Calculus is to consider a three-dimensional space in which several shapes reside, move and interact. Figure 1 shows a possible scenario at a certain time instant: on the left side there are simple 3D shapes (cubes, cylinders, etc.) or more complex ones, obtainable by "glueing" two given shapes on a common surface, moving freely in space. The arrows represent their instant velocity vectors. On the right side there is a composition of shapes enclosing a certain portion of the space. Their velocity vector is zero and it is intended to remain zero over time. These shapes can represents walls to the shapes inside and outside the enclosed region. Some of the pieces of the "walls" can represent doors that could open if some specific object hits them. We will call *network of 3D processes* a scenario like the one in figure.

While time flows shapes move according to their velocities, that can change over time both due to a general motion law - for instance as in a gravitational or in an electromagnetic field, or Brownian motion - and due to collisions that can occur between two or more shapes. Collisions can result in a bounce, that is to say *elastic* collisions. While, as it often happens for biological objects, colliding objects can bind and become a compound new object moving in a different way and possibly having a different behaviour. In this case we speak of *inelastic* collisions.

Naturally, the Shape Calculus can be used to represent a lot of scenarios at different scales in different fields. We can zoom into the atom, into a cell, into a tissue, into an organ of an organism. Or we can represent populations of animals, like fishes or birds, and their dynamics and interactions in a given environment. We can even zoom out and represent planets and their orbits.

However, our first motivation comes from the dynamics of molecules inside a cell, and thus we will mostly use this scenario in the paper for giving examples. We now let such biological metaphor guide us to the definition of behaviours of 3D shapes thinking of what it is known to happen in biochemical reactions. We can think that 3D shapes represent molecules swimming in a portion of a cell. We could be interested in just a homogeneous portion or, using the "walls", we could represent

membranes and different compartments inside the cell. Every species of molecule has a specific shape and we know from biology that the functions of a molecule are tightly related to its shape. For instance, in enzymatic reactions the functional sites that are active in the enzyme structure, at a given time, determine which substrate (one or two metabolites) can bind the enzyme and proceed to the catalysed reaction.

Figure 2 shows a (2D for simplicity) representation of a possible dynamic of an enzymatic reaction. Syntactically, we represent the larger shape, in this case playing the role of an enzyme, with the term $S_0[B_0]$ where S_0 is a term representing the shape and B_0 is a term representing the current behaviour of the shape. These two objects together constitute a 3D process. The term $S_1[B_1]$ represents a metabolite that is close to the given enzyme. Note that some surfaces of the shapes (the geometrical part of the 3D process) are highlighted: they are the *channels* that the current 3D processes exhibit to the environment. Channels are specified in the behaviours of processes and consist of two components: a channel name and an active surface. For instance, in Figure 2 $\langle a, X \rangle$ is an open channel of type a on the active site X of process $S_0[B_0]$. Note that X must be a portion of the surface of S_0 for $\langle a, X \rangle$ to be a valid channel. In this case, the enzyme has two open channels and the process is specified as follows: $S_0[\langle b, Y \rangle.B_0' + \langle a, X \rangle.B_0''']$. The operator $+$ represents the non-deterministic choice between the two possible communications on the channels. Note that this non-determinism is resolved during the evolution of the system depending on which 3D processes will collide with the enzyme and where.

Following the evolution proposed in the figure, after some time t elapsed (represented by the transition $\xrightarrow{t}$), after a detection and resolution of an inelastic collision (transition $\rightarrow_i$) and after a communication (action τ), we get one compound process represented by the term $S_0[B_0']\langle b, W \rangle S_1[B_1']$. Note that communication *is* the binding, and it can happen only if there is a collision between two processes that expose two compatible channels (name and co-name à la CCS) on their surface of contact. If the channels were not compatible, the collision would have been treated as elastic and the two 3D processes would have simply bounced. In this case, the surface of contact on which the bond is established is called W. The name b is a memory for the type of channels that bound.

Note that the component process of shape S_1 opened a new channel $\langle c, Y_1 \rangle$. This is possible because the behaviour of two composed 3D processes is the interleaving of the behaviours of the components. Indeed, it is $B_1' = \langle c, Y_1 \rangle.B_{other} + \omega(\bar{b}, Z).B_1 + \rho(\{\langle \bar{b}, Z \rangle.B_1''\})$, that is, the compound 3D process either can accept another communication on the channel $\langle c, Y_1 \rangle$ or can perform a *weak-splitting* on the bond established on his previous channel $\langle \bar{b}, Z \rangle$ (the ω action) or can perform a *strong-splitting* on the same bond.

The third stage of Figure 2 represents the case in which the non-deterministic weak-splitting was performed. Note that channels return to the previous situation. This evolution models naturally the behaviour of an enzyme binding with a substrate: it can happen for some reason that the bond is loose and the two molecules are free again. Weak-splitting is not an urgent action, thus it can be delayed of an unspecified time. This is another source of non-determinism in the calculus.

Figure 3 shows another possible evolution of the processes of Figure 2. In this case another substrate, process $S_2[B_2]$, binds - with its channel $\langle \bar{a}, X_1 \rangle$ on the common surface W_1 - together with the previously established compound process. Following our metaphor, in the terminology of biochemical reactions a final complex has been formed, and in this case the reaction must proceed and the products must be released. For modelling this behaviour, the calculus provide an urgent action, that we call strong-splitting. A strong splitting must occur as soon as it is enabled, i.e. all the involved components can release all the bonds. In this example the involved components are S_0B_0', $S_1[B_1']$ and $S_2[B_2']$ and the set of bonds is $L = \{\langle b, W \rangle, \langle a, W_1 \rangle\}$. Indeed, for the strong splitting to be enabled in this case it must hold that $B_0' \xrightarrow{\rho(a,X)}$, $B_0' \xrightarrow{\rho(b,Y)}$, $B_1' \xrightarrow{\rho(\bar{b},Z)}$ and $B_2' \xrightarrow{\rho(\bar{a},X_1)}$. Note, finally, that the enzyme returns to its original state, while the metabolites that are released exhibit a different behaviour according to what they have become.
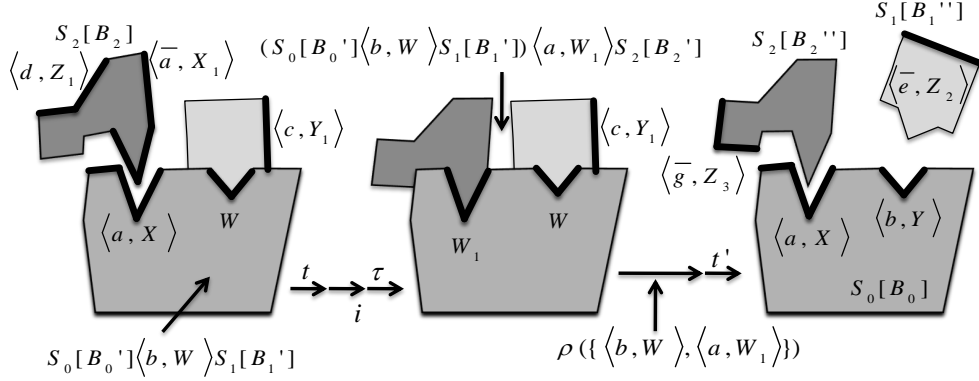
4

Figure 3: An example of complex formation and subsequent strong-splitting.

3   3D Shapes

We first introduce three dimensional shapes as terms of a suitable language, allowing simpler shapes to bind and form more complex shapes. From now on we consider assigned a *global* coordinate system in a three dimensional space represented by $\mathbb{R}^3$. Let $\mathbb{P}, \mathbb{V} = \mathbb{R}^3$ be the sets of positions and velocities, respectively, in this coordinate system.

For convenience we use, throughout the paper, relative coordinate systems that will always be w.r.t. a certain shape S, that is to say the origin of the relative system is a reference point $\mathbf{p}$ of S. We refer to this relative system as the *local* coordinate system of shape S. Given a point $\mathbf{p} \in \mathbb{P}$, expressed in the global coordinates, and a set of points $U \subseteq \mathbb{P}$, expressed in a local coordinate system whose origin is $\mathbf{p}$, we define $\mathsf{global}(U, \mathbf{p}) = U + \mathbf{p} = \{(\mathbf{u} + \mathbf{p}) \in \mathbb{P} \mid \mathbf{u} \in U\}$, i.e. the set of points U expressed in the global coordinates. Using the local system we can express parts of S - such as a certain face, a certain vertex, etc. - independently from the actual global position of the shape.

Definition 3.1 (Basic Shapes) *A basic shape σ is a tuple $\langle V, m, \mathbf{p}, \mathbf{v} \rangle$ where $V \subseteq \mathbb{P}$ is either a sphere, a cone, a cylinder or a convex polyhedron[1], $m \in \mathbb{R}^+$ is the mass of the shape, $\mathbf{p} \in \mathbb{P}$ is the centre of mass[2] of the shape and $\mathbf{v} \in \mathbb{V}$ is the vector representing the current velocity of the shape.*

We define the following operators on a basic shape σ: the points $\mathcal{P}(\sigma) = V$*, the* velocity $\mathcal{V}(\sigma) = \{\mathbf{v}\}$*, the* mass $\mathcal{M}(\sigma) = m$ *and the* reference point $\mathcal{R}(\sigma) = \mathbf{p}$*. The* boundary $\mathcal{B}(\sigma)$ *of σ is the subset of points of $\mathcal{P}(\sigma)$ that are on the surface of σ[3].*

The set of all possible basic shapes, ranged over by $\sigma, \sigma', \ldots$, is denoted by Basic.

Note that we use only very simple basic shapes that can be represented by suitable and efficient data structures and are handled by the most popular algorithms for motion simulation, collision detection and collision response [10]. Moreover, note that we consider only convex shapes. Recall that a set of points $U \subseteq \mathbb{P}$ is *convex* if and only if for every $\mathbf{x}, \mathbf{y}$ in U the set $\{(\lambda\mathbf{x} + (1-\lambda)\mathbf{y}) \in \mathbb{P} \mid 0 \leq \lambda \leq 1\}$ is contained in U.

Three dimensional shapes of any form can be approximated with arbitrary precision by composing basic shapes in the following sense: the composition of two shapes corresponds to the construction of a third shape by "glueing" the two components on a common surface. Consider the shape

---

[1]From a syntactical representation point of view, we assume that V is finitely represented by a suitable data structure, such as a formula or a set of vertices.

[2]We actually need only a reference point. Thus, any other point in V can be chosen.

[3]Note that we consider only closed shapes, i.e. they contain their boundary.
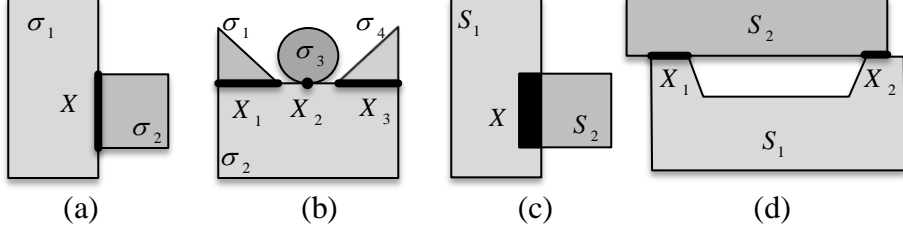
Figure 4: Some examples of 2D composed shapes.

shown in Figure 4(a). It is composed by the basic shape σ_1 "glued" with the basic shape σ_2 on the common surface X, called *surface of contact*. Note that no interpenetration between the composing shapes is allowed.

This concept can be generalised to the composition of two generic shapes either basic or compound under the same hypotheses, i.e. they bind on a common surface, but they do not interpenetrate.

Definition 3.2 (3D shapes) *The set* Shapes *of* 3D shapes, *ranged over by* $S, S', \ldots$ *is generated by the grammar* $S ::= \sigma \mid S \langle X \rangle S$ *where* $\sigma \in$ Basic *and* $X \subseteq \mathbb{P}$.

Starting from the same concepts defined for basic shapes, we inductively define the points, the velocity, the mass and the reference point of a compound shape $S = S_1 \langle X \rangle S_2$ as $\mathcal{P}(S) = \mathcal{P}(S_1) \cup \mathcal{P}(S_2)$, $\mathcal{V}(S) = \mathcal{V}(S_1) \cup \mathcal{V}(S_2)$, $\mathcal{M}(S) = \mathcal{M}(S_1) + \mathcal{M}(S_2)$ and $\mathcal{R}(S) = \mathcal{M}(S_1)\mathcal{R}(S_1) + \mathcal{M}(S_2)\mathcal{R}(S_2)^4$. The boundary of a compound shape S is defined as the surface of the resulting shape and is denoted by $\mathcal{B}(S)$. More formally, $\mathcal{B}(S_1 \langle X \rangle S_2) = (\mathcal{B}(S_1) \cup \mathcal{B}(S_2)) \setminus \{\mathbf{x} \in \mathbb{P} \mid \mathbf{x} \text{ is interior of } \mathcal{P}(S_1 \langle X \rangle S_2)\}$, where a point $\mathbf{x} \in U \subseteq \mathbb{P}$ is called *interior* of U if there exists an open ball with centre $\mathbf{x}$ which is completely contained in U.

In this paper we consider only *well-formed* shapes, i.e. basic shapes or compound shapes in which X is a surface of contact and the components do not interpenetrate. Moreover, all the components must have the same velocity.

Definition 3.3 (Well-formed shapes) *A basic shape* σ *is well-formed.*
A compound shape $S_1 \langle X \rangle S_2$ *is well-formed if and only if:*

1. *both* S_1 *and* S_2 *are well-formed*

2. *the set* $X = \mathcal{P}(S_1) \cap \mathcal{P}(S_2)$ *is* non-empty *and is equal to* $\mathcal{B}(S_1) \cap \mathcal{B}(S_2)$, *i.e. shapes* S_1 *and* S_2 *have some points in common, but all these points are on their boundaries. This means, in other words, that the shapes are in contact, but do not interpenetrate*

3. $\mathcal{V}(S_1 \langle X \rangle S_2)$ *is a singleton* $\{\mathbf{v}\}^5$

Given two well-formed shapes S_1 and S_2 we say that they interpenetrate *iff the set* $X = \mathcal{P}(S_1) \cap \mathcal{P}(S_2) \neq \emptyset$ *and* $X \not\subseteq \mathcal{B}(S_1) \cap \mathcal{B}(S_2)$. *Equivalently, we can say that the shapes interpenetrate if there exists a point* $\mathbf{x}$ *that is interior of both* $\mathcal{P}(S_1)$ *and* $\mathcal{P}(S_2)$.

If $S = S_1 \langle X \rangle S_2$ is well-formed, we say that X is a surface of contact *between* S_1 *and* S_2. If $\mathbf{x} \in X$ we say that $\mathbf{x}$ is a point of contact *between* S_1 *and* S_2.

---

[4]For simplicity, as above, we use the centre of mass as the reference point. Any other point can be chosen.
[5]With abuse of notation, throughout the paper, we use $\mathcal{V}(S)$ also to refer to the element $\mathbf{v}$ of the singleton $\{\mathbf{v}\}$ as this is not ambiguous when S is well-formed.

Example 3.5 (A Biological Example)

$S_a[\texttt{ATP}]$ $S_g[\texttt{G6P}]$ $S_h[\texttt{HEX}]$

hg

X_{ha}

$S_h[\texttt{HA}]\langle\texttt{atp},X\rangle S_a[\texttt{AH}]$
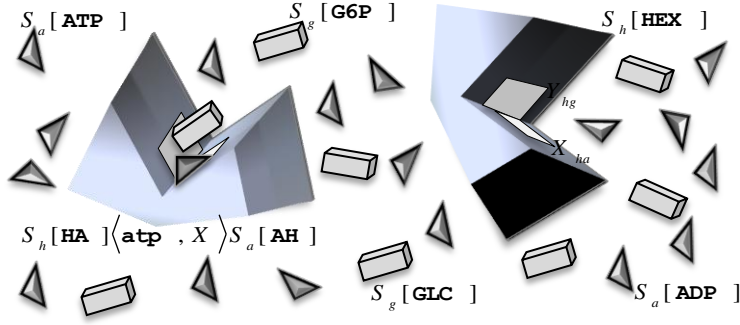
$S_g[\texttt{GLC}]$ $S_a[\texttt{ADP}]$

Figure 5: A network of 3D processes for describing the first reaction of the glycolysis pathway.

Note that condition 2) of the definition above guarantees that well-formed compound shapes touch but do not interpenetrate. The concept of touching without interpenetrating will be useful in the following when we define collision detection and compound 3D processes. By definition, X is always on the boundary of both S_1 and S_2. Thus, the set X can be a single point, a segment or a surface, depending on where the two shapes are touching without interpenetrating. Most of the time X is a (subset of a) *feature* of the basic shapes composing the 3D shape, i.e., a face, an edge or a vertex. Moreover, condition 3) imposes that all the basic shapes forming a compound shape have the same velocity, i.e., the compound shape moves as a unique body.

Figure 4 shows four examples of compound shapes. Note that while basic shapes are all convex, compound shapes can be non-convex, as those shown in figure. Shape in Figure 4(b) is composed of four basic shapes. A well-formed term representing this shape can be $((\sigma_1\langle X_1\rangle\sigma_2)\langle X_2\rangle\sigma_3)\langle X_3\rangle\sigma_4$. Note, for instance, that X_1 is exactly the intersection $\mathcal{B}(\sigma_1)\cap\mathcal{B}(\sigma_2)$ and that is equal to one feature (an edge) of σ_1. The surface of contact X_2 contains only one point of contact and is subset of $\mathcal{B}(\sigma_1\langle X_1\rangle\sigma_2)\cap\mathcal{B}(\sigma_3)$, i.e. its two immediate sub-components.

Figure 4(c) is an example of a not well-formed shape because there is interpenetration between S_1 and S_2.

In Figure 4(d) there is an example of a well-formed shape in which the intersection of (the boundaries of) the two components S_1 and S_2, called X in the figure, is *not* a connected set. Recall that a set U is *connected* if and only if the only pair of disjoint closed sets whose union is U is the pair $(\emptyset, U)$. Note that if the intersection (the boundaries of) two compound shapes is not connected it is always a finite union of connected sets. In this case we obtain a shape with a hole. We admit such shapes in the calculus since they can be formed by correct bindings of well-formed shapes.

Given a 3D shape S, it can be represented by arranging the basic shapes and the surfaces of contact in different ways. The following definition describes a structural congruence relation among terms representing shapes.

Definition 3.4 (Structural Congruence of Shapes) *Structural congruence over* Shapes, *denoted by $\equiv_S$, is the smallest relation that satisfies the following rules:*

1. $S_1\langle X\rangle S_2 \equiv_S S_2\langle X\rangle S_1$

2. $(S_1\langle X\rangle S_2)\langle Z\rangle S_3 \equiv_S S_1\langle X\rangle (S_2\langle Z\rangle S_3)$ *provided that $Z\subseteq\mathcal{B}(S_2)\cap\mathcal{B}(S_3)$*

The shape of Figure 4(b) can be represented by structural congruent terms, e.g. $((\sigma_3\langle X_2\rangle\sigma_2)\langle X_1\rangle\sigma_1)\langle X_3\rangle\sigma_4$ or $\sigma_1\langle X_1\rangle(\sigma_4\langle X_3\rangle(\sigma_3\langle X_2\rangle\sigma_2))$ etc.

We introduce an example in which of our calculus can be used by modelling a well-known biological scenario. The *glycolysis* pathway is part of the process by which individual cells produce and consume nutrient molecules. It consists of ten sequential reactions, all catalysed by a specific

enzyme. We focus, in this example, on the first reaction that can be described as *glucose, ATP* $\rightleftharpoons$ *glucose-6-phosphate, ADP, H⁺* where an ATP is consumed and a molecule of glucose (GLC) is phosphorylated to glucose 6-phosphate (G6P), releasing an ADP molecule and a positive hydrogen ion (Hydron). The enzyme catalysing this first reaction is *Hexokinase* (HEX). GLC, G6P, ATP, ADP and H^+ are metabolites. Both enzymes and metabolites are autonomous cellular entities that continuously move within the cytoplasm. The transformation of a metabolite into the one that follows in the "pipeline" of the pathway (in this case, GLC into G6P) depends on the encounter (collision in binding sites) of the right enzyme (in this example HEX) with the right metabolites, in this example GLC and ATP. The order of these bindings does not matter. After this binding the reaction takes place and the products[6] are released in the cytoplasm (i.e. a strong-splitting is performed). A special case occurs when the enzyme has bound one metabolite and an environmental event makes it release the metabolite and not proceed to the completion of the reaction (i.e. a weak-splitting is performed).

We model the shape of HEX, which we denote S_h, by a polyhedron approximating its real shape and mass, available at public databases (e.g. [1]). Figure 5 shows a network of 3D processes in which there are two hexokinases 3D processes and some GLC, G6P, ATP and ADP 3D processes. Note that we use a unique kind of shape for GLC ad G6P, denoted by S_g, and another unique kind of shape for ATP and ADP, denoted S_a. They are distinguished by their behaviours.

3.1 Trajectories of Shapes

Our shapes are intended to move in space along time. Given a well-formed term S, it represents shape S at a certain time instant t. The velocity of S in that instant is $\mathcal{V}(S)$. One of the choices to be made for the calculus is how the velocity of each shape changes over time. We believe that a continuous updating of the velocity, that would be a candidate for an "as precise as possible" approach of modelling, is not a convenient choice. The main reason is the well-known compromise between the benefits of approximation and the complexity of precision. Our choice, also common in the computer graphics field, is to approximate a continuous trajectory of a shape with a polygonal chain, i.e. a piecewise linear curve in which each segment is the result of a movement with a constant velocity. The vertices of the chain corresponds to the updates of the velocity of the shape (see Figure6(b)). To this purpose we define a global parameter $\Delta \in \mathbb{R}^+$, called *movement time step*, that represents the period of time after which the velocity of all shapes is updated. The time domain $\mathbb{T} = \mathbb{R}_0^+$ is then divided into an infinite sequence of movement time steps t_i such that $t_0 = 0$ and $t_i = t_{i-1} + \Delta$ for all $i > 0$. The quantification of Δ depends on the desired degree of approximation and also on other parameters connected to collision detection (see Section 3.2).

The updating of the velocities is represented by an operator $\mathsf{Move} \colon \mathsf{Shapes} \times \mathbb{T} \longrightarrow \mathbb{V}$ that gives the velocity vector $\mathsf{Move}(S, t)$ to assign to shape S at time t, which is intended to be one of the t_i defined above. Note that this approach gives the maximal flexibility for defining motion. Static shapes can be represented by assigning always the velocity $\mathbf{0}$ to them. A gravity field can be simulated by updating the velocities accordingly to the gravity acceleration (see Figure 6(a)). A Brownian motion can be simulated by choosing a random direction in 3D and then defining the length of the vector w.r.t. the mass and/or the volume of the shape.

For the sake of simplicity we do not consider, in this paper, movements by rotations. However, this kind of movement can be easily added to our shapes by assigning an angular velocity and a moment of inertia to a shape and then by performing a compound motion of translation and rotation along the movement time step. Let us define now some useful notation and properties.

Definition 3.6 (Time evolution of a shape) *Let $S \in \mathsf{Shapes}$ and $t \in \mathbb{T}$. We define, by induction on S, the shape $S + t$, i.e. S after t time units, as $\langle V + t \cdot \mathbf{v}, m, \mathbf{p} + t \cdot \mathbf{v}, \mathbf{v} \rangle$ if $S = \langle V, m, \mathbf{p}, \mathbf{v} \rangle$ and as $S_1 + t \langle X + t \cdot \mathcal{V}(S) \rangle S_2 + t$ if $S = S_1 \langle X \rangle S_2$.*

---

[6]In this example we neglect the hydron.

8

$$Move\ (S,t_i) = [0, -\frac{1}{2}g(i+1)\Delta, 0]m\,/\,s$$

$$t_i = t_{i-1} + \Delta$$

$$\Delta = 0.05\,s$$

$$v_1 = Move\ (S,t_0) = [0, -0.245, 0]m\,/\,s$$

$$v_2 = Move\ (S,t_1) = [0, -0.49, 0]m\,/\,s$$

$$v_3 = Move\ (S,t_2) = [0, -0.735, 0]m\,/\,s$$

$$S =$$

$$v_4 = Move\ (S,t_3) = [0, -0.98, 0]m\,/\,s$$

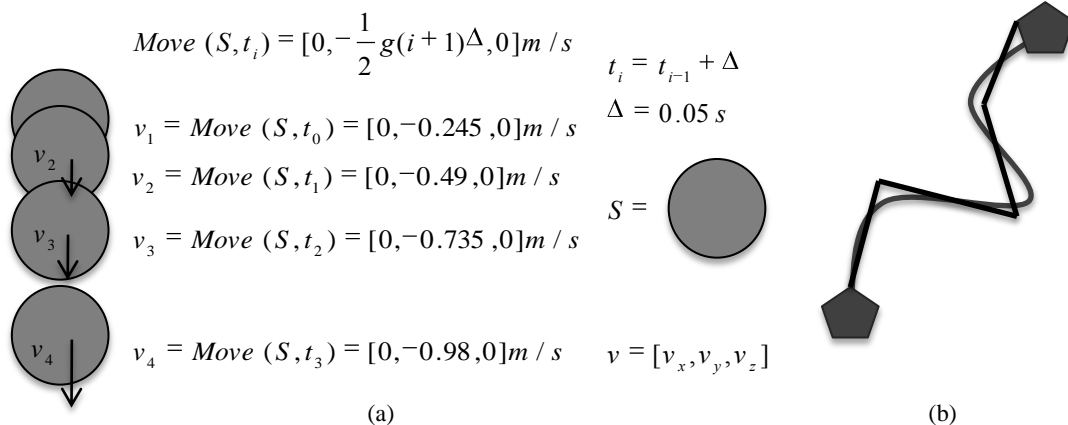$$v = [v_x, v_y, v_z]$$

(a)   (b)

Figure 6: An example of updating of the velocity and an approximated continuous trajectory of a shape.

Definition 3.7 (Velocity update of a shape) *Let $S \in$ Shapes and $\mathbf{w} \in \mathbb{V}$. We define, by induction on S, the shape $S[\![\mathbf{w}]\!]$, i.e. S updated with velocity $\mathbf{w}$, as $\langle V, m, \mathbf{p}, \mathbf{w} \rangle$ if $S = \langle V, m, \mathbf{p}, \mathbf{v} \rangle$ and as $S_1[\![\mathbf{w}]\!] \langle X \rangle S_2[\![\mathbf{w}]\!]$ if $S = S_1 \langle X \rangle S_2$.*

Proposition 3.8 *Let $S \in$ Shapes, $t \in \mathbb{T}$ and $\mathbf{w} \in \mathbb{V}$. If S is well-formed then $S + t$ and $S[\![\mathbf{w}]\!]$ are well-formed.*

In Example 3.5, as we model the molecules at the mesoscale (10^{-8} - 10^{-7} m) Brownian motion is generally considered a good approximation for their motion. Thus, the three kind of shapes S_h, S_g and S_a all are subject to the Brownian updating of velocity.

Our intent is to represent a lot of shapes moving simultaneously in space as described above. Inevitably, this scenario produces collisions between shapes when their trajectories encounter.

3.2 Collision Detection

There is a rich literature on collision detection systems, as this problem is fundamental in popular applications like computer games. Good introductions to existing methods for efficient collision detection are available and we refer to Ericson [10] and references therein for a detailed treatment.

For our purposes, it is sufficient to define an interface between our calculus and a typical collision detection system. We can then choose one of them according to their different characteristics, e.g. their applicability in large-scale environments or their robustness. It must be said, however, that the choice of the collision detection system may influence the kind of basic (or compound) shapes we can use, as, for instance, some systems may require the use of only convex shapes to be more efficient[7].

Typically, a collision detection algorithm assumes to start in a situation in which shapes do not interpenetrate. Then it tries to move all the shapes of a little time step - that we have already introduced as movement time step Δ - and check if interpenetrations occurred[8]. If so, it tries to consider only half of the original time step and repeat the interpentration check, i.e. it performs a binary search of the *first time of contact t* between two or more shapes, with some degree of

---

[7]The basic shapes that we consider in Definition 3.1 are typically accepted by most of the collision detection systems.

[8]Typically, the major efforts of optimisation are concentrated in this step since the number of checks is, in the worst case, $O(N^2)$ - where N is the number of shapes in the space - but the shapes that are likely to collide are only those that are very close to each other.
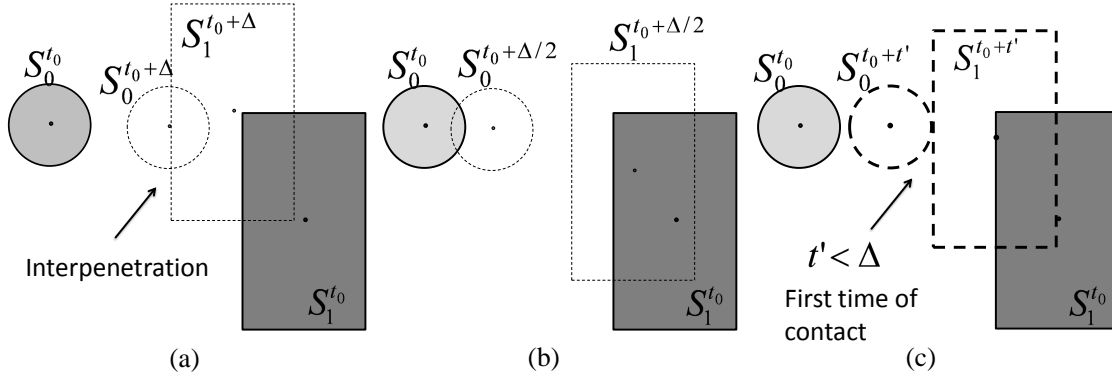
Figure 7: Some steps to determine the first time of contact between two shapes.

approximation. Figure 7 shows these steps. In case (a) the passage of the whole Δ results in an interpenetration. Then, in (b) the passage of $\Delta/2$ is tried resulting into a non-contact. After some iterations the situation in (c) is reached.

In addition to the first time of contact, a collision detection algorithm usually outputs the shapes that are colliding, i.e. are touching without interpenetrating after t, and some infomation about the surfaces or points of contact. We now define precisely what we expect to obtain from a collision detection system.

Definition 3.9 (First time of contact) *Let I be a non-empty finite set of indexes and let $\{S_i\}_{i\in I}$ be a set of well-formed shapes such that for all $i, j \in I$, S_i and S_j do not interpenetrate (Def. 3.2). The* first time of contact *of the shapes S_i, denoted $\mathsf{Ftoc}(\{S_i\}_{i\in I})$, is a number $t \in \mathbb{T}$ such that:*

1. *for all $t' \in \mathbb{T}$, $0 \leq t' \leq t$ and for all $i, j \in I$, $S_i + t'$ and $S_j + t'$ do not interpenetrate, i.e., from the starting point to t, shapes, while moving, could possibly touch but they do not interpenetrate*

2. *there exist $i, j \in I$, $i \neq j$, such that $\mathcal{B}(S_i + t) \cap \mathcal{B}(S_j + t) \neq \emptyset$, i.e., some shapes are touching at t*

3. *for all $\epsilon > 0$ there exists δ, $0 < \delta < \epsilon$, and $i, j \in I$, $i \neq j$, such that $S_i + (t+\delta)$ and $S_j + (t+\delta)$ interpenetrate, i.e., in t some shapes are touching and any further movement makes them to interpenetrate.*

Note that such a definition allows shapes that are touching without interpenetrating and with velocities that do not make them to interpenetrate (e.g., the same velocity) to move without triggering a first time of contact. This possibility will be useful in Section 5 when we split previously compound shapes. Giving them the same velocity vector after splitting we are guaranteed that the first time of contact currently in force is not affected by the splitting. Figure 8(a) shows a situation in which a collision is detected, while in cases (b) and (c) no collision is detected because letting any time pass, the two shapes will not interpenetrate.

A collision detection system usually returns, together with the first time of contact, some information useful to determine which shapes are colliding at that time and which are the points or surfaces of contact between them. We formalise this as follows.

Definition 3.10 (Collision information) *Let $\{S_i\}_{i\in I}$ be a set of well-formed shapes and $t = \mathsf{Ftoc}(\{S_i\}_{i\in I})$ be their first time of contact. With $\mathsf{colliding}(\{S_i\}_{i\in I}) \subseteq \mathsf{Shapes} \times \mathsf{Shapes} \times \wp(\mathbb{P})$ we denote the set of colliding shapes after t. A tuple $\langle S_i, S_j, X \rangle \in \mathsf{colliding}(\{S_i\}_{i\in I})$ iff*
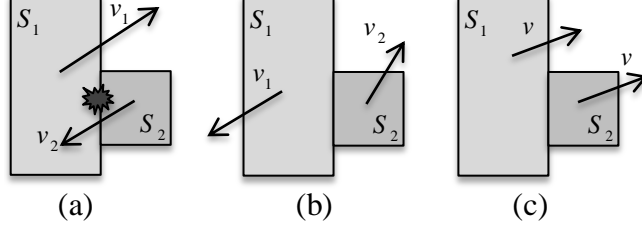
10

Figure 8: Some situations in which a collision is detected or not detected.

1. *the set* $X = \mathcal{P}(S_i + t) \cap \mathcal{P}(S_j + t)$ *is* non-empty *and is equal to* $\mathcal{B}(S_i + t) \cap \mathcal{B}(S_j + t)$

2. *for all* $\epsilon > 0$ *there exists* δ, $0 < \delta < \epsilon$, *such that* $S_i + (t + \delta)$ *and* $S_j + (t + \delta)$ *interpenetrate*

Conditions 1) and 2) control that S_i and S_j are really colliding after time t.

3.3 Collision Response

In this section, we address the problem of *collisions response* [13], i.e. how collisions, once detected, can be resolved. In what follows we distinguish between *elastic* collisions (those in which there is no loss in kinetic energy) and *perfectly inelastic* ones (in which kinetic energy is fully dissipated)[9]. After an elastic collision, two shapes will proceed independently to each other but their velocities will change according to the laws for conservation of linear momentum and kinetic energy (see Equations (1)-(2) in Definition 3.11). On the other hand, as a consequence of an inelastic collision, two shapes will bind together and will move as a *unique* body whose velocity is determined by the law for conservation of linear momentum only (see Equation (3), again in Definition 3.11).

Definition 3.11 (Elastic and inelastic collisions) *Let* $S_1, S_2 \in$ Shapes *and let* $X \subseteq \mathbb{P}$ *be a surface of contact between them. If* X *is neither an edge nor a vertex of the shape* S_1, *we set* $\mathbf{n}$ *to be the normal of contact away from* $X \subseteq \mathcal{B}(S_1)$ *(i.e.* $\mathbf{n}$ *is vector perpendicular to the face of* S_1 *that contains* X). *Otherwise,* $\mathbf{n}$ *is defined to be the normal of contact away from the shape* S_2.
  If $\mathbf{n}$ *is the normal of contact away from* S_1, *the velocities* $\mathbf{w}_1$ *and* $\mathbf{w}_2$ *of shapes* S_1 *and* S_2 *after an elastic collision in* X *are given by the following rules:*

$$(1) \quad \mathbf{w}_1 = \mathcal{V}(S_1) - \frac{\lambda}{\mathcal{M}(S_1)} \cdot \mathbf{n} \qquad\qquad (2) \quad \mathbf{w}_2 = \mathcal{V}(S_2) + \frac{\lambda}{\mathcal{M}(S_2)} \cdot \mathbf{n}$$

where

$$\lambda = 2 \cdot \frac{\mathcal{M}(S_1) \cdot \mathcal{M}(S_2)}{\mathcal{M}(S_1) + \mathcal{M}(S_2)} \cdot \frac{\mathcal{V}(S_1) \cdot \mathbf{n} - \mathcal{V}(S_2) \cdot \mathbf{n}}{\mathbf{n} \cdot \mathbf{n}}$$

If $\mathbf{n}$ *is the normal of contact away from* S_2, *the equations are symmetric. In both cases, we write* $S_1 \xleftrightarrow{X}_e S_2$ *to denote the pair of velocities* $(\mathbf{w}_1, \mathbf{w}_2)$.
  If S_1 *and* S_2 *collide inelastically in the surface of contact* X, *they will bind together as a unique body whose velocity (denoted with* $S_1 \xleftrightarrow{X}_i S_2$) *is given by:*

$$(3) \quad \mathbf{v} = \frac{\mathcal{M}(S_1)}{\mathcal{M}(S_1) + \mathcal{M}(S_2)} \cdot \mathcal{V}(S_1) + \frac{\mathcal{M}(S_2)}{\mathcal{M}(S_1) + \mathcal{M}(S_2)} \cdot \mathcal{V}(S_2)$$

In Figure 9(a) it is shown an example of collision response to an elastic collision along only one dimension. In Figure 9(b) there is another example of an inelastic collision.

---

[9]Other different kinds of collisions can be easily added to the calculus provided that the corresponding collision response laws are given.
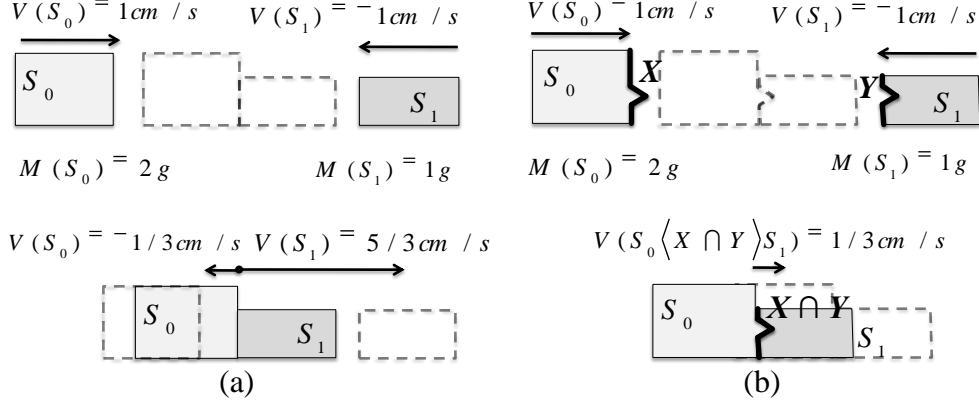
Figure 9: Examples of collision response of elastic and inelastic collision.

4 3D Processes

We first introduce the timed process algebra we use to define the *internal behaviour* of our shapes. This is a variation of Timed CCS [19], where basic actions provide information about binding capability and splittings of already established bonds.

We use the following notation. Let $\Lambda = \{a, b, \cdots\}$ be a countably infinite set of *channels names* (names, for short) and $\overline{\Lambda} = \{\overline{a} \,|\, a \in \Lambda\}$ its complementation. Let $\mathcal{A} = \Lambda \cup \overline{\Lambda}$; by convention we assume $\overline{\overline{a}} = a$ for each name a. Elements in $\mathcal{A}$ are ranged over by $\alpha, \beta, \cdots$.

A *channel* is a pair $\langle \alpha, X \rangle$ where $\alpha \in \mathcal{A}$ is a channel name and X is a *surface of contact*. We say that channels $\langle \alpha, X \rangle$ and $\langle \beta, Y \rangle$ are *compatible*, written $\langle \alpha, X \rangle \sim \langle \beta, Y \rangle$, if $\beta = \overline{\alpha}$ and $X \cap Y \neq \emptyset$. Otherwise, $\langle \alpha, X \rangle$ and $\langle \beta, Y \rangle$ are said to be *incompatible* (written $\langle \alpha, X \rangle \not\sim \langle \beta, Y \rangle$). Let $\mathcal{C}$ be the set of all channels, $\omega(\mathcal{C}) = \{\omega(\alpha, X) \,|\, \langle \alpha, X \rangle \in \mathcal{C}\}$ and $\rho(\mathcal{C}) = \{\rho(\alpha, X) \,|\, \langle \alpha, X \rangle \in \mathcal{C}\}$ be the sets of *weak-splitting actions* and *strong-splitting actions*, respectively. With an abuse of notation, we say that two weak-splitting actions $\omega(\alpha, X)$ and $\omega(\beta, Y)$ (as well as two strong-splitting actions $\rho(\alpha, X)$ and $\rho(\beta, Y)$) are compatible if so are the channels $\langle \alpha, X \rangle$ and $\langle \beta, Y \rangle$.

Let $\mathsf{Act} = \mathcal{C} \cup \omega(\mathcal{C}) \cup \rho(\mathcal{C})$ and and $\mathsf{Act}_\tau = \mathsf{Act} \cup \{\tau\}$ where, as usual in CCS [15], τ denotes internal activities. Our processes perform basic and *atomic* actions that belong to the set Act_τ whose elements are ranged over by $\mu, \mu', \cdots$. We finally assume a countably infinite collection $\mathcal{K}$ of *process name* or *process constants*.

Intuitively, an action of the form $\langle \alpha, X \rangle$ represents a *binding capability* in the surface of contact X, i.e. a portion of space (usually, a subset of the boundary of a given 3D shape) where the channel itself is active and where binding with other processes are possible. Moreover, channels's names allow us to introduce a notion of compatibility among channels and, hence, to distinguish between elastic and inelastic collisions (see Section 5).

Actions in $\omega(\mathcal{C}) \cup \rho(\mathcal{C})$ have been introduced to represent splitting of shape bonds. These actions behave differently w.r.t. to time passing. Indeed, while weak-splitting actions can be arbitrarily delayed, strong-splitting actions (as the internal ones) are *urgent* and, once enabled, must be performed before time can pass further.

Definition 4.1 (Shape behaviours) *The set $\mathbb{B}$ of* shape behaviours *is generated by the following grammar*

$$B ::= \mathsf{nil} \mid \tau.B \mid \langle \alpha, X \rangle.B \mid \omega(\alpha, X).B \mid \rho(L).B \mid \epsilon(t).B \mid B + B \mid K$$

where $\langle \alpha, X \rangle \in \mathcal{C}$, $L \subseteq \mathcal{C}$ (non-empty) whose elements are pairwise incompatible (i.e. for each pair $\langle \alpha, X \rangle, \langle \beta, Y \rangle \in L$ it is $\langle \alpha, X \rangle \not\sim \langle \beta, Y \rangle$), $t \in \mathbb{T}$ and K is a process name in $\mathcal{K}$.

12

$$\text{NIL}_t \frac{}{\text{nil} \xrightarrow{t} \text{nil}} \qquad\qquad \text{PREF}_t \frac{}{\langle \alpha, X \rangle.B \xrightarrow{t} \langle \alpha, X \rangle.B}$$

$$\text{SPLIT}_t \frac{}{\omega(\alpha, X).B \xrightarrow{t} \omega(\alpha, X).B} \qquad \text{DELAY}_t \frac{t' \geq t}{\epsilon(t').B \xrightarrow{t} \epsilon(t' - t).B}$$

$$\text{CHOICE}_t \frac{B_1 \xrightarrow{t} B_1' \quad B_2 \xrightarrow{t} B_2'}{B_1 + B_2 \xrightarrow{t} B_1' + B_2'} \qquad \text{DEF}_t \frac{B \xrightarrow{t} B'}{K \xrightarrow{t} B'} \quad \text{if } K \stackrel{\text{def}}{=} B$$

Table 1: Temporal behaviour of $\mathbb{B}$'s terms

A brief description of our operators now follows. nil is the Nil-behaviour, it can not perform any action but can let time pass without limits. A trailing nil will often be omitted, so e.g. we write $\tau + \langle a, X \rangle.\omega(a, X).$ to abbreviate $\tau.\text{nil} + \langle a, X \rangle.\omega(a, X).\text{nil}$

$\mu.B$, with $\mu \in \mathcal{C} \cup \omega(\mathcal{C}) \cup \{\tau\}$, is the action-prefixing known from CCS and represents a shape's behaviour that can perform a μ-action and then evolve in B. In particular, a term like $\langle \alpha, X \rangle.B$ represents the behaviour of a shape that exhibits a binding capability along the channel $\langle \alpha, X \rangle$; while $\omega(\alpha, X).B$ models the behaviour of a shape that, before evolving in B, wants to split a *single* bond established via the channel $\langle \alpha, X \rangle$. As in [19], we assume that internal actions are *urgent* and, hence, can not let time pass.

The *strong-splitting operator* $\rho(L).B$ is used to represent *simultaneous* strong-splittings of a set of shapes's bonds. Indeed, a behaviour like $\rho(L).B$ can evolve in B only if *all* the bonds established via channels in L can be simultaneously parted. Moreover, since each of such actions is urgent, we assume that a term like $\rho(L).B$ does not allow time passing.

$\epsilon(t).B$ is the delay-prefixing operator (see [19]) that introduces time delays in 3D processes; $t \in \mathbb{T}$ is the amount of time that has to elapse before the idling time is over (see rules DELAY_t and DELAY_a in Tables 1 and 2). Finally, $B_1 + B_2$ models a non-deterministic choice between B_1 and B_2 and K is a process definition.

In what follows we use terms in the set $\mathbb{B}$ to define the internal behaviour of 3D shapes. For this reason we assume that the behaviours of such shapes, and in particular sites in binding capabilities and in weak and strong splitting actions are expressed w.r.t. a *local* coordinate system whose origin is the reference point of the shape where they are embedded in.

Definition 4.2 (Temporal Behaviour of $\mathbb{B}$-terms) *Let $t \in \mathbb{T}$. The SOS-rules defining the transition relations $\xrightarrow{t} \subseteq (\mathbb{B} \times \mathbb{B})$ are given in Table 1. These transitions, also called* temporal transitions, *describe how $\mathbb{B}$-terms evolve by letting time t pass. As usual, we write $B \xrightarrow{t} B'$ if $(B, B') \in \xrightarrow{t}$ and $B \xrightarrow{t}$ if there exists a $B' \in \mathbb{B}$ such that $(B, B') \in \xrightarrow{t}$. Similar conventions will apply later on.*

Definition 4.3 (Functional Behaviour of $\mathbb{B}$-terms) *The SOS-rules defining the transition relations $\xrightarrow{\mu} \subseteq (\mathbb{B} \times \mathbb{B})$ for $\mu \in \text{Act}_\tau$ (the* action transitions, *define which basic actions that a shape's behaviour can perform) are given in Table 2.*

Rules in Table 1 are quite similar to those provided in [19]) and need no further explanations. Rules REAC_{a1} and REAC_{a2} in Table 2 state that a term like $\rho(L).B$ can do an action $\rho(\alpha, X)$ provided that the channel $\langle \alpha, X \rangle \in L$ and then evolves in either B (whenever $L = \{\langle \alpha, X \rangle\}$) or $\rho(L \setminus \{\langle \alpha, X \rangle\}).B$ (otherwise). Rule REAC_{a3} allows us to describe the evolution via $\rho(\alpha, X)$-action of nested terms as for instance $\rho(\{\langle a, X \rangle\}).\rho(\{\langle \bar{b}, Y \rangle\}).B$. Other rules are as expected.

$$\text{PREF}_a \frac{\mu \in \mathcal{C} \cup \omega(\mathcal{C}) \cup \{\tau\}}{\mu.B \xrightarrow{\mu} B} \qquad \text{REAC}_{a1} \frac{L = \{\langle \alpha, X \rangle\}}{\rho(L).B \xrightarrow{\rho(\alpha,X)} B}$$

$$\text{REAC}_{a2} \frac{\{\langle \alpha, X \rangle\} \subset L}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L \setminus \{\langle \alpha, X \rangle\}).B} \qquad \text{REAC}_{a3} \frac{B \xrightarrow{\rho(\alpha,X)} B'}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L).B'}$$

$$\text{DELAY}_a \frac{B \xrightarrow{\mu} B'}{\epsilon(0).B \xrightarrow{\mu} B'} \qquad \text{CHOICE}_a \frac{B_1 \xrightarrow{\mu} B'}{B_1 + B_2 \xrightarrow{\mu} B'}$$

$$\text{DEF}_a \frac{B \xrightarrow{\mu} B'}{K \xrightarrow{a} B'} \qquad \text{if } K \overset{\text{def}}{=} B$$

Table 2: Functional behaviour of $\mathbb{B}$-terms

Now we are ready to define our 3D processes that are simply or compound shapes with a given behaviour expressed as a $\mathbb{B}$-term.

Definition 4.4 (3D processes) *The set* 3DP *of* 3D processes *is generated by the grammar:*

$$P ::= S[B] \mid P \langle a, X \rangle P$$

where $S \in$ Shapes, $B \in \mathbb{B}$, $a \in \Lambda$ and X is a non-empty subset of $\mathbb{P}$. If P is a 3D process, we define $\text{shape}(P) \in$ Shapes by induction on P as follows:

Compound: $\text{shape}(P \langle a, X \rangle Q) = \text{shape}(P) \langle X \rangle \text{shape}(Q)$
Basic: $\text{shape}(S[B]) = S$

We also define $\mathcal{V}(P) = \mathcal{V}(\text{shape}(P))$ and $\mathcal{B}(P) = \mathcal{B}(\text{shape}(P))$. Finally, we define $\text{Move}(P, t) = P[\![\text{Move}(\text{shape}(P), t)]\!]$. Moreover, we often write $P \xleftarrow{X}_i Q$ and $P \xleftarrow{X}_e Q$ as shorthands for $\text{shape}(P) \xleftarrow{X}_i \text{shape}(Q)$ and for $\text{shape}(P) \xleftarrow{X}_e \text{shape}(Q)$, respectively.

If $\mathbf{v} \in \mathbb{V}$, we denote with $P[\![\mathbf{v}]\!]$ the 3D process we obtain by updating P's velocity with $\mathbf{v} \in \mathbb{V}$. $P[\![\mathbf{v}]\!]$ can be defined by induction on P as follows:

Compound: $(P \langle a, X \rangle Q)[\![\mathbf{v}]\!] = (P[\![\mathbf{v}]\!]) \langle a, X \rangle (Q[\![\mathbf{v}]\!])$
Basic: $(S[B])[\![\mathbf{v}]\!] = (S[\![\mathbf{v}]\!])[B]$

We say that a basic process $S[B]$ is well-formed if and only if the shape S is well-formed and, for each channel $\langle \alpha, X \rangle$ and for each action $\omega(\alpha, X)$ that syntactically occurs in B it is $\text{global}(X, \mathcal{R}(S)) \subseteq \mathcal{B}(S) = \mathcal{B}(P)$. A compound process $P \langle a, X \rangle Q$ is well-formed iff P and Q are well-formed processes with the same velocity (i.e. $\mathcal{V}(P) = \mathcal{V}(Q)$) and the site X (expressed w.r.t a global coordinate system) is a non-empty subset of $\mathcal{B}(P) \cap \mathcal{B}(Q)$. Notice that this also means that the set $\mathcal{P}(P) \cap \mathcal{P}(Q)$ is non-empty and equal to $\mathcal{B}(P) \cap \mathcal{B}(Q)$. Later on in this paper we only consider well-formed processes.

The following result easily follows from definitions of shapes and 3D processes well-formedness.

Proposition 4.5 *If $P \in$ 3DP well-formed then $\text{shape}(P)$ is a well-formed 3D shape.*

Example 4.6 (3D Processes for HEX, GLC and ATP) *Let us model the molecules involved in the reaction introduced in Example 3.5 as 3D processes. Hexokinase is modeled as $S_h[\text{HEX}]$*

$$\text{BASIC}_\tau \frac{B \xrightarrow{\tau} B'}{S[B] \xrightarrow{\tau} S[B']} \qquad \text{BASIC}_{ch} \frac{B \xrightarrow{\langle \alpha, X \rangle} B' \quad \mathbf{p} = \mathcal{R}(S)}{S[B] \xrightarrow{\langle \alpha, \mathsf{global}(X, \mathbf{p}) \rangle} S[B']}$$

$$\text{BASIC}_w \frac{B \xrightarrow{\omega(\alpha, X)} B' \quad \mathbf{p} = \mathcal{R}(S)}{S[B] \xrightarrow{\omega(\alpha, \mathsf{global}(X, \mathbf{p}))} S[B']} \qquad \text{BASIC}_s \frac{B \xrightarrow{\rho(\alpha, X)} B' \quad \mathbf{p} = \mathcal{R}(S)}{S[B] \xrightarrow{\rho(\alpha, \mathsf{global}(X, \mathbf{p}))} S[B']}$$

$$\text{COMP}_{a1} \frac{P \xrightarrow{\mu} P' \quad \mu \in \{\tau\} \cup \omega(\mathcal{C}) \cup \rho(\mathcal{C})}{P \langle a, X \rangle Q \xrightarrow{\mu} P' \langle a, X \rangle Q} \qquad \text{COMP}_{a2} \frac{P \xrightarrow{\langle \alpha, X_p \rangle} P' \quad X_p \subseteq \mathcal{B}(P \langle a, X \rangle Q)}{P \langle a, X \rangle Q \xrightarrow{\langle \alpha, X_p \rangle} P' \langle a, X \rangle Q}$$

$$\text{BASIC}_t \frac{B \xrightarrow{t} B'}{S[B] \xrightarrow{t} (S + t)[B']} \qquad \text{COMP}_t \frac{P \xrightarrow{t} P' \quad Q \xrightarrow{t} Q' \quad \mathbf{v} = \mathcal{V}(P)}{P \langle a, X + (t \cdot \mathbf{v}) \rangle Q \xrightarrow{t} P' \langle a, X \rangle Q'}$$

Table 3: Functional and temporal behaviour of 3DP-terms

where $\mathsf{HEX} = \langle \mathsf{atp}, X_{ha} \rangle.\mathsf{HA} + \langle \mathsf{glc}, Y_{hg} \rangle.\mathsf{HG}$. *The surfaces* X_{ha} *and* Y_{hg} *are those shown in Figure 5 on the internal part of the hexokinase shape. The process* $S_h[\mathsf{HEX}]$ *can, for instance, bind a 3D process* P *iff* P *has a channel* $\langle \overline{\mathsf{atp}}, X' \rangle$ *and* P *collide with it in such a way that* X' *has at least a point in common with* X_{ha}. *An example of this process is that modelling ATP, i.e.,* $S_a[\langle \overline{\mathsf{atp}}, X_{ah} \rangle.\epsilon(t_{atp}).(\rho(\{\langle \overline{\mathsf{atp}}, X_{ah} \rangle\}).\mathsf{ADP} + \omega(\overline{\mathsf{atp}}, X_{ah}).ATP)]$. *Here the surface* X_{ah} *is intended to be the whole boundary* $\mathcal{B}(S_a)$. *After a binding, the ATP process has to wait a delay* t_{atp} *that model an internal activity of adjusting and then can either non-deterministically release the established bond on its channel - and thus return free as ATP - or participate in the reaction and become an ADP. The process modelling the GLC is very similar:* $S_g[\langle \overline{\mathsf{glc}}, X_{gh} \rangle.\epsilon(t_{glc}).(\rho(\{\langle \overline{\mathsf{glc}}, X_{gh} \rangle\}).\mathsf{G6P} + \omega(\overline{\mathsf{glc}}, X_{gh}).GLC)]$. *To conclude we specify the rest of the behaviour of HEX:*

$\mathsf{HA} = \omega(\langle \mathsf{atp}, X_{ha} \rangle).\mathsf{HEX} + (\langle \mathsf{glc}, X_{hg} \rangle.\rho(\{\langle \mathsf{atp}, X_{ha} \rangle, \langle \mathsf{glc}, Y_{hg} \rangle\}).\mathsf{HEX})$, *i.e., it can either choose to do a weak split and come back to HEX or if the binding with a GLC occur then a reaction must occur - because* ρ *is an urgent action - as soon as all the component involved in the split are ready. The result is the splitting of the complex in the three original shapes with the same behaviour for HEX and different behaviours for ATP and GLC.* HG *is similar and we leave unspecified the behaviours* $\mathsf{G6P}$ *and* ADP.

We are now ready to define the timed operational semantics of 3D processes.

Definition 4.7 (Temporal and Functional Behaviour of 3DP-terms) *Rules in Table 3 define the transition relations* $\xrightarrow{t} \subseteq (3DP \times 3DP)$ *and* $\xrightarrow{\mu} \subseteq 3DP \times 3DP$ *for* $t \in \mathbb{T}$ *and* $\mu \in \mathsf{Act}_\tau$, *respectively. We often write* $P \xrightarrow{\theta}\!\!\!\!/\,$ *and* $P \xrightarrow{\omega}\!\!\!\!/\,$ *as a shorthands for* $P \xrightarrow{\rho(\alpha, X)}\!\!\!\!\!\!\!\!\!\!/\,\,\,\,\,$ *and* $P \xrightarrow{\omega(\alpha, X)}\!\!\!\!\!\!\!\!\!\!/\,\,\,\,\,$ *for any* $\langle \alpha, X \rangle \in \mathcal{C}$. *Two processes* P *and* Q *are* compatible *(written* $P \sim Q$*) if there exist two compatible channels* $\langle \alpha, X \rangle, \langle \overline{\alpha}, Y \rangle \in \mathcal{C}$ *such that* $P \xrightarrow{\langle \alpha, X \rangle}$ *and* $Q \xrightarrow{\langle \overline{\alpha}, Y \rangle}$; *otherwise,* P *and* Q *are said to be* incompatible *that we denote with* $P \not\sim Q$.

Rules in Table 3 say that a 3D process inherits its functional and temporal behaviour from the $\mathbb{B}$-terms we use to describe its internal behaviour. We only remark that now sites of binding capabilities and splitting actions are expressed w. r. t. a *global* coordinate system.

The following proposition (whose proof has been moved to Appendix B) is needed to prove that processes well-formedness is closed with respect to transitions $\xrightarrow{\mu}$ and $\xrightarrow{t}$.

Proposition 4.8 Let $P, Q \in$ 3DP with P well-formed; let, moreover, $t \in \mathbb{T}$ and $\mu \in \mathsf{Act}_\tau$.

1. $P \xrightarrow{t} Q$ implies $\mathsf{shape}(Q) = \mathsf{shape}(P) + t$;

2. $P \xrightarrow{\mu} Q$ implies $\mathsf{shape}(Q) = \mathsf{shape}(P)$;

3. If $P \xrightarrow{t} Q$ or $P \xrightarrow{\mu} Q$ then Q well-formed.

Note that, at this stage, the functional behaviour of a compound process is obtained as the interleaving of the behaviours of its components and no synchronisations between such components are possible. Actually, both binding of compatible processes and splitting of processes' bonds require synchronisation among 3D processes. Synchronisation due to binding of compatible processes will be introduced in Section 5 (see Rules INEL in Table 7). This mainly originates from the fact that this kind of synchronisations occurs only as a consequence of collisions between two compatible 3D processes. In a more detail, if P and Q are compatible processes (i.e. if there are two compatible channels $\langle \alpha, X_p \rangle, \langle \overline{\alpha}, X_q \rangle \in \mathcal{C}$ such that $P \xrightarrow{\langle \alpha, X_p \rangle} P'$ and $Q \xrightarrow{\langle \overline{\alpha}, X_q \rangle} Q'$) that collide in the site $X = X_p \cap X_q$, then the result of such a collision will be a compound shape of the form $(P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]$ where $a \in \Lambda$ such that $\alpha \in \{a, \overline{a}\}$ and $\mathbf{v} = P \xleftarrow{X}_i Q = \mathsf{shape}(P) \xleftarrow{X}_i \mathsf{shape}(Q)$. Vice versa, if P and Q are not compatible (i.e. if no synchronisation between compatible channels is possible) any possible collision between P and Q is considered to be an elastic collision. Thus, P and Q (actually, the processes we obtain by changing the velocities of P and Q according to Equations (1) and (2) in Definition 3.11 - see Rule ELAS in Table 6) will proceed independently to each other.

On the other hand, the bond $\langle a, X \rangle$ of the compound process $P \langle a, X \rangle Q$ can be *strongly* splitted only if its components P and Q are able to synchronise on the execution of two compatible actions $\rho(\alpha, X_p)$ and $\rho(\overline{\alpha}, X_q)$, with $\alpha \in \{a, \overline{a}\}$ and $X = X_p \cap X_q$. As an example, assume $P = S_p[\rho(\{\langle a, X_p \rangle\}).B]$, $Q = S_q[\rho(\{\langle \overline{a}, X_q \rangle\}).B']$ and consider the compound process $P \langle a, X_p \cap X_q \rangle Q$. Furthermore, the result of such a splitting operation will be that of producing two independent 3D processes, i.e. a network (see again Section 5 for the definition of networks of 3D processes) that consists of the processes $S_p[B]$ and $S_q[B']$. Similarly, bonds are *weakly* splitted only due to synchronisations among compatible $\omega(\text{-})$ actions. Moreover, also weak splitting operations produce, as a result, networks of 3D processes.

To properly define this kind of behaviours some technical details are needed. First, we define two transition relations $\xrightarrow{\rho(a,X)}$ and $\xrightarrow{\omega(a,X)}$ in order to allow synchronisation on compatible $\rho(\text{-})$ and $\omega(\text{-})$ actions, respectively. Basically we want that, if P and Q are the same processes we have considered above, then $P \langle a, X_p \cap X_q \rangle Q \xrightarrow{\rho(a,X)} S_p[B] \langle a, X_p \cap X_q \rangle S_q[B']$. Now, to obtain the network of processes we are interested in, it still remains to remove the bond $\langle a, X \rangle$. This can be done by exploiting the function split over 3D processes we provide in the next section.

Definition 4.9 (Semantics of strong and weak splittings for 3D processes) *Let $\rho(a, X) \in \rho(\mathcal{C})$. The SOS-rules that define the transition relations $\xrightarrow{\rho(a,X)} \subseteq$ 3DP $\times$ 3DP are given in Table 4; additionally, there is a symmetric rule for STRPAR for $\rho(\text{-})$ actions of Q.*

For the sake of simplicity we omit the SOS-rules defining the transition relations $\xrightarrow{\omega(a,X)} \subseteq$ 3DP $\times$ 3DP for $\omega(a, X) \in \omega(\mathcal{C})$. These can be obtained by replacing each occurrence of a $\rho(\text{-})$ action in Table 4 with the corresponding $\omega(\text{-})$ action.

We final observe that strong-splittings of multiple shape bonds must be performed simultaneously, i.e. can only be performed if the involved components are *all together* ready to synchronise on a proper set of compatible $\rho(\text{-})$ actions. If this is the case, we say that the 3D process we are considering is able to *complete a reaction*, i.e. it can satisfy all the "pending strong-splitting requests".

16

Otherwise, i.e. if there is at least a synchronisation partner that is not currently able to contribute, such shapes's bonds can not be splitted at all. We formalise these concepts as follows.

Definition 4.10 (Bonds of 3DP-terms) *The function* bonds : 3DP $\rightarrow \wp(\mathcal{C})$ *returns the bonds currently established in a given 3D process. It can be defined by induction on $P \in$ 3DP as follows:*

Compound: $\mathsf{bonds}(P \langle a, X \rangle Q) = \mathsf{bonds}(P) \cup \mathsf{bonds}(Q) \cup \{\langle a, X \rangle\}$
Basic: $\mathsf{bonds}(S[B]) = \emptyset$

We say that $P \in$ 3DP is able to complete a reaction, *written $P \searrow$, iff either*

1. $P \not\stackrel{\theta}{\rightarrow}$, *or*

2. $P \stackrel{\rho(a,X)}{\Rightarrow} Q$, *for some $\rho(a, X) \in \rho(\mathcal{C})$, and $Q \searrow$.*

Example 4.11 Consider $P = S_p[\rho(\{\langle a, X_p \rangle, \langle \bar{b}, Y_p \rangle\}).\mathsf{nil}]$, $Q = S_q[\rho(\{\langle \bar{a}, X_q \rangle\}).\mathsf{nil}]$ and $R = S_r[\tau.\rho(\{\langle b, Y_r \rangle\}).\mathsf{nil}]$, and the compound 3D process $(P \langle a, X \rangle Q) \langle b, Y \rangle R$ where $X = X_p \cap X_q \neq \emptyset$ and $Y = Y_p \cap Y_r \neq \emptyset$. $(P \langle a, X \rangle Q) \langle b, Y \rangle R$ is not able to complete a reaction because the component R is not able to synchronise with P on the execution of $\rho(b, Y)$. More formally (according to Definition 4.10): $(P \langle a, X \rangle Q) \langle b, Y \rangle R \stackrel{\rho(a,X)}{\Rightarrow} (S_p[\rho(\{\langle \bar{b}, Y_p \rangle\})] \langle a, X \rangle S_q[\mathsf{nil}]) \langle b, Y \rangle R = P'$ with P' not able to complete a reaction (it can still perform the action $\rho(\bar{b}, Y_p)$ but no synchronisations are possible). But, after performing the R's internal action, we obtain a 3D process

$$(P \langle a, X \rangle Q) \langle b, Y \rangle (S_r[\rho(\{\langle b, Y_r \rangle\}).\mathsf{nil}]) \qquad\qquad \stackrel{\rho(a,X)}{\Rightarrow}$$
$$(S_p[\rho(\{\langle \bar{b}, Y_p \rangle\}).\mathsf{nil}] \langle a, X \rangle S_q[\mathsf{nil}]) \langle b, Y \rangle (S_r[\rho(\{\langle b, Y_r \rangle\}).\mathsf{nil}] \qquad \stackrel{(b,Y)}{\Rightarrow}$$
$$(S_p[\mathsf{nil}] \langle a, X \rangle S_q[\mathsf{nil}]) \langle b, Y \rangle S_r[\mathsf{nil}] \qquad\qquad\qquad \searrow$$

So we have that $(P \langle a, X \rangle Q) \langle b, Y \rangle (S_r[\rho(\{\langle b, Y_r \rangle\}).\mathsf{nil}]) \searrow$.

We also use a structural congruence over 3D processes to be defined below.

Definition 4.12 (Structural congruence over 3D processes) *Structural congruence over processes in* 3DP, *denoted by $\equiv_P$, is the smallest relation that satisfies the following axioms:*

- $S[B] \equiv_P S'[B]$ *provided that $S \equiv_S S'$;*

- $P \langle a, X \rangle Q \equiv_P Q \langle a, X \rangle P$;

- $P \equiv_P Q$ *implies* $P \langle a, X \rangle R \equiv_P Q \langle a, X \rangle R$;

- $(P \langle a, X \rangle Q) \langle b, Y \rangle R \equiv_P Q \langle a, X \rangle (Q \langle b, Y \rangle R)$ *provided that $Y \subseteq \mathcal{B}(Q) \cap \mathcal{B}(R)$*

The following result allows us to state that the function split we define in Section 5 (up to structural congruence over 3D processes) is well-defined.

$$\text{STRSYNC} \frac{P \xrightarrow{\rho(\alpha, X_p)} P' \quad Q \xrightarrow{\rho(\bar{\alpha}, X_q)} Q' \quad \alpha \in \{a, \bar{a}\} \quad X = X_p \cap X_q}{P \langle a, X \rangle Q \stackrel{\rho(a,X)}{\Rightarrow} P' \langle a, X \rangle Q'}$$

$$\text{STRPAR} \frac{P \stackrel{\rho(b,Y)}{\Rightarrow} P'}{P \langle a, X \rangle Q \stackrel{\rho(b,Y)}{\Rightarrow} P' \langle a, X \rangle Q}$$

Table 4: Transitional semantics for strong-splitting actions for 3D processes

17

Proposition 4.13 *Let $P \in$ 3DP well-formed. If $\langle a, X \rangle \in$ bonds(P) there are $Q, R \in$ 3DP well-formed such that $X \subseteq \mathcal{B}(Q) \cap \mathcal{B}(R)$, $\mathcal{V}(Q) = \mathcal{V}(R) = \mathcal{V}(P)$, and $P \equiv_P Q \langle a, X \rangle R$.*

We also need to following closure result.

Proposition 4.14 *Let $P, Q \in$ 3DP with P well-formed, and $\mu \in \omega(\mathcal{C}) \cup \rho(\mathcal{C})$. Then:*

1. *$P \overset{\mu}{\Rightarrow} Q$ implies shape$(Q) =$ shape(P);*

2. *$P \overset{\mu}{\Rightarrow} Q$ implies Q well-formed.*

5   Networks or 3D processes

Now we can define a network of 3D processes as a collection of 3D processes that freely moving in the same 3D space.

Definition 5.1 (Networks of 3D processes) *The set $\mathbb{N}$ of networks of 3D processes is generated by the grammar*

$$N ::= \mathsf{Nil} \mid P \mid N \parallel N$$

where $P \in$ 3DP. We say that a network N is well-formed iff each 3D process composing the network is well-formed and, for each pair of distinct processes P and Q in the network, shape(P) and shape(Q) do not interpenetrate. Moreover, we extend the definition of Move on networks in the natural way, i.e. such that each process of the network is updated simultaneously.

In our running example we construct a network of processes containing a proper number of HEX, ATP and GLC processes in order to replicate the conditions in a portion of cytoplasm.

Definition 5.2 (Splitting bonds) *Let $P \in$ 3DP and $C \subseteq \mathcal{C}$. We define split(P, C) as follows:*

$$\mathsf{split}(P, C) = \begin{cases} \mathsf{split}(Q, C) \parallel \mathsf{split}(R, C) & \text{if } \exists \langle a, X \rangle \in C \cap \mathsf{bonds}(P) \text{ s.t. } P \equiv Q \langle a, X \rangle R \\ P & \text{otherwise} \end{cases}$$

Note that we do not change the velocities of splitted shapes. Thus, they maintain the same velocity until the next occurrence of a movement time step. As we mentioned above, this is not a problem because they will not trigger a collision and, thus, a shorter first time of contact.

Proposition 5.3 *Let $P \in$ 3DP well-formed and $C \subseteq \mathcal{C}$. Then split(P, C) is a well-formed network of 3D processes.*

Definition 5.4 (Semantics of weak and strong splittings) *Let $P \in$ 3DP with P able to complete a reaction, and $N \in \mathbb{N}$. We write that $P \overset{\rho}{\rightarrow} N \in \mathbb{N}$ iff there is a non empty set of channels $C = \{\langle a_1, X_1 \rangle, \cdots, \langle a_n, X_n \rangle\} \subseteq$ bonds(P) such that $P = P_0 \overset{\rho(a_1, X_1)}{\Rightarrow} P_1 \cdots \overset{\rho(a_n, X_n)}{\Rightarrow} P_n \overset{\rho}{\nrightarrow}$ and $N = \mathsf{split}(P_n, C)$.*

Let $P \in$ 3DP and $N \in \mathbb{N}$. We write that $P \overset{\omega}{\rightarrow} N$ iff there exists $\langle a, X \rangle \in$ bonds(P) such that $P \overset{\omega(a, X)}{\Rightarrow} Q$ and $N = \mathsf{split}(Q, \{\langle a, X \rangle\})$.

Recall that bonds of a given shape can be weakly parted as a consequence of a synchronisation between just a pair of 3D processes. For this reason, when defining semantics of weak splittings, we do not need to require that P is able to complete a reaction, but the condition $P \overset{\omega(a, X)}{\Rightarrow} Q$ suffices for our aims.

$$\text{EMPTY}_t \frac{}{\mathsf{Nil} \xrightarrow{t} \mathsf{Nil}} \qquad \text{PAR}_t \frac{N \xrightarrow{t} N' \quad M \xrightarrow{t} M'}{N \parallel M \xrightarrow{t} N' \parallel M'} \qquad \text{PAR}_a \frac{N \xrightarrow{\mu} N'}{N \parallel M \xrightarrow{\mu} N' \parallel M}$$

Table 5: Temporal and functional behaviour of networks of 3D processes

Example 5.5 *As an application of the definitions given so far, let us consider the 3D process* $P = H \langle \mathsf{atp}, X_a \rangle (A \langle \mathsf{glc}, Y_g \rangle G)$ *where:*

$$H = S_h[\, \rho(\{\langle \mathsf{atp}, X_{ha} \rangle, \langle \mathsf{glc}, Y_{hg} \rangle\}).\mathsf{HEX}\,],$$

$$A = S_a[\, \rho(\{\langle \overline{\mathsf{atp}}, X_{ah} \rangle\}).\mathsf{ADP} + \omega(\overline{\mathsf{atp}}, X_{ah}).\mathsf{ATP}\,],$$

$$G = S_g[\rho(\{\langle \overline{\mathsf{glc}}, Y_{gh} \rangle\}).\mathsf{G6P} + \omega(\overline{\mathsf{glc}}, Y_{gh}).\mathsf{GLC}]$$

and $X_{ha} \cap X_{ah} = X_a \neq \emptyset$ *and* $Y_{hg} \cap Y_{gh} = Y_g \neq \emptyset$. *Then:*

$$\begin{array}{llll} P & \stackrel{\rho(\mathsf{atp}, X_a)}{\Rightarrow} & S_h[\rho(\{\langle \mathsf{glc}, Y_{hg} \rangle\}).\mathsf{HEX}] \langle \mathsf{atp}, X_a \rangle (S_a[\mathsf{ADP}] \langle \mathsf{glc}, Y_g \rangle G) & = & Q \\ & \stackrel{\rho(\mathsf{glc}, Y_g)}{\Rightarrow} & S_h[\mathsf{HEX}] \langle \mathsf{atp}, X_a \rangle (S_a[\mathsf{ADP}] \langle \mathsf{glc}, Y_g \rangle S_g[\mathsf{G6P}]) & = & R \end{array}$$

with $R \stackrel{\theta}{\nrightarrow}$. *By Definition 5.4, R, Q and, hence, P are able to complete a reaction. Moreover,* $\mathsf{split}(R, \{\langle \mathsf{atp}, X_a \rangle, \langle \mathsf{glc}, Y_g \rangle\}) = S_a[\mathsf{HEX}] \parallel \mathsf{split}(S_a[\mathsf{ADP}] \langle \mathsf{glc}, Y_g \rangle S_g[\mathsf{G6P}], \{\langle \mathsf{atp}, X_a \rangle, \langle \mathsf{glc}, Y_g \rangle\}) = S_h[\mathsf{HEX}] \parallel (S_a[\mathsf{ADP}] \parallel S_g[\mathsf{G6P}])$ *implies that* $P \stackrel{\rho}{\rightarrow} S_h[\mathsf{HEX}] \parallel (S_a[\mathsf{ADP}] \parallel S_g[\mathsf{G6P}])$.

Now, we define the temporal and functional behaviour of networks of 3D processes. Here, we assume that a network of 3D processes performs basic actions that belong to set $\{\omega, \rho, \tau\}$, where we use ω and ρ to denote, respectively, weak and a strong splittings of 3D process bonds as a unique action (at a network level we only see if shape bonds can be splitted or not). In the following, we also let elements of the set $\{\omega, \rho, \tau\} \cup \mathbb{T}$ to be ranged over by $\nu, \nu', \cdots$.

Definition 5.6 (Temporal and Functional Behaviour of $\mathbb{N}$-terms) *Rules in Table 5 (plus an additional rule symmetric of* PAR_a *for actions of M) defines the transition relations* $\stackrel{t}{\rightarrow} \subseteq \mathbb{N} \times \mathbb{N}$ *for* $t \in \mathbb{T}$ *and* $\stackrel{\mu}{\rightarrow} \subseteq \mathbb{N} \times \mathbb{N}$ *for* $\mu \in \{\omega, \rho, \tau\}$. *A timed trace from a net N is a finite sequence of steps of the form*

$$N = N_0 \stackrel{\nu_1}{\longrightarrow} N_1 \stackrel{\nu_2}{\longrightarrow} \cdots \stackrel{\nu_n}{\longrightarrow} N_n = M$$

We finally write that $N \stackrel{t}{\Rightarrow} M$ *if there exists a timed trace* $N = N_0 \stackrel{\nu_1}{\longrightarrow} N_1 \stackrel{\nu_2}{\longrightarrow} \cdots \stackrel{\nu_n}{\longrightarrow} N_n = M$ *such that* $t = \sum_{i=0}^{n} \{\nu_i \,|\, \nu_i \in \mathbb{R}^+\}$.

Proposition 5.7 *Let* $P \in \mathsf{3DP}$, $N \in \mathbb{N}$ *with P and Q well-formed; let, moreover,* $t \in \mathbb{T}$.

1. $P \stackrel{\omega}{\rightarrow} N$ *and* $P \stackrel{\rho}{\rightarrow} N$ *implies* $N \in \mathbb{N}$ *well-formed.*

2. $N \stackrel{t}{\rightarrow} M$ *implies M well-formed;*

3. $N \stackrel{t}{\Rightarrow} M$ *implies M well-formed.*

$$\text{ELAS}_{\equiv}\frac{N \equiv N' \quad N' \xrightarrow{\langle P,Q,X\rangle}_e M}{N \xrightarrow{\langle P,Q,X\rangle}_e M} \qquad \text{ELAS}\frac{P \xleftrightarrow{X}_e Q = (\mathbf{v}_p, \mathbf{v}_q)}{(P \parallel Q) \parallel N \xrightarrow{\langle P,Q,X\rangle}_e (P[\![\mathbf{v}_p]\!] \parallel Q[\![\mathbf{v}_q]\!]) \parallel N}$$

Table 6: Reaction rules for elastic collisions

$$\text{INEL}_{\equiv}\frac{N \equiv N' \quad N' \xrightarrow{\langle P,Q,X\rangle}_i M}{N \xrightarrow{\langle P,Q,X\rangle}_i M}$$

$$\text{INEL}\frac{P \xrightarrow{\langle \alpha, X_p\rangle} P' \quad Q \xrightarrow{\langle \overline{\alpha}, X_q\rangle} Q' \quad \alpha \in \{a, \overline{a}\} \quad X = X_p \cap X_q \neq \emptyset \quad P \xleftrightarrow{X}_i Q = \mathbf{v}}{(P \parallel Q) \parallel N \xrightarrow{\langle P,Q,X\rangle}_i ((P' \langle a, X\rangle Q')[\![\mathbf{v}]\!]) \parallel N}$$

Table 7: Reaction rules for inelastic collisions

5.1 Collision response

In this subsection, we describe the semantics we use to address the problem of *collisions response*. To this aim, we introduce two different kinds of reduction relations over networks of 3D processes: $\xrightarrow{\langle P,Q,X\rangle}_e$ and $\xrightarrow{\langle P,Q,X\rangle}_i$, where P, Q are 3D processes and X i a surface of contact. Intuitively, if $N \xrightarrow{\langle P,Q,X\rangle}_e M$ ($N \xrightarrow{\langle P,Q,X\rangle}_e M$) then M is the network we obtain once an elastic (respectively inelastic) collisions between P and Q in the surface of contact X has been resolved. These reduction relations (given in Definition 5.9) use the structural congruence over nets of 3D processes defined below.

Definition 5.8 (Structural congruence over nets of 3D processes) *We define the structural congruence over terms in* $\mathbb{N}$*, we denote with* $\equiv$*, is the smallest relation that satisfies the following axioms:*

- Nil $\parallel N \equiv N$, $N \parallel M \equiv M \parallel N$ *and* $N \parallel (M \parallel R) \equiv (N \parallel M) \parallel R$;

- $P \parallel N \equiv Q \parallel N$ *provided that* $P \equiv_P Q$.

Let I *a finite set of indexes. We often write* $(\parallel P_i)_{i \in I}$ *to denote the network that consists of all 3D processes* P_i *such that* $i \in I$ *(If* $I = \emptyset$*,* $(\parallel P_i)_{i \in I} = $ Nil*). Finally, for* $N = (\parallel P_i)_{i \in I}$ *we define* colliding(N) *to be the set of all tuples* $\langle P, Q, X\rangle$ *such that* $\langle$shape(P), shape(Q), $X\rangle \in$ colliding$(\{$shape$(P_i)\}_{i \in I})$.

Definition 5.9 (Resolving elastic and inelastic collisions) *Let* $N \in \mathbb{N}$ *and* $\langle P, Q, X\rangle$ *a tuple in* colliding(N)*. We write that* $N \xrightarrow{\langle P,Q,X\rangle} M$ *if either* $P \sim Q$ *and* $N \xrightarrow{\langle P,Q,X\rangle}_e M$ *or* $P \not\sim Q$ *and* $N \xrightarrow{\langle P,Q,X\rangle}_i M$*. We write that* $N \leftrightarrow M$ *if there a finite sequence of reduction of reduction steps of the form* $N = N_0 \xrightarrow{\langle P_1,Q_1,X_1\rangle} N_1 \cdots \xrightarrow{\langle P_k,Q_k,X_k\rangle} N_k = M$ *where:*

1. *for each* $i \in [1, k]$ *it is* $\langle P_i, Q_i, X_i\rangle \in$ colliding(N_{i-1})

2. colliding$(N_k) = \emptyset$.

A brief description of rules in Tables 6 and 7 now follows. As already discussed, collisions among incompatible processes are treated as inelastic ones and, hence, resolved by means of the reaction relations $\xrightarrow{\langle P,Q,X \rangle}_e$. Rules ELAS in Table 6 simply changes velocities of two colliding and incompatible processes as stated by Equations (1) and (2) in Definition 3.11. Moreover in Rule ELAS$_\equiv$ we also consider structural congruence over nets of processes.

On the other hand, rules in Table 7 describe how inelastic collision (i.e. collisions between two compatible processes P and Q) can be resolved. Rule INEL joins two compatible processes P and Q to obtain a compound process whose velocity is given by Equation (3) in Definition 3.11. Note that we force P and Q to synchronise on the execution of two compatible actions $\langle \alpha, X_p \rangle$ and $\langle \overline{\alpha}, X_q \rangle$ before joining them.

Let also note that, at any given time t, colliding(N) can be obtained from the set of all the pairs of processes in N that are touching at that time. This set and hence colliding(N) is surely finite and changes only when we resolve some inelastic collision (this is because, after an inelastic collision one or more binding sites can possibly become internal points of a compound process, and hence are not available anymore). Moreover a collision between pairs of processes with the same shape can not be resolved twice. This is either because two processes P and Q have been bond in a compound process as a consequence of an inelastic collision, or because P and Q collide elastically and their velocities have been changed according to Equations (1) and (2) in Definition 3.11 in order to obtain two processes that do not collide anymore (see Proposition 6.4 in Appendix C). Thus, we can always decide if there is a finite sequence of reduction steps that allows us to resolve all collisions listed in colliding(N) and hence obtain a network M with colliding$(M) = \emptyset$.

Proposition 5.10 Let $N \in \mathbb{N}$, $P, Q \in$ 3DP and X a not-emptyset subset of $\mathbb{R}^3$. Then N well-formed and $N \xrightarrow{\langle P,Q,X \rangle} M$ implies $M \in \mathbb{N}$ well-formed.

Iterative applications of Proposition 5.10 (see Appendix C for the proof) allow us to state that following result.

Lemma 5.11 Let $N, M \in \mathbb{N}$, $P, Q \in$ 3DP. Then N well-formed and $N \leftrightarrow M$ implies M well-formed.

We are now ready to define how a network of 3D processes evolves by performing an infinite number of *movement time steps*, where each movement time step describes the evolution of the system when we let time Δ pass.

Definition 5.12 (Movement time steps and system evolution) *Let $N, M \in \mathbb{N}$ and $t \in \mathbb{T}$. We say that $(N, t) \overset{\Delta}{\Rightarrow} (M, t + \Delta)$ iff one of the following two conditions holds:*

1. *there is a finite sequence of $n + 1$ (with $n \geq 0$) steps from $N = N_0$ of the form*

$$N_0 \overset{t_0}{\Rightarrow} M_0 \leftrightarrow N_1 \overset{t_1}{\Rightarrow} M_1 \leftrightarrow N_2 \cdots N_n \overset{t_n}{\Rightarrow} M_n$$

such that: (1) $\Delta = \sum_{i=0}^n t_i$, (2) for $i \in [0, n-1]$, $t_i = $ Ftoc(N_i) and $t_n = \Delta - \sum_{i=0}^{n-1} t_i <$ Ftoc(N_n) (note that, whenever $n = 0$, $t_0 = \Delta <$ Ftoc(N_0) and $N_0 \overset{t_0}{\Rightarrow} M_0$, i.e. we have no collisions to resolve), and (3) $M = $ Move$(M_n, t + \Delta)$.

2. *there is a finite sequence of $n + 1$ (with $n \geq 0$) steps from $N = N_0$ of the form*

$$N_0 \overset{t_0}{\Rightarrow} M_0 \leftrightarrow N_1 \overset{t_1}{\Rightarrow} M_1 \leftrightarrow N_2 \cdots N_n \overset{t_n}{\Rightarrow} M_n \leftrightarrow N_{n+1}$$

such that: (1) $\Delta = \sum_{i=0}^n t_i$, (2) for $i \in [0, n]$, $t_i = $ Ftoc(N_i) (in this case, if $n = 0$ then $t_0 = $ Ftoc$(N_0) = \Delta$ and $N_0 \overset{t_0}{\Rightarrow} N_0' \leftrightarrow N_1$), and (3) $M = $ Move$(N_{n+1}, t + \Delta)$.

A system evolution is a infinite sequence of movement time steps of the form: $(N_0, 0) \stackrel{\Delta}{\Rightarrow} (N_1, \Delta) \stackrel{\Delta}{\Rightarrow} (N_2, 2\Delta) \cdots (N_i, i\Delta) \stackrel{\Delta}{\Rightarrow} (N_{i+1}, (i+1)\Delta) \stackrel{\Delta}{\Rightarrow} \cdots$.

In order to make sure that processes in the network will never interpenetrate during a system evolution, a movement time step consists actually of a finite sequence of intermediate steps of the form $N_i \stackrel{t_i}{\Rightarrow} M_i \leftrightarrow N_{i+1}$ along which we first calculate the next first time of contact (i.e. $t_i = \mathsf{Ftoc}(N_i)$), and then resolve all the collisions that happen after that time t_i. Notice that, at the end of each movement time step, we also apply the changes suggested by the function $\mathsf{Move}(\text{-})$ as described in Section 3.1.

We can prove the following basic property of the Shape Calculus stating that any system evolution does not introduce space inconsistencies like interpenetration of 3D processes or not well-formed processes.

Theorem 5.13 (Closure w.r.t. well-formedness) *Let N be a well-formed network of 3D processes. If $(N, t) \stackrel{\Delta}{\Rightarrow} (M, t + \Delta)$ then M is well-formed.*

Proof: The statement follows easily because, by Proposition 5.7-3 and Lemma 5.11, N_i well-formed and $N_i \stackrel{t_i}{\Rightarrow} M_i \leftrightarrow N_{i+1}$ implies N_{i+1} well-formed. $\square$

6 Conclusions and Future Work

We have defined a Shape Calculus that takes into account space, time, shapes, movement and collisions among shapes. The features and the expressiveness of the calculus are shown with several examples in the biological domain. We proved a correctness property of the calculus regarding the conservation of well-formedness during the evolution of the system. We are currently working on an implementatio of a simulator whose basic low-level language is the Shape Calculus. As future work we intend to study the possibility to include in the calculus some new useful, but in some cases complex, concepts such as re-shaping, message passing of values, and communication by perception of a compatible process in the neighbourhood.

References

[1] http://www.rcsb.org, RCSB - Protein Data Bank.

[2] R. Barbuti, A. Maggiolo-Schettini, P. Milazzo, and G. Pardini. Spatial Calculus of Looping Sequences. *Electr. Notes Theor. Comput. Sci.*, 229(1):21–39, 2009. FBTC 2008.

[3] E. Bartocci, M. R. Di Berardini, F. Corradini, M. Emanuela, and L. Tesei. A Shape Calculus for Biological Processes. In *ICTCS 2009*, pages 30–33, 2009.

[4] L. Bortolussi and A. Policriti. Stochastic concurrent constraint programming and differential equations. *Electr. Notes Theor. Comput. Sci.*, 190(3):27–42, 2007.

[5] N. Cannata, F. Corradini, E. Merelli, and L. Tesei. A spatial model and simulator for metabolic pathways. In *NETTAB '08 - Bioinformatics Methods for Biomedical Complex System Applications*, pages 40–42, Varenna (LC), Italy, May 2008.

[6] N. Cannata, F. Corradini, E. Merelli, and L. Tesei. A spatial simulator for metabolic pathways. In *MAS&BIO 2008*, pages 31–46, Cagliari, Italy, September 2008.

[7] L. Cardelli. Brane calculi. In *CMSB*, pages 257–278, 2004.

[8] L. Cardelli and P. Gardner. Processes in Space. Unpublished, 2009.

[9] F. Ciocchetta and J. Hillston. Bio-pepa: An extension of the process algebra pepa for biochemical networks. *Electr. Notes Theor. Comput. Sci.*, 194(3):103–117, 2008.

[10] C. Ericson. *Real-time collision detection*. Elsevier North-Holland, Inc., 2005.

[11] A. Finkelstein, J. Hetherington, L. Li, O. Margoninski, P. Saffrey, R. Seymour, and A. Warner. Computational challenges of systems biology. *IEEE Computer*, 37(5):26–33, 2004.

[12] D. T. Gillespie. Simulation methods in systems biology. In *SFM08*, pages 125–167.

[13] C. Hecker. Physics, part 3: Collision response. *Game Developer Magazine*, pages 11–18, 1997.

[14] M. John, R. Ewald, and A. Uhrmacher. A spatial extension to the π calculus. *Electronic Notes in Theoretical Computer Science*, 194(3):133–148, 2008. FBTC 2007.

[15] R. Milner. *Communication and concurrency*. Prentice-Hall, Inc. Upper Saddle River, NJ, USA, 1989.

[16] C. Priami and P. Quaglia. Beta binders for biological interactions. In *CMSB*, pages 20–33, 2004.

[17] A. Regev, E. Panina, W. Silverman, L. Cardelli, and E. Shapiro. Bioambients: an abstraction for biological compartments. *Theoretical Computer Science*, 325(1):141–167, 2004.

[18] K. Takahashi, S. Arjunan, and M. Tomita. Space in systems biology of signaling pathways–towards intracellular molecular crowding in silico. *FEBS letters*, 579(8):1783–1788, 2005.

[19] W. Yi. Real-time behaviour of asynchronous agents. In *CONCUR*, pages 502–520, 1990.

Appendix A: some useful properties

Proposition 6.1 Let $S \in \mathsf{Shapes}$ well-formed, $t \in \mathbb{T}$. Then:

1. $\mathcal{V}(S + t) = \mathcal{V}(S)$ and $\mathcal{M}(S + t) = \mathcal{M}(S)$;

2. $\mathcal{R}(S + t) = \mathcal{R}(S) + t \cdot \mathcal{V}(S)$;

3. $\mathcal{P}(S + t) = \mathcal{P}(S) + t \cdot \mathcal{V}(S)$;

4. $\mathcal{B}(S + t) = \mathcal{B}(S) + t \cdot \mathcal{V}(S)$.

Proof: Item 4 follows directly from Item 3. We prove Items 1, 2 and 3 all together by induction on $S \in \mathsf{Shapes}$ well-formed.

Basic: $S = \langle V, m, \mathbf{p}, \mathbf{v} \rangle]$ In such a case $S + t = \langle V + (t \cdot \mathbf{v}), m, \mathbf{p} + (t \cdot \mathbf{v}), \mathbf{v} \rangle$. So $\mathcal{V}(S + t) = \mathbf{v} = \mathcal{V}(S)$, $\mathcal{M}(S + t) = m = \mathcal{M}(S)$ and $\mathcal{R}(S + t) = \mathbf{p} + (t \cdot \mathbf{v}) = \mathcal{R}(S) + (t \cdot \mathbf{v})$. Moreover $\mathcal{P}(S + t) = V + (t \cdot \mathcal{V}(S)) = \mathcal{P}(S) + (t \cdot \mathcal{V}(S))$.

Compound: $S = S_1 \langle X \rangle S_2$ and $S + t = (S_1 + t) \langle X + (t \cdot \mathcal{V}(S)) \rangle (S_2 + t)$. By induction hypothesis:

1. $\mathcal{V}(S_i + t) = \mathcal{V}(S_i) = \mathcal{V}(S)$ and $\mathcal{M}(S_i + t) = \mathcal{M}(S_i)$ for $i = 1, 2$. Thus $\mathcal{V}(S + t) = \mathcal{V}(S)$ and $\mathcal{M}(()S + t) = \mathcal{M}(S_1 + t) + \mathcal{M}(S_2 + t) = \mathcal{M}(S_i) + \mathcal{M}(S_2) = \mathcal{M}(S)$.

2. $\mathcal{R}(S_i + t) = \mathcal{R}(S_i)$ for $i = 1, 2$. Thus $\mathcal{R}(S + t) = \mathcal{M}(S_1 + t) \cdot \mathcal{R}(S_1 + t) + \mathcal{M}(S_2 + t) \cdot \mathcal{R}(S_2 + t) = \mathcal{M}(S_1) \cdot \mathcal{R}(S_1) + \mathcal{M}(S_2) \cdot \mathcal{R}(S_2) = \mathcal{R}(S)$.

3. $\mathcal{P}(S + t) = \mathcal{P}(S_1 + t) \cup \mathcal{P}(S_2 + t) = \mathcal{P}(S_1) \cup \mathcal{P}(S_2) = \mathcal{P}(S)$.

$\square$

Proposition 3.8 Let $S \in \mathsf{Shapes}$, $t \in \mathbb{T}$ and $\mathbf{w} \in \mathbb{V}$. If S is well-formed then $S + t$ and $S[\![\mathbf{w}]\!]$ are well-formed.

Proof: We prove these statement by induction in $S \in \mathsf{Shapes}$.

Basic: $S = \langle V, m, \mathbf{p}, \mathbf{v} \rangle$. In such a case, $S + t = \langle V + t \cdot \mathbf{v}, m, p + t \cdot \mathbf{v}, \mathbf{v} \rangle$ and $S[\![\mathbf{w}]\!] = \langle V, m, \mathbf{p}, \mathbf{w} \rangle$ are well-formed shapes.

Compound: $S = S_1 \langle X \rangle S_2$. By Definitions 3.6 and 3.7 $S + t = S_1 + t \langle X + t \cdot \mathcal{V}(S) \rangle S_2 + t$ and $S[\![\mathbf{w}]\!] = S_1[\![\mathbf{w}]\!] \langle X \rangle S_2[\![\mathbf{w}]\!]$. By induction hypothesis both $S_1 + t$ and $S_2 + t$ are well-formed. By Prop. 6.1, we have also that: (1) the set $X + t \cdot \mathcal{V}(S) = \mathcal{P}(S_1 + t) \cap \mathcal{P}(S_2 + t) = (\mathcal{P}(S_1) + t \cdot \mathcal{V}(S_1)) \cap (\mathcal{P}(S_2) + t \cdot \mathcal{V}(S_2)) = (\mathcal{P}(S_1) + t \cdot \mathcal{V}(S)) \cap (\mathcal{P}(S_2) + t \cdot \mathcal{V}(S)) \subseteq \mathcal{B}(S_1 + t) \cap \mathcal{B}(S_2 + t)$, (2) $\mathcal{V}(S_1 + t \langle X + t \cdot \mathcal{V}(S) \rangle S_2 + t)$ is the singleton $\mathbf{v} = \mathcal{V}(S)$.

Again by induction hypothesis we have that $S_1[\![\mathbf{w}]\!]$ and $S_2[\![\mathbf{w}]\!]$ are well-formed shapes. Moreover, for $i = 1, 2$ it is $\mathcal{P}(S_i[\![\mathbf{w}]\!]) = \mathcal{P}(S_i)$. Thus, $X = \mathcal{P}(S_1) \cap \mathcal{P}(S_2) = \mathcal{P}(S_1[\![\mathbf{w}]\!]) \cap \mathcal{P}(S_2[\![\mathbf{w}]\!])$ is a non-empty subset of $\mathcal{B}(S_1) \cap \mathcal{B}(S_2) = \mathcal{B}(S_1[\![\mathbf{w}]\!]) \cap \mathcal{B}(S_2[\![\mathbf{w}]\!])$. Finally $\mathcal{V}(S_1[\![\mathbf{w}]\!] \langle X \rangle S_2[\![\mathbf{w}]\!]) = \{\mathbf{w}\}$.

$\square$

Proposition 4.5 If $P \in \mathsf{3DP}$ well-formed then $\mathsf{shape}(P)$ is a well-formed 3D shape.

Proof:

Basic: $P = S[B]$. In such a case, trivially, P well-formed implies $\mathsf{shape}(P) = S$ well-formed.

Compound: $P = P_1 \langle a, X \rangle P_2$. In such a case $\mathsf{shape}(P) = \mathsf{shape}(P_1) \langle X \rangle \mathsf{shape}(P_2)$. By induction hypothesis $\mathsf{shape}(P_i)$ is a well-formed shape for $i = 1, 2$. Moreover, P well-formed implies $X \subseteq \mathcal{P}(S_1) \cap \mathcal{P}(S_2) \subseteq \mathcal{B}(S_1) \cap \mathcal{B}(S_2)$ and $\mathcal{V}(\mathsf{shape}(P)) = \{\mathbf{v}\}$ where $\mathbf{v} = \mathcal{V}(P_1) = \mathcal{V}(P_2)$.

$\square$

Appendix B: Proofs of Section 4

In this section we prove the results stated in Section 4.

Proposition 4.8 Let $P, Q \in \mathsf{3DP}$ with P well-formed; let moreover $t \in \mathbb{T}$ and $\mu \in \mathsf{Act}_\tau$. Then:

1. $P \xrightarrow{t} Q$ implies $\mathsf{shape}(Q) = \mathsf{shape}(P) + t$;

2. $P \xrightarrow{\mu} Q$ implies $\mathsf{shape}(Q) = \mathsf{shape}(P)$;

3. either $P \xrightarrow{t} Q$ or $P \xrightarrow{\mu} Q$ imply Q well-formed.

Proof: We first prove Items 1 and 2 by induction on $P \in \mathsf{3DP}$.

Basic: $P = S[B]$.

1. $P \xrightarrow{t} Q$ implies $B \xrightarrow{t} B'$ and $Q = (S+t)[B']$. In such a case $\mathsf{shape}(Q) = (S+t) = \mathsf{shape}(P) + t$.

2. $P \xrightarrow{\mu} Q$ implies $Q = S[B']$ for a proper $B' \in \mathbb{B}$ (see rules in table 3). Then: $\mathsf{shape}(Q) = S = \mathsf{shape}(P)$.

Compound: $P = P_1 \langle a, X \rangle P_2$.

1. $P \xrightarrow{t} Q$ implies $P_1 \xrightarrow{t} P_1'$, $P_2 \xrightarrow{t} P_2'$, and $Q = P_1' \langle a, X' \rangle P_2'$ where $X' = X + (t \cdot \mathcal{V}(P))$. In such a case, by induction hypothesis, we have that $\mathsf{shape}(Q) = \mathsf{shape}(P_1') \langle X' \rangle \mathsf{shape}(P_2') = (\mathsf{shape}(P_1) + t) \langle X' \rangle (\mathsf{shape}(P_2) + t) = \mathsf{shape}(P) + t$.

2. $P \xrightarrow{\mu} Q$ implies either $P_1 \xrightarrow{\mu} P_1'$ and $Q = P_1' \langle a, X \rangle P_2$ or $P_2 \xrightarrow{\mu} P_2'$ and $Q = P_1 \langle a, X \rangle P_2'$. Let us consider the former case (the latter one is similar). Then, again by induction hypothesis, $\mathsf{shape}(Q) = \mathsf{shape}(P_1') \langle X \rangle \mathsf{shape}(P_2) = \mathsf{shape}(P_1) \langle X \rangle \mathsf{shape}(P_2) = \mathsf{shape}(P)$.

Now we prove that P well-formed and $P \xrightarrow{t} Q$ imply Q well-formed. We proceed by induction on P.

Basic: $P = S[B]$. $P \xrightarrow{t} Q$ implies $B \xrightarrow{t} B'$ and $Q = (S + t)[B']$. In such a case, S well-formed implies $\mathsf{shape}(Q) = S + t$ well-formed. Moreover for each $\langle \alpha, X \rangle$ and $\omega(\alpha, X)$ that occurs in B' and, hence, in B we have that $\mathsf{global}(X, \mathcal{R}(P)) \subseteq \mathcal{B}(P)$. Thus, $\mathsf{global}(X, \mathcal{R}(Q)) = \mathsf{global}(X, \mathcal{R}(P) + (t \cdot \mathcal{V}(P)) = \mathsf{global}(X, \mathcal{R}(P)) + (t \cdot \mathcal{V}(P)) \subseteq \mathcal{B}(P) + (t \cdot \mathcal{V}(P)) = \mathcal{B}(Q)$ by Proposition 6.1-4. Thus, we can conclude Q is well-formed.

Compound: $P = P_1 \langle a, X \rangle P_2$ with P_i well-formed for $i = 1, 2$ and $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$.

$P \xrightarrow{t} Q$ implies $P_1 \xrightarrow{t} P_1'$, $P_2 \xrightarrow{t} P_2'$, and $Q = P_1' \langle a, X' \rangle P_2'$ where $X' = X + (t \cdot \mathcal{V}(P))$. By induction hypothesis, both P_1' and P_2' are well-formed. Moreover, since $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$, we also have $X' = X + (t \cdot \mathcal{V}(P)) \subseteq (\mathcal{B}(P_1) \cap \mathcal{B}(P_2)) + (t \cdot \mathcal{V}(P)) = (\mathcal{B}(P_1) + (t \cdot \mathcal{V}(P))) \cap (\mathcal{B}(P_2) + (t \cdot \mathcal{V}(P))) = \mathcal{B}(P_1') \cap \mathcal{B}(P_2')$.

It remains to prove that P well-formed and $P \xrightarrow{\mu} Q$ imply Q well-formed. We proceed, again, by induction on P.

Basic: $P = S[B]$. $P \xrightarrow{\mu} Q$ implies $B \xrightarrow{\mu'} B'$ for a proper $\mu \in \mathsf{Act}_\tau$ (see rules in Table 3) and $Q = S[B']$. P well-formed implies S well-formed. Moreover, for each $\langle \alpha, X \rangle$ and $\omega(\alpha, X)$ that occurs in B we have $\mathsf{global}(X, \mathcal{R}(P)) \subseteq \mathcal{B}(P) = \mathcal{B}(S) = \mathcal{B}(Q)$. Thus, the well-formedness of Q follows since each $\langle \alpha, X \rangle$ and $\omega(\alpha, X)$ that occurs in B' must also occurs in B.

Compound: $P = P_1 \langle a, X \rangle P_2$ with P_i well-formed for $i = 1, 2$ and $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$.

$P \xrightarrow{\mu} Q$ implies either $P_1 \xrightarrow{\mu} P_1'$ and $Q = P_1' \langle a, X \rangle P_2$ or $P_2 \xrightarrow{\mu} P_2'$ and $Q = P_1 \langle a, X \rangle P_2'$. Let us consider the former case (the latter one is similar). By induction hypothesis, P_1' is well-formed and by Proposition 6.1 we have also $\mathsf{shape}(P_1') = \mathsf{shape}(P_1)$ and, hence, $\mathcal{B}(P_1') = \mathcal{B}(P_1)$.

Thus, we can conclude that both P_1' and P_2 are well-formed and $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2) = \mathcal{B}(P_1') \cap \mathcal{B}(P_2)$ and, hence, that Q is well-formed.

$\square$

Proposition 4.13 Let $P \in \mathsf{3DP}$ well-formed. If $\langle a, X \rangle \in \mathsf{bonds}(P)$ there are $Q, R \in \mathsf{3DP}$ well-formed such that $X \subseteq \mathcal{B}(Q) \cap \mathcal{B}(R)$, $\mathcal{V}(Q) = \mathcal{V}(R) = \mathcal{V}(P)$, and $P \equiv_P Q \langle a, X \rangle R$.

Proof: By induction on P

Basic: $P = S[B]$. Not possible since $\mathsf{bonds}(P) = \emptyset$

Compound: $P = P_1 \langle b, Y \rangle P_2$ with P_i well-formed for $i = 1, 2$ and $Y \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$.

If $\langle a, X \rangle = \langle b, Y \rangle$ the statement follows easily (indeed we can choose $Q = P_1$ and $R = P_2$). Assume that $\langle a, X \rangle \in \mathsf{bonds}(P_1)$ (whenever $\langle a, X \rangle \in \mathsf{bonds}(P_2)$ the statement can be proved similarly). Then, by induction hypothesis, there exist $Q_1, R_1 \in \mathsf{3DP}$ well-formed such that $X \subseteq \mathcal{B}(Q_1) \cap \mathcal{B}(R_1)$, $\mathcal{V}(Q_1) = \mathcal{V}(R_1) = \mathcal{V}(P_1)$, and $P_1 \equiv_P Q_1 \langle a, X \rangle R_1$. Thus $P = P_1 \langle b, Y \rangle P_2 \equiv_P (Q_1 \langle a, X \rangle R_1) \langle b, Y \rangle P_2$. At this point, we can distinguish two possible subcases: (1) $Y \subseteq \mathcal{B}(R_1)$ and (2) $Y \subseteq \mathcal{B}(Q_1)$.

In the former case we have that $P \equiv_P Q_1 \langle a, X \rangle (R_1 \langle b, Y \rangle P_2)$ and we choose $Q = Q_1$ and $R = R_1 \langle b, Y \rangle P_2$. Moreover:

- we prove that $X \subseteq \mathcal{B}(Q) \cap \mathcal{B}(R) = \mathcal{B}(Q_1) \cap \mathcal{B}(R)$ by contradiction. Let $\mathbf{x} \in X$ such that $\mathbf{x} \notin \mathcal{B}(Q_1) \cap \mathcal{B}(R)$. Since $\mathcal{B}(R) = (\mathcal{B}(R_1) \cup \mathcal{B}(P_2)) \setminus \{\mathbf{z} \mid \mathbf{z} \text{ is interior of } \mathcal{P}(R_1) \cup \mathcal{P}(P_2)\}$ and $X \subseteq \mathcal{B}(Q_1) \cap \mathcal{B}(R_1)$, then $\mathbf{x} \notin \mathcal{B}(Q_1) \cap \mathcal{B}(R)$ implies that $\mathbf{x}$ is an interior point of $\mathcal{P}(R_1) \cup \mathcal{P}(P_2)$. Moreover $\mathbf{x} \in X \subseteq \mathcal{B}(Q_1) \cap \mathcal{B}(R_1)$ implies $\mathbf{x}$ interior of $P_1 \equiv_P Q_1 \langle a, X \rangle R_1$ and hence $\mathbf{x}$ can not be interior of $\mathcal{P}(P_2)$ (otherwise P_1 and P_2 interpenetrate and P could not be a well-formed process.) Thus we can conclude that $\mathbf{x}$ must be an interior point of $\mathcal{P}(R_1)$. But this is impossible since no point can be (at the same time) an interior point and a boundary point of a 3D shape.

- we already know that $Q = Q_1$ is well-formed; moreover, since both R_1 and P_2 are well-formed, to prove that R is well-formed too, we have to prove that $Y \subseteq \mathcal{B}(R_1) \cap \mathcal{B}(P_2)$. We proceed by contradiction. Thus let $\mathbf{y} \in Y$ such that $\mathbf{y} \notin \mathcal{B}(R_1) \cap \mathcal{B}(P_2)$ i.e. (since $Y \subseteq \mathcal{B}(R_1)$) such that $\mathbf{y} \notin \mathcal{B}(P_2)$. Then $\mathbf{y} \notin \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$. But this is impossible because $Y \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$.

- Let $\mathbf{v} = \mathcal{V}(P)$; then $\mathcal{V}(Q) = \mathcal{V}(P_1) = \mathbf{v}$; moreover, $\mathcal{V}(R_1) = \mathcal{V}(P_1) = \mathcal{V}(P_2) = \mathbf{v}$ implies $\mathcal{V}(R) = \mathbf{v}$.

Now let $Y \subseteq \mathcal{B}(Q_1)$. In such a case, $P \equiv_P (Q_1 \langle a, X \rangle R_1) \langle b, Y \rangle P_2 \equiv_P (R_1 \langle a, X \rangle Q_1) \langle b, Y \rangle P_2 \equiv_P R_1 \langle a, X \rangle (Q_1 \langle b, Y \rangle P_2)$ and we can choose $Q = R_1$ and $R = Q_1 \langle b, Y \rangle P_2$. The proof is omitted because it is similar to the above one.

$\square$

Proposition 4.14 Let $P, Q \in \mathsf{3DP}$ with P well-formed, and $\mu \in \omega(\mathcal{C}) \cup \rho(\mathcal{C})$. Then:

1. $P \stackrel{\mu}{\Rightarrow} Q$ implies $\mathsf{shape}(Q) = \mathsf{shape}(P)$;

2. $P \stackrel{\mu}{\Rightarrow} Q$ implies Q well-formed.

Proof: We only prove the statement for $\mu = \rho(a, X) \in \rho(\mathcal{C})$ (if $\mu = \in \omega(\mathcal{C})$ the proof is similarly).

Basic: $P = S[B]$. This case is not possible since $P \not\stackrel{\rho(a,X)}{\Rightarrow}$.

Compound: $P = P_1 \langle b, Y \rangle P_2$ with P_i well-formed for $i = 1, 2$ and $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$. We distinguish two possible subcases:

- $\langle b, Y \rangle = \langle a, X \rangle$, $P_1 \xrightarrow{\rho(\alpha, X_1)} P_1'$, $P_2 \xrightarrow{\rho(\overline{\alpha}, X_2)} P_2'$ (with $\alpha \in \{a, \overline{a}\}$ and $X = X_1 \cap X_2$), and $Q = P_1' \langle a, X \rangle P_2'$.

  1. In this case, by Proposition 4.8-2, $\mathsf{shape}(P_i') = \mathsf{shape}(P_i)$ for $i = 1, 2$ and, hence, $\mathsf{shape}(Q) = \mathsf{shape}(P_1') \langle X \rangle \mathsf{shape}(P_2') = \mathsf{shape}(P_1) \langle X \rangle \mathsf{shape}(P_2) = \mathsf{shape}(P)$.

2. By induction hypotheses, P_i well-formed implies P_i' well-formed, for $i = 1, 2$. Moreover $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2)$ and (again by Proposition 4.8-2) $\mathsf{shape}(P_i') = \mathsf{shape}(P_i)$ for $i = 1, 2$ imply also $X \subseteq \mathcal{B}(P_1') \cap \mathcal{B}(P_2')$. So we can conclude that Q is well formed.

- $P_1 \stackrel{\rho(a,X)}{\Rightarrow} P_1'$ and $Q = P_1' \langle a, X \rangle P_2$.

1. In this case, by Item 1, $\mathsf{shape}(P_1') = \mathsf{shape}(P_1)$ and, as above, we can prove that $\mathsf{shape}(Q) = \mathsf{shape}(P)$.

2. By induction hypotheses, P_1 well-formed implies P_1' well-formed. Moreover, since (by Item 1) $\mathsf{shape}(P_1') = \mathsf{shape}(P_1)$, $X \subseteq \mathcal{B}(P_1) \cap \mathcal{B}(P_2) = \mathcal{B}(P_1') \cap \mathcal{B}(P_2)$. We can conclude that Q is well formed.

$\square$

Appendix C: Proofs of Section 5

Proposition 6.2 Let $P \in \mathsf{3DP}$ well-formed, $C \subseteq \mathcal{C}$ and $N = \mathsf{split}(P, C) \in \mathbb{N}$. If N contains the 3D process $Q \in \mathsf{3DP}$ (i.e. if $N \equiv Q \| M$ for a proper net M) then we have that either $Q = P$ or Q is a component of P such that $\mathsf{bonds}(Q) \cap C = \emptyset$.

Proof: By induction on the number of channels in $\mathsf{bonds}(P) \cap C$.

$\mathsf{bonds}(P) \cap C = \emptyset$. In such a case $\mathsf{split}(P, C) = P$ contains a 3D process Q only if $Q = P$.

$\langle a, X \rangle \in \mathsf{bonds}(P) \cap C \neq \emptyset$. By Proposition 4.13, there exist two well-formed $P_1, P_2 \in \mathsf{3DP}$ such that $P \equiv_P P_1 \langle a, X \rangle P_2$. As a consequence, $\mathsf{bonds}(P) = \mathsf{bonds}(P_1) \cup \{\langle a, X \rangle\} \cup \mathsf{bonds}(P_2)$ and, hence, $|\mathsf{bonds}(P_1) \cap C|, |\mathsf{bonds}(P_2) \cap C| < |\mathsf{bonds}(P) \cap C|$. Moreover, $\mathsf{split}(P, C) = \mathsf{split}(P_1, C) \| \mathsf{split}(P_2, C)$.

Now, if Q is contained in $\mathsf{split}(P, C)$ we have either Q in $\mathsf{split}(P_1, C)$ or Q in $\mathsf{split}(P_2, C)$. Assume Q in $\mathsf{split}(P_i, C)$ (for $i = 1, 2$). By induction hypothesis we have that either $Q = P_i$ (this also means that $\mathsf{bonds}(P_i) \cap C = \emptyset$) or Q is a component of P_i (and, hence, of P) such that $\mathsf{bonds}(Q) \cap C = \emptyset$.

$\square$

Proposition 5.3 Let $P \in \mathsf{3DP}$ well-formed and $C \subseteq \mathcal{C}$. Then $\mathsf{split}(P, C)$ is a well-formed network of 3D processes.

Proof: By induction on the number of channels in $\mathsf{bonds}(P) \cap C$.

$\mathsf{bonds}(P) \cap C = \emptyset$. In such a case $\mathsf{split}(P, C) = P$ that is a well-formed network of processes by definition.

$\langle a, X \rangle \in \mathsf{bonds}(P) \cap C \neq \emptyset$. Again by Proposition 4.13, there exist two well-formed $P_1, P_2 \in \mathsf{3DP}$ such that $P \equiv_P P_1 \langle a, X \rangle P_2$ and $\mathsf{split}(P, C) = \mathsf{split}(P_1, C) \| \mathsf{split}(P_2, C) = N_1 \| N_2$. By induction hypothesis N_i is a well-formed network of 3D processes for $i = 1, 2$. Now, in order to prove that $\mathsf{split}(P, C)$ is a well-formed network, it still remains to prove that if Q_1 and Q_2 are two 3D processes contained, respectively, in N_1 and N_2 then Q_1 and Q_2 do not interpenetrate.

Assume, towards a contradiction, that there Q_1 and Q_2 in N_1 and N_2, respectively, such that Q_1 and Q_2 interpenetrate. By Proposition 6.2, we have either that, for $i = 1, 2$, either $Q_i = P_i$ or Q_i is a component of P_i. Now, if Q_1 and Q_2 interpenetrate, there is at least a point $\mathbf{x}$ that is an interior point of both $\mathcal{P}(Q_1) \subseteq \mathcal{P}(P_1)$ and $\mathcal{P}(Q_2) \subseteq \mathcal{P}(P_2)$ and, thus, also P_1 and P_2 interpenetrate. But this is not possible since $P \equiv_P P_1 \langle a, X \rangle P_2$ and P is well-formed.

$\square$

Proposition 6.3 Let $N, M \in \mathbb{N}$, $P, Q \in \mathsf{3DP}$ and $t \in \mathbb{T}$ such that $N \overset{t}{\to} M$ and $P \overset{t}{\to} Q$. The network N contains P iff M contains Q.

Proof: By induction on $N \in \mathbb{N}$.

$N = \mathsf{Nil}$. $N \overset{t}{\to} \mathsf{Nil}$ and Nil does not contain any 3D process.

$N = P$ with $P \in \mathsf{3DP}$. By our operational semantics, $N \overset{t}{\to} M$ iff $M = Q$ and $P \overset{t}{\to} Q$.

$N = N_1 \,\|\, N_2$. $N \overset{t}{\to} M_1 \,\|\, M_2 = M$ iff $N_i \overset{t}{\to} M_i$ for $i = 1, 2$. Thus, P is contained in N iff P is contained either in N_1 or in N_1 iff (by induction hypothesis) and Q is contained either in M_1 or in M_1, i.e. iff Q is contained in M.

$\square$

Proposition 5.7 Let $P \in \mathsf{3DP}$, $N \in \mathbb{N}$ with P and N well-formed; let, moreover, $t \in \mathbb{T}$.

1. $P \overset{\omega}{\to} N$ and $P \overset{\rho}{\to} N$ implies $N \in \mathbb{N}$ well-formed.

2. $N \overset{t}{\to} M$ implies M well-formed;

3. $N \overset{t}{\Rightarrow} M$ implies M well-formed.

Proof: Item 1 can be proved by iterative applications of Proposition 4.14-2 and due to Proposition 5.3. Moreover, by Definition 5.6, Item 3 follows directly from Items 1 and 3. In what follows we prove Item 2 by induction on $N \in \mathbb{N}$.

$N = \mathsf{Nil}$. In such a case $N \overset{t}{\to} M$ implies $M = \mathsf{Nil}$ that is always well-formed.

$N = P$ with $P \in \mathsf{3DP}$. In such a case the statement follows by Proposition 4.8-3.

$N = N_1 \,\|\, N_2$. By our operational rules, $N \overset{t}{\to} M$ implies that $N_i \overset{t}{\to} M_i$, for $i = 1, 2$, and $M = M_1 \,\|\, M_2$. By induction hypothesis we have that both M_1 and M_2 are well-formed. Now, to prove that M is well-formed, it still remains to prove that if Q_1 and Q_2 are 3D processes that compose the networks M_1 and M_2, respectively, then Q_1 and Q_2 do not interpenetrate. We proceed by contradiction.

Thus, let us assume that there are Q_1 in M_1 and Q_2 in M_2 such that Q_1 and Q_2 interpenetrate. By Proposition 6.3, M_i contains Q_i iff N_i contains P_i for some $P_i \in \mathsf{3DP}$ such that $P_i \overset{t}{\to} Q_i$. Moreover, by Proposition 4.8-1, $\mathsf{shape}(Q_i) = \mathsf{shape}(P_i) + t$. Thus, we can conclude that if Q_1 and Q_2 interpenetrate the same do P_1 and P_2. But this not possible since N is well-formed.

$\square$

Proposition 6.4 Let $N, M \in \mathbb{N}$, $\langle P, Q, X \rangle \in \mathsf{colliding}(N)$ such that $N \xrightarrow{\langle P, Q, X \rangle} M$. If P' and Q' are two processes in M with $\mathsf{shape}(P') = \mathsf{shape}(P)$ and $\mathsf{shape}(Q') = \mathsf{shape}(Q)$, $\langle P', Q', Y \rangle \notin \mathsf{colliding}(M)$ for any $Y \subseteq \mathbb{R}^3$.

Proof: Let us assume $N = (P \,\|\, Q) \,\|\, N'$. By rules in Table 6, $N \xrightarrow{\langle P, Q, X \rangle}_e M$ implies $M \equiv (P[\![\mathbf{v}_p]\!] \,\|\, Q[\![\mathbf{v}_q]\!]) \,\|\, N'$ where $(\mathbf{v}_p, \mathbf{v}_q) = P \xleftrightarrow{X}_e Q$. Moreover, Equations (1) and (2) in Definition 3.11 and the velocities they provide ensure that $P[\![\mathbf{v}_p]\!]$ and $Q[\![\mathbf{v}_q]\!]$ (the only processes in M that have the same shapes of P and Q respectively) can not collide anymore.

If, otherwise, $N \xrightarrow{\langle P,Q,X \rangle}_i M$ then there exist $\langle \alpha, X_p \rangle, \langle \overline{\alpha}, X_q \rangle \in \mathcal{C}$, with $\alpha \in \{a, \overline{a}\}$, such that $P \xrightarrow{\langle \alpha, X_p \rangle} P'$, $Q \xrightarrow{\langle \overline{\alpha}, X_q \rangle} Q'$ and $M \equiv ((P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]) \parallel N'$ where $X = X_p \cap X_q \neq \emptyset$ and $P \xleftarrow{X}_i Q = \mathbf{v}$. In such a case the statement follows easily because there no processes P' and Q' in M with $\mathsf{shape}(P') = \mathsf{shape}(P)$ and $\mathsf{shape}(Q') = \mathsf{shape}(Q)$.

$\square$

Proposition 5.10 Let $N \in \mathbb{N}$, $P, Q \in \mathsf{3DP}$ and X a not-emptyset subset of $\mathbb{R}^3$. Then N well-formed and $N \xrightarrow{\langle P,Q,X \rangle} M$ implies M well-formed.

Proof:

Assume $N = (P \parallel Q) \parallel N'$. By Definition 5.1, N well-formed implies P, Q and N' well-formed. Moreover, both P and Q do not interpenetrate with any 3D process that compose the network N'

Now, if $N \xrightarrow{\langle P,Q,X \rangle}_e M$ then $M \equiv (P[\![\mathbf{v}_p]\!] \parallel Q[\![\mathbf{v}_q]\!]) \parallel N'$ where $(\mathbf{v}_p, \mathbf{v}_q) = P \xleftarrow{X}_e Q$ and $P[\![\mathbf{v}_p]\!]$ and $Q[\![\mathbf{v}_q]\!]$ well-formed (this is because so are both P and Q). Moreover $\mathsf{shape}(P[\![\mathbf{v}_p]\!]) = \mathsf{shape}(P)$ and $\mathsf{shape}(Q[\![\mathbf{v}_q]\!]) = \mathsf{shape}(Q)$. Thus, as P and Q, $P[\![\mathbf{v}_p]\!]$ and $Q[\![\mathbf{v}_q]\!]$ do not interpenetrate with any 3D process that compose the network N'. Finally we can conclude that the network M is well-formed.

Now assume that $N \xrightarrow{\langle P,Q,X \rangle}_i M$. Then, according to Rule INEL, there are $\langle \alpha, X_p \rangle, \langle \overline{\alpha}, X_q \rangle \in \mathcal{C}$, with $\alpha \in \{a, \overline{a}\}$, such that $P \xrightarrow{\langle \alpha, X_p \rangle} P'$, $Q \xrightarrow{\langle \overline{\alpha}, X_q \rangle} Q'$ and $M \equiv ((P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]) \parallel N'$ where $X = X_p \cap X_q \neq \emptyset$ and $P \xleftarrow{X}_i Q = \mathbf{v}$. By Proposition 4.8-3, P and Q well-formed implies P' and Q' well-formed. Moreover:

- P (Q) well-formed and $P \xrightarrow{\langle \alpha, X_p \rangle} P'$ ($Q \xrightarrow{\langle \overline{\alpha}, X_q \rangle} Q'$) implies $X_p \subseteq \mathcal{B}(P)$ ($X_q \subseteq \mathcal{B}(Q)$, respectively) – see Rules BASIC_{ch} and COMP_{a2} in Table 3. Thus $X = X_p \cap X_q \subseteq \mathcal{B}(P) \cap \mathcal{B}(Q)$, and $P' \langle a, X \rangle Q'$, as well as $(P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]$, is well-formed.

- $\mathsf{shape}((P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]) = \mathsf{shape}(P' \langle a, X \rangle Q') = \mathsf{shape}(P') \langle X \rangle \mathsf{shape}(Q') = \mathcal{P}(P') \cup \mathcal{P}(Q') = \mathcal{P}(P) \cup \mathcal{P}(Q)$ (this is because Proposition 4.8-2 implies $\mathsf{shape}(P') = \mathsf{shape}(P)$ and $\mathsf{shape}(Q') = \mathsf{shape}(Q)$), implies that $(P' \langle a, X \rangle Q')[\![\mathbf{v}]\!]$ can not interpenetrate any 3D process that compose the network N' (otherwise either P or Q would interpenetrate the same process).

Finally, we can conclude that M is well-formed.

$\square$