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# Timed Operational Semantics and Well-Formedness of Shape Calculus

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**Abstract**

The Shape Calculus is 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. In this paper, the full formal timed operational semantics of the calculus is provided, together with examples that illustrate the use of the calculus in a well-known biological scenario. Moreover, a result of well-formedness about the evolution of a given network of well-formed 3D processes is proved.

## 1 Introduction

The language of the Shape Calculus was previously introduced in this volume [2] with the aim of gently and incrementally present all its features and their relative semantics. The motivations behind the type and nature of the calculus operators were discussed and a great variety of scenarios in which the calculus may be used effectively were described. The Shape Calculus is intended to be a core language providing basic operators to describe a large variety of biological scenarios. A network of 3D processes, as introduced in [2], represents a virtual environment in which biological entities with

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their physical 3D shape are placed. The dynamics of the calculus describes how they can interact through their channels, bumping or binding. In case of binding, the composed process can exhibit new channels and interact in a different way. Moreover, a composed process can split weakly - non-deterministically at any time on one bond - producing two pieces, or strongly - on a set of bonds as soon as the whole strong-split is possible - producing several pieces like in a biochemical reaction.

A formal definition of the timed operational semantics of the calculus is needed to integrate and complete the partially informal description given in [2]. It is also the starting point for constructing both a suitable simulator for the calculus and several verification tools that can be used to prove properties of the defined model or of an abstraction of it. In this paper, such a semantics is fully provided. Moreover, we present a first fundamental result of correctness and suitability of the calculus. A concept of well-formedness is introduced, starting from shapes and porting it to more complex calculus objects such as 3D processes and, ultimately, networks of 3D processes. Well-formedness is a standard concept used to avoid strange and unwanted situations in which a term can be legally written by syntax rules, but that semantically corresponds to a contradictory situation. In our case, an example of such a situation is, for instance, a composed shape whose pieces move in different directions. We prove that a given well-formed network of 3D processes always evolves into a well-formed network of 3D processes, that is to say, no temporal and spatial inconsistencies are introduced by the dynamics of the calculus.

The reader of this paper is strongly encouraged to read [2] first, in order to get familiar with the fundamental concepts of the calculus and, thus, to follow more easily the technical definitions and results. The proofs of several results are omitted here. They can be found in [1], an extended version of this paper that contains also a larger introduction to the general concepts of the Shape Calculus. The rest of the paper is organized as follows. Section 2 introduces 3D shapes, shape composition, movement, collision detection and collision response. Section 3 defines behaviours and 3D processes giving them full semantics. Section 4 puts all the pieces together and specifies precisely networks of 3D processes and a general result of dynamic well-formedness is proven.

## 2 3D Shapes

Let $\mathbb{P}, \mathbb{V} = \mathbb{R}^3$ be the sets of positions and velocities, respectively, in a *global* three dimensional coordinate system. We also assume relative coordinate systems that will always be w.r.t. a certain shape $S$. We refer to this relative system as the *local* coordinate system of shape $S$. Using local coordinate systems we can express parts of a given shape, such as faces and vertexes, independently from its actual global position. If $\mathbf{p} \in \mathbb{P}$ is a position expressed in global coordinates, and $V \subseteq \mathbb{P}$ is a set of points expressed w.r.t. a local coordinate system whose origin is $\mathbf{p}$, $\mathsf{global}(V, \mathbf{p}) = V + \mathbf{p} = \{\mathbf{x} + \mathbf{p} \,|\, \mathbf{x} \in V\}$ denotes the set $V$ w.r.t. the global coordinates.

**Definition 1 (Basic Shapes)** *A basic shape $\sigma$ is a tuple $\langle V, m, \mathbf{p}, \mathbf{v}\rangle$ where $V \subseteq \mathbb{P}$ is a* convex polyhedron *(e.g. a* sphere*, a* cone*, a* cylinder*, etc.)*[2] *that represents the set of shape points; $m \in \mathbb{R}^+$, $\mathbf{p} \in \mathbb{P}$ and $\mathbf{v} \in \mathbb{V}$ are, resp., the mass, the centre of mass*[3] *and the velocity of $\sigma$. All possible basic shapes are ranged over by $\sigma, \sigma', \cdots$. We also define the* boundary *$\mathcal{B}(\sigma)$ of $\sigma$ to be the subset of points of $V$ that are on the surface of $\sigma$*[4]*.*

Three dimensional shapes of any form can be approximated - with arbitrary precision - by "gluing" basic shapes on a common surface. This concept is generalized by the following definition.

**Definition 2 (3D shapes)** *The set $\mathbb{S}$ of the* 3D shapes*, ranged over by $S, S', \cdots$, is generated by the grammar: $S ::= \sigma \mid S \langle X \rangle S$ where $\sigma$ is a basic shape and $X \subseteq \mathbb{P}$. If $S = \sigma = \langle V, m, \mathbf{p}, \mathbf{v}\rangle$, we define $\mathcal{P}(S) = V$, $m(S) = m$, $\mathcal{R}(S) = \mathbf{p}$, $\mathbf{v}(S) = \{\mathbf{v}\}$ to be, resp., the* set of points*, the* mass*, the* reference point *and the* velocity *of $S$. If $S = S_1 \langle X \rangle S_2$ is a compound shape, then: $\mathcal{P}(S) = \mathcal{P}(S_1) \cup \mathcal{P}(S_2)$, $m(S) = m(S_1) + m(S_2)$, $\mathcal{R}(S) = \big(m(S_1) \cdot \mathcal{R}(S_1) + m(S_2) \cdot \mathcal{R}(S_2)\big) / \big(m(S_1) + m(S_2)\big)$*[5] *and $\mathbf{v}(S) = \mathbf{v}(S_1) \cup \mathbf{v}(S_2)$. Finally, the boundary of $S$ is defined to be the set $\mathcal{B}(S) = \big(\mathcal{B}(S_1) \cup \mathcal{B}(S_2)\big) \setminus \{\mathbf{x} \in \mathbb{P} \mid \mathbf{x}$ is interior of $\mathcal{P}(S_1 \langle X \rangle S_2)\}$, where a point $\mathbf{x} \in V \subseteq \mathbb{P}$ is said to be* interior *if there exists an open ball with centre $\mathbf{x}$ which is completely contained in $V$.*

[2] 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.

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

[4] Note that we consider only closed shapes, i.e. they contain their boundary.

[5] Again for simplicity, we use the centre of mass as the reference point. Any other point can also be chosen.

In the following, we only consider shapes that are *well-formed* according to the following definition.

**Definition 3 (Well-formed shapes)** *Each basic shape $\sigma$ is well-formed. A compound shape $S_1 \langle X \rangle S_2$ is well-formed iff:*

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 equal to $\mathcal{B}(S_1) \cap \mathcal{B}(S_2)$;*
3. *$\mathbf{v}(S_1 \langle X \rangle S_2)$ is a singleton $\{\mathbf{v}\}$[6] where $\mathbf{v} = \mathbf{v}(S_1) = \mathbf{v}(S_2)$.*

*We say that two shapes $S_1$ and $S_2$* interpenetrate *each other if there exists a point $\mathbf{x}$ that is interior of both $\mathcal{P}(S_1)$ and $\mathcal{P}(S_2)$. In other terms, they* interpenetrate *iff the set $X = \mathcal{P}(S_1) \cap \mathcal{P}(S_2) \neq \emptyset$ is not a subset of $\mathcal{B}(S_1) \cap \mathcal{B}(S_2)$. If $S = S_1 \langle X \rangle S_2$ is well-formed, $X$ is said to be the* surface of contact *between $S_1$ and $S_2$; moreover, each $\mathbf{x} \in X$ is a* point of contact.

Condition (2) guarantees that well-formed compound shapes touch but do not interpenetrate; the surface of contact $X$ (a single point, a segment or a surface) is always on the boundary of both $S_1$ and $S_2$. 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. Condition (3) imposes that all the shapes forming a compound shape have the same velocity; thus, the compound shape moves as a unique body. Since a compound 3D shape $S$ can be represented in a number of different ways by rearranging its basic shapes and surfaces of contact, a structural congruence is defined to 'equate' all these possible representations.

**Definition 4 (Structural Congruence of 3D Shapes)** *The structural congruence relation over $\mathbb{S}$, denoted by $\equiv_S$, is the smallest relation that satisfies the following rules:*

- $S_1 \langle X \rangle S_2 \equiv_S S_2 \langle X \rangle S_1$;
- $(S_1 \langle X \rangle S_2) \langle Y \rangle S_3 \equiv_S S_1 \langle X \rangle (S_2 \langle Y \rangle S_3)$, *where* $Y \subseteq \mathcal{B}(S_2) \cap \mathcal{B}(S_3)$.

[6] With abuse of notation, throughout the paper, we write $\mathbf{v}(S)$ also to refer to the element $\mathbf{v}$ of the singleton $\{\mathbf{v}\}$ as this is not ambiguous when $S$ is well-formed.

## 2.1 Trajectories of Shapes

The general idea of the Shape Calculus is to consider a three-dimensional space in which several shapes reside, move and interact. Variations of shape velocities over time are treated by approximating 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 and vertices of the chain corresponds to velocity updates [3].

In detail, a global parameter $\Delta \in \mathbb{R}^+$, called *movement time step*, represents the maximum period of time after which the velocities of all shapes are updated. The quantification of $\Delta$ depends on the desired degree of approximation and also on other parameters connected to collision detection. In some situations, the time of updating can be shorter than $\Delta$ because, before that time, collisions between moving shapes can occur. These collisions must be resolved and the whole system must re-adapt itself to the new situation. The time domain $\mathbb{T} = \mathbb{R}_0^+$ is then divided into an infinite sequence of time steps $t_i$ such that $t_0 = 0$ and $t_i \leq t_{i-1} + \Delta$ for all $i > 0$. The updating of velocities is performed by exploiting a function $\mathsf{steer}\colon \mathbb{T} \to (\mathbb{S} \hookrightarrow \mathbb{V})$ that describes how the velocity of all existing shapes (i.e. all shapes that are currently moving in the space) at each time $t$ is changed. We assume that, at any given time instant $t \in \mathbb{T}$, $\mathsf{steer}\ t\ S$ is undefined iff shape $S$ does not exist and, hence, its velocity has not to be changed.

**Definition 5 (Evolution of shapes over time)** *Let $S \in \mathbb{S}$ and $t \in \mathbb{T}$; $S + t$, i.e. the shape $S$ after $t$ time units, is defined by induction on $S$:*
*Basic:* $\langle V, m, \mathbf{p}, \mathbf{v}\rangle + t = \langle V + (t \cdot \mathbf{v}), m, \mathbf{p} + (t \cdot \mathbf{v}), \mathbf{v}\rangle$
*Comp:* $(S_1 \langle X \rangle S_2) + t = (S_1 + t) \langle X + t \cdot \mathbf{v}(S)\rangle (S_2 + t)$

**Definition 6 (Updating shape velocity)** *Let $S \in \mathbb{S}$ and $\mathbf{w} \in \mathbb{V}$. We define the shape $S[\![\mathbf{w}]\!]$, i.e. $S$ whose velocity is updated with $\mathbf{w}$, as follows:*
*Basic:* $\langle V, m, \mathbf{p}, \mathbf{v}\rangle[\![\mathbf{w}]\!] = \langle V, m, \mathbf{p}, \mathbf{w}\rangle$
*Comp:* $(S_1 \langle X \rangle S_2)[\![\mathbf{w}]\!] = (S_1[\![\mathbf{w}]\!]) \langle X \rangle (S_2[\![\mathbf{w}]\!])$

The following result comes directly from Def. 3.

**Proposition 1** *Let $S \in \mathbb{S}$, $t \in \mathbb{T}$ and $\mathbf{w} \in \mathbb{V}$. If $S$ is well-formed then $S + t$ and $S[\![\mathbf{w}]\!]$ are well-formed.*

## 2.2 Collisions: Detection and Response

The intent to represent a lot of shapes moving simultaneously in space produces inevitably a scenario where collisions among shapes are possible. There is a rich literature on collision detection systems. For our purposes, it is sufficient to define an interface between our calculus and a typical collision detection system pivoting on the notions described in the following.

**Definition 7 (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 (see Def. 3). 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. *$\forall t' \in \mathbb{T}.\ 0 \leq t' \leq t$ and $\forall i, j \in I.\ S_i{+}t'$ and $S_j{+}t'$ do not interpenetrate;*
2. *$\exists i, j \in I.\ i \neq j$, such that $\mathcal{B}(S_i + t) \cap \mathcal{B}(S_j + t) \neq \emptyset$, i.e., some shapes are touching at $t$;*
3. *$\forall \epsilon > 0\ \exists \delta.\ 0 < \delta < \epsilon$ and $\exists i, j \in I.\ i \neq j$, 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.*

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 will be useful in Section 4 when we split previously compound shapes. Indeed, after the split these shapes have the same velocity and, hence, do not affect the next first time of contact.

**Definition 8 (Collision information)** *Let $\{S_i\}_{i\in I}$ be a set of well-formed shapes and let $t = \mathsf{Ftoc}(\{S_i\}_{i\in I})$ be their first time of contact. The* set of colliding shapes *after time $t$ is denoted by $\mathsf{colliding}(\{S_i\}_{i\in I}) \subseteq \mathbb{S} \times \mathbb{S} \times \wp(\mathbb{P})$. A tuple $\langle S_i, S_j, X\rangle \in \mathsf{colliding}(\{S_i\}_{i\in I})$ iff:*

1. *$\mathcal{P}(S_i{+}t) \cap \mathcal{P}(S_j{+}t)$ is* non-empty *and is equal to $\mathcal{B}(S_i{+}t) \cap \mathcal{B}(S_j{+}t)$;*
2. *$\forall \epsilon > 0\ \exists \delta.\ 0 < \delta < \epsilon$, such that $S_i{+}(t{+}\delta)$ and $S_j{+}(t{+}\delta)$ interpenetrate.*

The problem of *collisions response* [4], i.e. how collisions, once detected, are resolved, is treated by distinguishing between *elastic* collisions (those in which there is no loss in kinetic energy) and *perfectly inelastic* ones (in

which kinetic energy is fully dissipated)[7]. After an elastic collision, the two shapes will proceed independently to each other but their velocities will be changed according to the laws for conservation of linear momentum and kinetic energy - Equations (1)-(2) in Def. 9. On the contrary, two shapes that collide inelastically will bind together and will move as a *unique* body whose velocity is given by the law for conservation of linear momentum only - Equation (3), in Def. 9.

**Definition 9 (Collision Response)** *Let $S_1, S_2 \in \mathbb{S}$ and let $X \subseteq \mathbb{P}$ be a surface of contact. If $X$ is neither an edge nor a vertex of $S_1$, the velocities $\mathbf{w}_1$ and $\mathbf{w}_2$ of these shapes after an elastic collision in $X$ are given by:*

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

*where $\mathbf{n}$ is the normal of contact away from $X \subseteq \mathcal{B}(S_1)$, i.e. the unit vector perpendicular to the face of $S_1$ that contains $X$, and*

$$\lambda = 2\,\frac{m(S_1)\,m(S_2)}{m(S_1)+m(S_2)}\,\frac{\mathbf{v}(S_1)\cdot\mathbf{n} - \mathbf{v}(S_2)\cdot\mathbf{n}}{\mathbf{n}\cdot\mathbf{n}}$$

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

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

## 3 3D Processes

Now we introduce the timed process algebra whose terms describe the *internal behaviour* of our 3D shapes. We briefly recall the definitions of *shape behaviours*, as well as the associated temporal and functional semantics.

**Definition 10 (Shape behaviours)** *The set of* shape behaviours, *denoted by $\mathbb{B}$, is generated by the grammar:*

[7] Other different kinds of collisions can be easily added to the calculus provided that the corresponding collision response laws are given.

$$\textsc{Nil}_t\frac{}{\mathsf{nil} \overset{t}{\rightsquigarrow} \mathsf{nil}} \quad \textsc{Pref}_t\frac{\mu \in \mathcal{C} \cup \omega(\mathcal{C})}{\mu.B \overset{t}{\rightsquigarrow} \mu.B} \quad \textsc{Str}_t\frac{}{\rho(L).B \overset{t}{\rightsquigarrow} \rho(L).B}$$

$$\textsc{Sum}_t\frac{B_1 \overset{t}{\rightsquigarrow} B_1' \quad B_2 \overset{t}{\rightsquigarrow} B_2'}{B_1 + B_2 \overset{t}{\rightsquigarrow} B_1' + B_2'} \quad \textsc{Del}_t\frac{t' \geq t}{\epsilon(t').B \overset{t}{\rightsquigarrow} \epsilon(t'-t).B} \quad \textsc{Def}_t\frac{B \overset{t}{\rightsquigarrow} B' \;\; K \overset{\text{def}}{=} B}{K \overset{t}{\rightsquigarrow} B'}$$

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

$$\textsc{Pref}_a\frac{\mu \in \mathcal{C} \cup \omega(\mathcal{C})}{\mu.B \xrightarrow{\mu} B} \quad \textsc{Del}_a\frac{B \xrightarrow{\mu} B'}{\epsilon(0).B \xrightarrow{\mu} B'} \quad \textsc{Sum}_a\frac{B_1 \xrightarrow{\mu} B'}{B_1 + B_2 \xrightarrow{\mu} B'}$$

$$\textsc{Def}_a\frac{B \xrightarrow{\mu} B' \;\; K \overset{\text{def}}{=} B}{K \xrightarrow{\mu} B'} \qquad \textsc{Str}_1\frac{L = \{\langle \alpha, X\rangle\}}{\rho(L).B \xrightarrow{\rho(\alpha,X)} B}$$

$$\textsc{Str}_2\frac{L = \{\langle \alpha, X\rangle\} \cup L' \;\; L' \neq \emptyset}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L').B} \quad \textsc{Str}_3\frac{B \xrightarrow{\rho(\alpha,X)} B'}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L).B'}$$

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

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

**Definition 11 (Operational semantics of shape behaviours)** *The SOS-rules that define the* temporal transition *relations* $\overset{t}{\rightsquigarrow} \subseteq (\mathbb{B} \times \mathbb{B})$ *for* $t \in \mathbb{T}$*, that describe how shape behaviours evolve by letting time* $t$ *pass, are provided in Table 1. We write* $B \overset{t}{\rightsquigarrow} B'$ *if* $(B, B') \in \overset{t}{\rightsquigarrow}$ *and* $B \overset{t}{\rightsquigarrow}$ *if there is* $B' \in \mathbb{B}$ *such that* $(B, B') \in \overset{t}{\rightsquigarrow}$[8]*. Rules in Table 2 define the* action transition *relations* $\xrightarrow{\mu} \subseteq (\mathbb{B} \times \mathbb{B})$ *for* $\mu \in \mathsf{Act}$*, describing which basic actions a shape behaviour can perform.*

Now we are ready to define 3D processes, i.e. simple or compound shapes whose behaviour is expressed by a process in $\mathbb{B}$.

[8]Similar conventions will apply later on.

**Definition 12 (3D processes)** *The set* 3DP *of* 3D processes *is generated by the following grammar:* $P ::= S[B] \mid P \langle a, X \rangle P$ *where* $S \in \mathbb{S}$, $B \in \mathbb{B}$, $a \in \Lambda$ *and* $X$ *is a non-empty subset of* $\mathbb{P}$. *The shape of each* $P \in \mathsf{3DP}$ *is defined by induction on* $P$ *as follows:*

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

*We also define* $\mathbf{v}(P) = \mathbf{v}(\mathsf{shape}(P))$ *and* $\mathcal{B}(P) = \mathcal{B}(\mathsf{shape}(P))$. *Below we often write* $P \overset{X}{\longleftrightarrow}_i Q$ *and* $P \overset{X}{\longleftrightarrow}_e Q$ *as shorthand for* $\mathsf{shape}(P) \overset{X}{\longleftrightarrow}_i \mathsf{shape}(Q)$ *and* $\mathsf{shape}(P) \overset{X}{\longleftrightarrow}_e \mathsf{shape}(Q)$, *resp. Finally,* $P[\![\mathbf{v}]\!]$ *is the 3D process we obtain by updating* $P$*'s velocity as follows:*

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

*We finally write* $\mathsf{steer}\ t\ P$ *to denote* $P[\![\mathsf{steer}\ t\ \mathsf{shape}(P)]\!]$. *We say that a basic process* $S[B]$ *is* well-formed *iff the shape* $S$ *is well-formed and, for each* $X \subseteq \mathbb{P}$ *that occurs in* $B$, $\mathsf{global}(X, \mathcal{R}(S)) \subseteq \mathcal{B}(S)$. *A compound process* $P \langle a, X \rangle Q$ *is well-formed iff* $P$ *and* $Q$ *are well-formed,* $\mathbf{v}(P) = \mathbf{v}(Q)$ *and the site* $X$ *expressed w.r.t. a global coordinate system is a non-empty subset of* $\mathcal{B}(P) \cap \mathcal{B}(Q)$. *This also means that* $\mathcal{P}(P) \cap \mathcal{P}(Q)$ *is non-empty and equal to* $\mathcal{B}(P) \cap \mathcal{B}(Q)$.

Later on we only consider well-formed processes. The following proposition is an easy consequence of well-formedness of shapes and 3D processes.

**Proposition 2** *For each* $P \in \mathsf{3DP}$ *well-formed,* $\mathsf{shape}(P)$ *is well-formed.*

Let us recall a running example, taken from [2], based on the well-known biochemical pathway of glycolysis. We consider only one reaction, catalyzed by the Hexokinase enzyme (HEX). GLC, G6P, ATP and ADP are metabolites. The transformation of a metabolite (GLC) into another (G6P) depends on the meeting (collision in binding sites) of the right enzyme (HEX) with the right metabolites (GLC and ATP). After this binding the reaction takes place and the products (G6P and ADP) are released. 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. We denote by $S_h$, $S_g$ and $S_a$ the shape of HEX, GLC (and G6P) and ATP (and ADP), respectively.

**Example 1 (3D Processes for $HEX$, $GLC$ and $ATP$)** *An Hexokinase molecule can be modelled as* $HEX = S_h[\mathsf{HEX}]$ *where* $\mathsf{HEX} = \langle \mathsf{atp}, X_{ha}\rangle.\mathsf{HA} + \langle \mathsf{glc}, X_{hg}\rangle.\mathsf{HG}$, $\mathsf{HA} = \omega(\mathsf{atp}, X_{ha}).\mathsf{HEX} + \epsilon(t_h).\langle \mathsf{glc}, X_{hg}\rangle.$ $\rho(\{\langle \mathsf{atp}, X_{ha}\rangle, \langle \mathsf{glc}, Y_{hg}\rangle\}).\mathsf{HEX}$, $\mathsf{HG} = \omega(\mathsf{glc}, X_{hg}).\mathsf{HEX} + \epsilon(t_h).\langle \mathsf{atp}, X_{ha}\rangle.$ $\rho(\{\langle \mathsf{atp}, X_{ha}\rangle, \langle \mathsf{glc}, Y_{hg}\rangle\}).\mathsf{HEX}$, *and* $X_{ha}, Y_{hg}$ *are proper surfaces of contact.*

$ATP = S_a[\mathsf{ATP}]$ *models an ATP molecule where* $\mathsf{ATP} = \langle \overline{\mathsf{atp}}, X_{ah}\rangle.$ $(\epsilon(t_a).\rho(\{\langle \overline{\mathsf{atp}}, X_{ah}\rangle\}).\mathsf{ADP} + \omega(\overline{\mathsf{atp}}, X_{ah}).\mathsf{ATP})$ *and the surface of contact* $X_{ah}$ *is the whole boundary* $\mathcal{B}(S_a)$*. The process modelling a molecule of glucose is similar:* $GLC = S_g[\mathsf{GLC}]$ *where* $\mathsf{GLC} = \langle \overline{\mathsf{glc}}, X_{gh}\rangle.(\epsilon(t_g).$ $\rho(\{\langle \overline{\mathsf{glc}}, X_{gh}\rangle\}).\mathsf{G6P} + \omega(\overline{\mathsf{glc}}, X_{gh}).\mathsf{GLC}$*. We leave unspecified the behaviours* G6P *and* ADP.

HEX *has two binding capabilities along the channels* $\langle \mathsf{atp}, X_{ha}\rangle$ *and* $\langle \mathsf{glc}, Y_{hg}\rangle$ *to bind, resp., with an ATP and a GLC molecule. By performing an action* $\langle \mathsf{atp}, X_{ha}\rangle$*,* HEX *evolves in* HA*.* HA *can perform either a weak-split action* $\omega(\mathsf{atp}, X_{ha})$ *to come back to* HEX*, or can wait at most* $t_h$ *units of time, perform* $\langle \mathsf{glc}, Y_{hg}\rangle$ *and then evolve in* $\rho(\{\langle \mathsf{atp}, X_{ha}\rangle, \langle \mathsf{glc}, Y_{hg}\rangle\}).\mathsf{HEX}$*. Now, two strong-split actions are enabled after which we come back to* HEX*. Note that, after an action* $\langle \mathsf{glc}, Y_{hg}\rangle$*,* HEX *becomes* HG *that behaves symmetrically. An ATP molecule performs a* $\langle \overline{\mathsf{atp}}, X_{ah}\rangle$*-action, waits* $t_r$ *units of time, and then can release the bond established on the channel* $\langle \overline{\mathsf{atp}}, X_{ah}\rangle$ *– and thus return free as ATP – or can participate in the reaction and become an ADP. As we will see in Section 4, the result is the split of the complex in the three original shapes whose behaviours are* HEX*,* ADP *and* G6P*, resp. We omit the description of the behaviour of* GLC *since it is similar to that of* ATP*.*

The timed operational semantics of 3D processes is defined below.

**Definition 13 (Transitional semantics of 3D processes)** *Rules in Table 3 define the transition relations* $\overset{t}{\rightsquigarrow} \subseteq (\mathsf{3DP} \times \mathsf{3DP})$ *for* $t \in \mathbb{T}$*, and* $\xrightarrow{\mu} \subseteq \mathsf{3DP} \times \mathsf{3DP}$ *for* $\mu \in \mathsf{Act}$*. Two 3D processes* $P$ *and* $Q$ *are said to be* compatible*, written* $P \sim Q$*, if* $P \xrightarrow{\langle \alpha, X\rangle}$ *and* $Q \xrightarrow{\langle \overline{\alpha}, Y\rangle}$ *for some compatible channels* $\langle \alpha, X\rangle$ *and* $\langle \overline{\alpha}, Y\rangle$*; otherwise,* $P$ *and* $Q$ *are* incompatible*, written* $P \not\sim Q$*. We often write* $P \overset{\rho}{\not\rightarrow}$ *and* $P \overset{\omega}{\not\rightarrow}$ *as shorthand for* $P \xrightarrow{\rho(\alpha, X)}$ *and* $P \xrightarrow{\omega(\alpha, X)}$*, resp., for any* $\langle \alpha, X\rangle$*.*

The following proposition shows that 3D processes well-formedness is closed w.r.t. transitions $\overset{t}{\rightsquigarrow}$ and $\xrightarrow{\mu}$.

$$\textsc{Basic}_t \frac{B \overset{t}{\rightsquigarrow} B'}{S[B] \overset{t}{\rightsquigarrow} (S+t)[B']} \qquad \textsc{Comp}_t \frac{P \overset{t}{\rightsquigarrow} P' \;\; Q \overset{t}{\rightsquigarrow} Q' \wedge X' = X + (t \cdot \mathbf{v}(P))}{P \langle a, X \rangle Q \overset{t}{\rightsquigarrow} P' \langle a, X' \rangle Q'}$$

$$\textsc{Basic}_c \frac{B \xrightarrow{\langle \alpha, X \rangle} B' \;\; Y = \mathsf{global}(X, \mathcal{R}(S))}{S[B] \xrightarrow{\langle \alpha, Y \rangle} S[B']} \qquad \textsc{Comp}_s \frac{P \xrightarrow{\rho(\alpha, Y)} P'}{P \langle a, X \rangle Q \xrightarrow{\rho(\alpha, Y)} P' \langle a, X \rangle Q}$$

$$\textsc{Basic}_s \frac{B \xrightarrow{\rho(\alpha, X)} B' \;\; Y = \mathsf{global}(X, \mathcal{R}(S))}{S[B] \xrightarrow{\rho(\alpha, Y)} S[B']}$$

$$\textsc{Comp}_w \frac{P \xrightarrow{\omega(\alpha, Y)} P'}{P \langle a, X \rangle Q \xrightarrow{\omega(\alpha, Y)} P' \langle a, X \rangle Q} \qquad \textsc{Comp}_c \frac{P \xrightarrow{\langle \alpha, Y \rangle} P' \;\; Y \subseteq \mathcal{B}(P \langle a, X \rangle Q)}{P \langle a, X \rangle Q \xrightarrow{\langle \alpha, Y \rangle} P' \langle a, X \rangle Q}$$

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

**Proposition 3** *Let $P \in$ 3DP well-formed. Either $P \overset{t}{\rightsquigarrow} Q$ or $P \xrightarrow{\mu} Q$ implies $Q \in$ 3DP well-formed.*

Notice that the operational rules in Table 3 do not allow synchronization between components of compound process that proceed independently to each other. Consider, as an example, $P = S_p[\rho(\{a, X_p\}).B_p]$, $Q = S_q[\rho(\{\overline{a}, X_q\}).B_q]$, and $P \langle a, X \rangle Q$ where $X = X'_p \cap X'_q$ and, for each $i \in \{p, q\}$, $X'_i = \mathsf{global}(X_i, \mathcal{R}(S_i))$, i.e. $X'_i$ is the site $X_i$ w.r.t. the global coordinate system. As stand-alone processes, $P$ and $Q$ can perform two compatible strong-split actions, namely $\rho(a, X'_p)$ and $\rho(\overline{a}, X'_q)$ and evolve, resp., in $S_p[B_p]$ and $S_q[B_q]$. As a consequence, $P \langle a, X \rangle Q$ becomes either $S_p[B_p] \langle a, X \rangle Q$ or $P \langle a, X \rangle S_p[B_q]$.

Being these actions compatible, $P$ and $Q$ have to synchronize on their execution in order to split the bond $\langle a, X \rangle$ (i.e., a strong-split operation is enabled). Such an operation must be performed before time can pass further and must produce as a result two independent 3D processes, i.e. the *network* of 3D processes (see Section 4) that contains both $S_p[B_p]$ and $S_q[B_q]$. Similarly, we would allow synchronizations between compatible weak-split action in order to perform a weak-split operation. To properly deal with this kind of behaviours some technical details are still needed.

We first allow synchronization on compatible split actions by introducing the transition relations $\stackrel{\rho(a,X)}{\Rightarrow}$ and $\stackrel{\omega(a,X)}{\Rightarrow}$. Intuitively, we want that $P\,\langle a,X\rangle\,Q \stackrel{\rho(a,X)}{\Rightarrow} S_p[B_p]\,\langle a,X\rangle\,S_q[B_q]$. Now, we can 'physically' remove the bond $\langle a,X\rangle$ (this will be done by exploiting the function split over 3D processes we provide in the next section) and obtain the network of processes we are interested in.

**Definition 14 (Semantics of strong and weak splits)** *The SOS-rules that define the transition relations* $\stackrel{\rho(a,X)}{\Rightarrow} \subseteq \mathsf{3DP} \times \mathsf{3DP}$ *where* $\rho(\alpha,X) \in \rho(\mathcal{C})$ *are given in Table 4. We omit symmetric rules and those ones defining the transition relations* $\stackrel{\omega(a,X)}{\Rightarrow} \subseteq \mathsf{3DP} \times \mathsf{3DP}$ *for* $\omega(a,X) \in \omega(\mathcal{C})$*, since these can be obtained from those in Table 4 by replacing each action* $\rho(\text{-})$ *with the corresponding action* $\omega(\text{-})$*.*

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

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

Table 4: Transitional semantics for strong-split actions

Recall that strong-split operations require simultaneous split of multiple bonds. In this case, all the components involved in the reaction must *all together* be ready to synchronize on a proper set of compatible strong-split actions. This concept is formalized by the definition below.

**Definition 15 (Bonds of 3DP-terms)** *The function* $\mathsf{bonds} : \mathsf{3DP} \to \wp(\mathcal{C})$ *returns the set of bonds that are currently established in* $P$*. It is defined by induction on* $P \in \mathsf{3DP}$*:*
*Basic:* $\mathsf{bonds}(S[B]) = \emptyset$
*Comp:* $\mathsf{bonds}(P\,\langle a,X\rangle\,Q) = \mathsf{bonds}(P) \cup \mathsf{bonds}(Q) \cup \{\langle a,X\rangle\}$

*By induction on* $P$ *we can prove that* $P \stackrel{\rho(a,X)}{\Rightarrow}$ *implies* $\langle a,X\rangle \in \mathsf{bonds}(P)$*. Moreover, we say that* $P \in \mathsf{3DP}$ *is* able to complete a reaction*, written* $P \searrow$*, iff either (1)* $P \stackrel{\beta}{\not\to}$*, or (2)* $P \stackrel{\rho(a,X)}{\Rightarrow} Q$ *for some* $\rho(a,X)$ *and* $Q$ *such that* $Q \searrow$*.*

Finally, if $P$ is able to complete a reaction and there is at a least a bond that has to be strongly split (i.e. if $P \stackrel{\rho}{\not\rightarrow}$ does not hold), a reaction can actually take place and, as a consequence, time cannot pass further. Below we restrict the timed operational semantics of 3D processes as it has been defined in Def. 13 in order to take this aspect into account.

**Definition 16** *Let $P \in \mathsf{3DP}$. We say that $P \stackrel{t}{\rightarrow} Q$ if $P \stackrel{t}{\rightsquigarrow} Q$ and either $P \stackrel{\rho}{\not\rightarrow}$ or $P$ is* not *able to complete a reaction.*

Proposition 4 states that the function $\mathsf{split}$ is well-defined up to structural congruence over 3D processes we define below.

**Definition 17 (Structural congruence over 3D processes)** *We define the structural congruence over processes in $\mathsf{3DP}$, which we denote by $\equiv_P$, as 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* $P \langle a, X \rangle R \equiv_P Q \langle a, X \rangle R$;
- $Y \subseteq \mathcal{B}(Q) \cap \mathcal{B}(R)$ *implies* $(P \langle a, X \rangle Q) \langle b, Y \rangle R \equiv_P P \langle a, X \rangle (Q \langle b, Y \rangle R)$.

**Proposition 4** *Let $P \in \mathsf{3DP}$ well-formed. If $\langle a, X \rangle \in \mathsf{bonds}(P)$ there is a well-formed 3D process $Q \langle a, X \rangle R \equiv_P P$.*

We also need the following closure result.

**Proposition 5** *Let $P, Q \in \mathsf{3DP}$ 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. $P$ well-formed and $P \stackrel{\mu}{\Rightarrow} Q$ implies $Q$ well-formed.*

# 4 Networks or 3D processes

In the following, we recall the definition of a 3D network, i.e. a collection of 3D processes moving in the same 3D space.

**Definition 18 (Networks of 3D processes)** *The set $\mathbb{N}$ of* networks of 3D processes *(3D networks, for short) is generated by the grammar:*
$N ::= \mathsf{Nil} \mid P \mid N \parallel N$ *where $P \in \mathsf{3DP}$. Given a finite set of indexes $I$, we often write $(\parallel P_i)_{i \in I}$ to denote the network that consists of all $P_i$ with*

$i \in I$. *We assume that* $I = \emptyset$ *implies* $(\|\, P_i)_{i\in I} = \mathsf{Nil}$. *For* $N = (\|\, P_i)_{i\in I}$ *we let* $S_i = \mathsf{shape}(P_i)$, *for* $i \in I$, *and define* $\mathsf{colliding}(N)$ *as the set of all tuples* $\langle P_i, P_j, X\rangle$ *such that* $\langle S_i, S_j, X\rangle \in \mathsf{colliding}(\{S_i\}_{i\in I})$ *(see Def. 8). A network* $N = (\|\, P_i)_{i\in I}$ *is said to be well-formed iff each* $P_i$ *is well-formed and, for each pair of distinct processes* $P_i$ *and* $P_j$, *the shapes* $S_i$ *and* $S_j$ do not interpenetrate. *Moreover,* $\mathsf{steer}\ t\ (\|\, P_i)_{i\in I} = (\|\, \mathsf{steer}\ t\ P_i)_{i\in I}$.

**Definition 19 (Splitting bonds)** *The function* $\mathsf{split} : \mathsf{3DP} \times \wp(\mathcal{C}) \to \mathbb{N}$ *is defined as follows: If* $\langle a, X\rangle \in \mathsf{bonds}(P) \cap C$ *and* $P \equiv_P Q\,\langle a, X\rangle\, R$ *then* $\mathsf{split}(P, C) = \mathsf{split}(Q, C) \,\|\, \mathsf{split}(R, C)$; *if, otherwise,* $\mathsf{bonds}(P) \cap C = \emptyset$, *then* $\mathsf{split}(P, C) = P$.

It is worth noting that split shapes 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 6** *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.*

**Definition 20 (Semantics of weak- and strong-split operation)** *Let* $P \in \mathsf{3DP}$ *a 3D process. If* $P \searrow$, *we write that* $P \xrightarrow{\rho} N \in \mathbb{N}$ *iff there is a non empty set* $C = \{\langle a_1, X_1\rangle, \cdots, \langle a_n, X_n\rangle\} \subseteq \mathsf{bonds}(P)$ *such that* $P = P_0 \overset{\rho(a_1,X_1)}{\Rightarrow} P_1 \cdots \overset{\rho(a_n,X_n)}{\Rightarrow} P_n$, $P_n \overset{\rho}{\not\to}$ *and* $N = \mathsf{split}(P_n, C)$. *Similarly,* $P \xrightarrow{\omega} N$ *iff* $\exists\langle a, X\rangle \in \mathsf{bonds}(P)$ *such that* $P \overset{\omega(a,X)}{\Rightarrow} Q$ *and* $N = \mathsf{split}(Q, \{\langle a, X\rangle\})$.

Since weak-split operations are due to a synchronization between just a pair of 3D processes, condition '$P$ is able to complete a reaction' is not needed, but '$P \overset{\omega(a,X)}{\Rightarrow} Q$' suffices to our aim.

**Example 2** *Let us consider the 3D process* $P = H\,\langle \mathsf{atp}, X\rangle\,(A\,\langle \mathsf{glc}, Y\rangle\ G)$ *where* $H = S_h[\,\rho(\{\langle \mathsf{atp}, X_{ha}\rangle, \langle \mathsf{glc}, Y_{hg}\rangle\}).\mathsf{HEX}\,]$, $A = S_a[\,\rho(\{\langle \overline{\mathsf{atp}}, X_{ah}\rangle\}).\mathsf{ADP} + \omega(\overline{\mathsf{atp}}, X_{ah}).\mathsf{ATP}\,]$,$G = S_g[\rho(\{\langle \overline{\mathsf{glc}}, Y_{gh}\rangle\}).\mathsf{G6P} + \omega(\overline{\mathsf{glc}}, Y_{gh}).\mathsf{GLC}]$, $X'_{ha} \cap X'_{ah} = X$ *(here* $X'_{ha}$ *and* $X'_{ah}$ *are the sites* $X_{ha}$ *and* $X_{ah}$ *expressed w.r.t. a global coordinate system; this convention will be applied later on) and* $Y'_{hg} \cap Y'_{gh} = Y$. *According to the definitions given so far,* $P$ *is* able to complete a reaction *since:*

$$\begin{array}{lll} P & \overset{\rho(\mathsf{atp},X)}{\Rightarrow} & S_h[\rho(\{\langle \mathsf{glc}, Y_{hg}\rangle\}).\mathsf{HEX}]\,\langle \mathsf{atp}, X\rangle\,(S_a[\mathsf{ADP}]\,\langle \mathsf{glc}, Y\rangle\ G) \\ & \overset{\rho(\mathsf{glc},Y)}{\Rightarrow} & S_h[\mathsf{HEX}]\,\langle \mathsf{atp}, X\rangle\,(S_a[\mathsf{ADP}]\,\langle \mathsf{glc}, Y\rangle\, S_g[\mathsf{G6P}]) = R \end{array}$$

*Moreover,* $R \stackrel{\rho}{\not\to}$ *and*

$$\begin{array}{rcl} \mathsf{split}(R, C) & = & S_a[\mathsf{HEX}] \parallel \mathsf{split}(S_a[\mathsf{ADP}]\,\langle \mathsf{glc}, Y\rangle\, S_g[\mathsf{G6P}], C) \\ & = & S_h[\mathsf{HEX}] \parallel (S_a[\mathsf{ADP}] \parallel S_g[\mathsf{G6P}]) = N, \end{array}$$

*where* $C = \{\langle \mathsf{atp}, X\rangle, \langle \mathsf{glc}, Y\rangle\}$*, implies* $P \stackrel{\rho}{\to} N$*. Moreover, let us note that, for each* $t \in \mathbb{T}$*,* $P \stackrel{t}{\rightsquigarrow} P$ *but* $P \stackrel{t}{\not\to}$ *since* $P$ *is able to complete a reaction and* $P \stackrel{\rho}{\not\to}$ *does not hold.*

Below we recall the temporal and functional behaviour of 3D networks. Symmetric rules have been omitted.

**Definition 21 (Temporal and Functional Behaviour of $\mathbb{N}$-terms)** *The following rules defines the transition relations* $\stackrel{t}{\to} \subseteq \mathbb{N} \times \mathbb{N}$ *for* $t \in \mathbb{T}$ *and* $\stackrel{\nu}{\to} \subseteq \mathbb{N} \times \mathbb{N}$ *for* $\nu \in \{\omega, \rho\}$*:*

$$\textsc{Empty}_t \frac{}{\mathsf{Nil} \stackrel{t}{\to} \mathsf{Nil}} \qquad \textsc{Par}_t \frac{N \stackrel{t}{\to} N' \quad M \stackrel{t}{\to} M'}{N \parallel M \stackrel{t}{\to} N' \parallel M'} \qquad \textsc{Par}_a \frac{N \stackrel{\nu}{\to} N'}{N \parallel M \stackrel{\nu}{\to} N' \parallel M}$$

*A* timed trace *from* $N$ *is a finite sequence of steps of the form* $N = N_0 \stackrel{\nu_1}{\longrightarrow} N_1 \cdots \stackrel{\nu_n}{\longrightarrow} N_n = M$*. We also write that* $N \stackrel{t}{\Rightarrow} M$ *if there is a timed trace* $N = N_0 \stackrel{\nu_1}{\longrightarrow} N_1 \cdots \stackrel{\nu_n}{\longrightarrow} N_n = M$ *such that* $t = \sum_{i=0}^{n} \{\nu_i \mid \nu_i \in \mathbb{T}\}$*.*

**Proposition 7** *Let* $t \in \mathbb{T}$*,* $P \in \mathsf{3DP}$*,* $N \in \mathbb{N}$*, with* $P$ *and* $N$ *well-formed.*

1. $P \stackrel{\omega}{\to} N$ *and* $P \stackrel{\rho}{\to} N$ *implies* $N \in \mathbb{N}$ *well-formed.*
2. $N \stackrel{t}{\to} M$ *implies* $M$ *well-formed;*
3. $N \stackrel{t}{\Rightarrow} M$ *implies* $M$ *well-formed.*

## 4.1 Collision response

In this section we describe the semantics of *collisions response*. The notion of compatibility between channels (and, hence, processes) has been introduced to distinguish between elastic and inelastic collision. In particular, collisions among compatible processes are always inelastic. So, if $P \stackrel{\langle a, X_p\rangle}{\longrightarrow} P'$ and $Q \stackrel{\langle \overline{a}, X_q\rangle}{\longrightarrow} Q'$, with $\langle a, X_p\rangle$ and $\langle \overline{a}, X_q\rangle$ compatible, and $P$ and $Q$ collide in the non-empty site $X = X_p \cap X_q$ we get a compound process $(P'\,\langle a, X\rangle\, Q')[\![\mathbf{v}]\!]$ where the velocity $\mathbf{v}$ is provided by Equation (3) in Def. 9. Vice versa, a collision between two incompatible processes $P$ and $Q$ is treated as an elastic

one. After such a collision, $P$ and $Q$ (actually the processes we obtain by updating their velocities according to Equations (1) and (2) in Def. 9) will proceed independently to each other. To resolve collisions, we introduce two different kinds of *reduction relations* over 3D networks, namely $\xrightarrow{\langle P,Q,X\rangle}_e$ and $\xrightarrow{\langle P,Q,X\rangle}_i$, where $P, Q$ are 3D processes and $X$ is a surface of contact (see Table 5). Intuitively, if $N \xrightarrow{\langle P,Q,X\rangle}_e M$ ($N \xrightarrow{\langle P,Q,X\rangle}_i M$), then $M$ is the 3D network we obtain once an elastic (inelastic, resp.) collision between $P$ and $Q$ in the surface of contact $X$ has been resolved. These reduction relations also use the structural congruence over 3D networks.

**Definition 22 (Structural congruence over 3D networks)** *The structural congruence over terms in $\mathbb{N}$, that we denote with $\equiv$, is the smallest relation that satisfies the following axioms:*

- $\mathsf{Nil} \parallel N \equiv N$, $N \parallel M \equiv M \parallel N$ *and* $N \parallel (M \parallel R) \equiv (N \parallel M) \parallel R$;
- $P \parallel N \equiv Q \parallel N$ *provided that* $P \equiv_P Q$.

Rule ELAS in Table 5 simply changes velocities of two colliding but incompatible processes guided by Equations (1) and (2) in Def. 9, while rule INEL joins two compatible processes $P$ and $Q$ to obtain a compound process whose velocity is given by Equation (3) in Def. 9. We force $P$ and $Q$ to synchronize on the execution of two compatible actions $\langle \alpha, X_p\rangle$ and $\langle \overline{\alpha}, X_q\rangle$ before joining them. In rules ELAS$_\equiv$ and INELAS$_\equiv$ we also consider structural congruence over nets of processes. In Def. 23 we collect together all the reduction-steps needed to solve collisions listed in a given set of collisions $\mathsf{colliding}(N)$; clearly $N$ is a generic 3D network.

**Definition 23 (Resolving collisions)** *Let $N \in \mathbb{N}$ and $\langle P, Q, X\rangle$ a tuple in $\mathsf{colliding}(N)$. $N \xrightarrow{\langle P,Q,X\rangle} M$ if either $P \sim Q$ and $N \xrightarrow{\langle P,Q,X\rangle}_i M$ or $P \not\sim Q$ and $N \xrightarrow{\langle P,Q,X\rangle}_e M$. Moreover, we write that $N \xrightarrow{\kappa} M$ if either $\mathsf{colliding}(N) = \emptyset$ and $N = M$ or $\mathsf{colliding}(N) \neq \emptyset$ and there is a finite sequence of reduction steps $N = N_0 \xrightarrow{\langle P_1,Q_1,X_1\rangle} N_1 \cdots \xrightarrow{\langle P_k,Q_k,X_k\rangle} N_k = M$ such that:*

1. $\langle P_i, Q_i, X_i\rangle \in \mathsf{colliding}(N_{i-1})$ *for each* $i \in [1, k]$;
2. $\mathsf{colliding}(N_k) = \emptyset$.

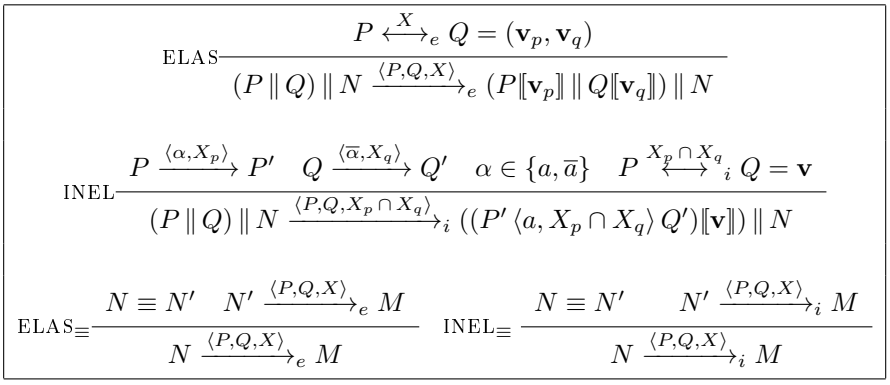

Table 5: Reaction rules for elastic and inelastic collisions

Let also note that, at any given time $t$, $\mathsf{colliding}(N)$ can be obtained from the set of all the pairs of processes in $N$ that are touching at that time. This set and hence $\mathsf{colliding}(N)$ 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 any more). 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 bound 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 Def. 9 in order to obtain two processes that do not collide any more. Thus, we can always decide if there is a finite sequence of reduction steps that allows us to resolve all collisions listed in $\mathsf{colliding}(N)$ and hence obtain a network $M$ with $\mathsf{colliding}(M) = \emptyset$.

**Proposition 8** *Let $N \in \mathbb{N}$, $P, Q \in \mathsf{3DP}$ and $X$ a non-empty subset of $\mathbb{P}$. Then $N$ well-formed and $N \xrightarrow{\langle P,Q,X\rangle} M$ implies $M$ well-formed.*

Iterating Proposition 8 it is also:

**Lemma 1** *Let $N \in \mathbb{N}$ well-formed and $N \xrightarrow{\kappa} M$. Then $M$ is well-formed.*

We are now ready to define how a network of 3D processes evolves by performing an infinite number of *movement time steps*.

**Definition 24 (System evolution)** *Let $N, M \in \mathbb{N}$ and $t, t' \in \mathbb{T}$. We say that $(N,t) \stackrel{t'}{\Rightarrow} (M, t+t')$ iff one of the following conditions holds:*

1. *$t' = \mathsf{Ftoc}(N) \leq \Delta$ and $N \stackrel{t'}{\Rightarrow} N' \stackrel{\kappa}{\rightarrow} N''$ and $M = \mathsf{steer}\ (t+t')\ N''$;*
2. *$t' = \Delta < \mathsf{Ftoc}(N)$ and $N \stackrel{t'}{\Rightarrow} N'$ and $M = \mathsf{steer}\ (t+t')\ N'$.*

*A* system evolution *is any infinite sequence of time steps of the form:*

$$(N_0, 0) \stackrel{t_1}{\Rightarrow} (N_1, t_1) \stackrel{t_2}{\Rightarrow} (N_2, t_1 + t_2) \cdots (N_{i-1}, \sum_{j=1}^{i-1} t_j) \stackrel{t_i}{\Rightarrow} (N_i, \sum_{j=1}^{i} t_j) \stackrel{t_{i+1}}{\Rightarrow} \cdots$$

Note that, for each $i \geq 1$, $t_i = \min\{\mathsf{Ftoc}(N_{i-1}), \Delta\}$. Moreover, in order to make sure that processes will never interpenetrate during a system evolution, if $\mathsf{Ftoc}(N_{i-1}) \leq \Delta$, we first resolve all the collisions that happen after time $t_i = \mathsf{Ftoc}(N_{i-1})$ (by means of transition $\stackrel{\kappa}{\rightarrow}$) and then apply the changes suggested by the function steer as described in Section 2.1.

**Example 3** *This example shows a possible evolution of the 3D network $N_0 = (HEX \parallel ATP) \parallel GLC$ where $HEX$, $ATP$ and $GLC$ are the 3D processes of Example 1. Below we use the following notation:*

- *$H(t) = (S_h + t)[\mathsf{HEX}]$, $A(t) = (S_a + t)[\mathsf{ATP}]$ and $G(t) = (S_g + t)[\mathsf{GLC}]$ for each $t \in \mathbb{T}$. Note that $HEX = H(0)$, $ATP = A(0)$ and $GLC = G(0)$;*
- *$\mathsf{C} = \rho(\{\langle \mathsf{atp}, X_{ha}\rangle, \langle \mathsf{glc}, X_{hg}\rangle\}).\mathsf{HEX}$ and, for any $t \leq t_h$, $\mathsf{HA}(t) = \omega(\mathsf{atp}, X_{ha}).\mathsf{HEX} + \epsilon(t_h - t).\langle \mathsf{glc}, X_{hg}\rangle.\mathsf{C}$;*
- *$\mathsf{AH}(t) = \omega(\overline{\mathsf{atp}}, X_{ah}).\mathsf{ATP} + \epsilon(t_a - t).\rho(\{\overline{\mathsf{atp}}, X_{ah}\}).\mathsf{ADP}$ for any $t \in \mathbb{T}$ with $t \leq t_a$;*
- *$\mathsf{GH}(t) = \omega(\overline{\mathsf{glc}}, X_{gh}).\mathsf{GLC} + \epsilon(t_g - t).\rho(\{\overline{\mathsf{glc}}, X_{gh}\}).\mathsf{G6P}$ for any $t \leq t_g$.*

*Let $t_1 = \mathsf{Ftoc}(N_0)$ and assume $t_1 \leq \Delta$. By the operational rules, it is $N_0 \stackrel{t_1}{\Rightarrow} H(t_1) \parallel A(t_1) \parallel G(t_1) = N_0'$. We also assume that $\mathsf{colliding}(N_0') = \{\langle H(t_1), A(t_1), X\rangle\}$ where $X = X_{ha}' \cap X_{ah}' \neq \emptyset$, $X_{ha}' = \mathsf{global}(X_{ha}, \mathcal{R}(S_h + t_1))$ and $X_{ah}' = \mathsf{global}(X_{ah}, \mathcal{R}(S_a + t_1))$. Then: $N_0' \stackrel{\kappa}{\rightarrow} P(t_1) \parallel G(t_1) = N_0''$ where $P(t_1) = \big((S_h + t_1)[\mathsf{HA}(0)]\langle \mathsf{atp}, X\rangle(S_a + t_1)[\mathsf{AH}(0)]\big)[\![\mathbf{v}_{ha}]\!]$ and $\mathbf{v}_{ha} = H(t_1) \stackrel{X}{\longleftrightarrow}_i A(t_1)$.*

***Finally:*** $(N_0,0) \stackrel{t_1}{\Rightarrow} (N_1,t_1)$ *where* $N_1 = \mathsf{steer}\, t_1\, N_0'' = \mathsf{steer}\, t_1\, P(t_1) \parallel \mathsf{steer}\, t_1\, G(t_1) = P(t_1)[\![\mathbf{v}_1]\!] \parallel G(t_1)[\![\mathbf{v}_2]\!]$. *Note that:*

$$\begin{array}{rcl} P(t_1)[\![\mathbf{v}_1]\!] & = & \big((S_h+t_1)[\mathsf{HA}(0)]\langle \mathsf{atp}, X\rangle (S_a+t_1)[\mathsf{AH}(0)]\big)[\![\mathbf{v}_1]\!] \\ & = & \big(S_h^1[\mathsf{HA}(0)]\langle \mathsf{atp}, X\rangle S_a^1[\mathsf{AH}(0)]\big) \end{array}$$

*where* $S_h^1 = ((S_h+t_1)[\![\mathbf{v}_1]\!])$ *and* $S_a^1 = ((S_a+t_1)[\![\mathbf{v}_1]\!])$. *Moreover,* $G(t_1)[\![\mathbf{v}_2]\!] = ((S_g+t_1)[\![\mathbf{v}_2]\!][\mathsf{GLC}] = S_g^1[\mathsf{GLC}]$.

*Let* $t_2 = \mathsf{Ftoc}(N_1)$ *and assume* $t_2 = t_h \leq \min\{t_a, \Delta\}$[9]. *Below we write* $G'(t_2)$ *and* $P'(t_2)$ *to denote, respectively, the 3D processes* $(S_g^1+t_2)[\mathsf{GLC}]$ *and* $\big((S_h^1+t_2)[\mathsf{HA}(t_h)]\langle \mathsf{atp}, X+t_2\cdot\mathbf{v}_1\rangle (S_a^1+t_2)[\mathsf{AH}(t_2)]\big)$. *Again by the operational rules,* $N_1 \stackrel{t_2}{\Rightarrow} P'(t_2) \parallel G'(t_2) = N_1'$.

*Let* $\mathsf{colliding}(N_1') = \{\langle P'(t_2), G'(t_2), Y\rangle\}$ *where* $Y = X'_{hg} \cap X'_{gh} \neq \emptyset$, $X'_{hg} = \mathsf{global}(X_{hg}, \mathcal{R}(S_h^1 + t_2))$ *and* $X'_{gh} = \mathsf{global}(X_{gh}, \mathcal{R}(S_g^1 + t_2)) \subseteq \mathcal{B}(P'(t_2))$. *If* $\mathbf{v}_{gh} = P'(t_2) \stackrel{Y}{\longleftrightarrow}_i G'(t_2)$, *then*
$N_1' \stackrel{\kappa}{\rightarrow} \big(P(t_2)\,\langle \mathsf{glc}, Y\rangle\, G(t_2)\big)[\![\mathbf{v}_{gh}]\!] = N_1''$ *where* $G(t_2) = (S_g^1 + t_2)[\mathsf{GH}(0)]$ *and* $P(t_2) = \big((S_h^1 + t_2)[\mathsf{C}]\langle \mathsf{atp}, X + t_2\cdot\mathbf{v}_1\rangle (S_a^1 + t_2)[\mathsf{AH}(t_2)]\big)$.

***Finally:*** $(N_1,t_1) \stackrel{t_2}{\Rightarrow} (N_2, t_1+t_2)$ *where* $N_2 = \mathsf{steer}\ (t_1+t_2)\ N_1'' = \big(P(t_2)\,\langle \mathsf{glc}, Y\rangle\, G(t_2)\big)[\![\mathbf{v}_3]\!]$. *Observe that:*
$\big(P(t_2)\,\langle \mathsf{glc}, Y\rangle\, G(t_2)\big)[\![\mathbf{v}_3]\!] = \big(P(t_2)[\![\mathbf{v}_3]\!]\big)\,\langle \mathsf{glc}, Y\rangle\,\big(G(t_2)[\![\mathbf{v}_3]\!]\big) =$
$\big(S_h^2[\mathsf{C}]\,\langle \mathsf{atp}, X + t_2\cdot\mathbf{v}_1\rangle\, S_a^2[\mathsf{AH}(t_2)]\big)\,\langle \mathsf{glc}, Y\rangle\, S_g^2[\mathsf{GH}(0)]$
*where* $S_h^2 = (S_h^1 + t_2)[\![\mathbf{v}_3]\!]$, $S_a^2 = (S_a^1 + t_2)[\![\mathbf{v}_3]\!]$ *and* $S_g^2 = (S_g^1 + t_2)[\![\mathbf{v}_3]\!]$.
*At this stage the network contains just one process and, as a consequence, no collisions are possible. Thus,* $\mathsf{Ftoc}(N_2) = \infty$. *Assume* $t_g = t_a - t_2 \leq \Delta$[10].
*If we let* $X_g = (X + t_2\cdot\mathbf{v}_1) + t_g\cdot\mathbf{v}_3$ *and* $Y_g = Y + t_g\cdot\mathbf{v}_3$, *then:*
$N_2 \stackrel{t_g}{\Rightarrow} ((S_h^2 + t_g)[\mathsf{C}]\,\langle \mathsf{atp}, X_g\rangle\,(S_a^2 + t_g)[\mathsf{AH}(t_a)])\,\langle \mathsf{glc}, Y_g\rangle (S_g^2 + t_g)[\mathsf{GH}(t_g)] \stackrel{\rho}{\rightarrow}$
$((S_h^2 + t_g)[\mathsf{HEX}] \parallel (S_a^2 + t_g)[\mathsf{ADP}]) \parallel (S_g^2 + t_g)[\mathsf{G6P}] \stackrel{\Delta - t_g}{\Rightarrow}$
$((S_h^2 + \Delta)[\mathsf{HEX}] \parallel (S_a^2 + \Delta)[\mathsf{ADP}]) \parallel (S_g^2 + \Delta)[\mathsf{G6P}] = N_2'$.

***Thus:*** $(N_2, t_1+t_2) \stackrel{\Delta}{\Rightarrow} (N_3, t_1+t_2+\Delta)$ *where* $N_3 = \mathsf{steer}\ (t_1+t_2+\Delta)\ N_2' = (S_h^3[\mathsf{HEX}] \parallel S_a^3[\mathsf{ADP}]) \parallel S_g^3[\mathsf{G6P}]$, $S_i^3 = (S_i^2 + \Delta)[\![\mathbf{v}_i]\!]$ *and* $\mathbf{v}_i = \mathsf{steer}\ (t_1+t_2+\Delta)\ (S_i^2 + \Delta)$ *for each* $i \in \{h, a, g\}$.

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[9] If were $t_2 < t_h$. the 3D processes $\mathsf{HA}(t_2)$ and $\mathsf{GLC}$ would be no more compatible, and a collision between them would be treated as elastic. On the other hand, if were $t_2 = t_a$ the idling time for $\mathsf{AH}(t_a)$ would be over. As a consequence, time would pass further only after the execution of a weak-split operation that splits the bond between the Hexokinases and the Atp molecules

[10] If were $t_g \neq t_a - t_2$ the reaction could never proceed since the involved molecules would never be able to release - all together - the bonds. Thus the system would deadlock.

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

**Theorem 1 (Closure w.r.t. well-formedness)** *Let $N \in \mathbb{N}$ well-formed. If $(N,t) \stackrel{t'}{\Rightarrow} (M, t+t')$ then $M$ is well-formed.*

**Proof:** Assume that $(N,t) \stackrel{t'}{\Rightarrow} (M, t+t')$ because of $N \stackrel{t'}{\Rightarrow} N' \stackrel{\kappa}{\rightarrow} N''$ and $M = \mathsf{steer}\ (t+t')\ N''$ (the other case – see Def. 24 – is similar). Then, by Proposition 7 (item 3) and Lemma 1, $N$ well-formed and $N \stackrel{t'}{\Rightarrow} N' \stackrel{\kappa}{\rightarrow} N''$ implies $N''$ and hence $M = \mathsf{steer}\ (t+t')\ N''$ well-formed.

## 5 Conclusions and Future Work

We have formally defined the full timed operational semantics of the Shape Calculus. Moreover, a result of well-formedness has been proven: any well-formed 3D network will evolve in a well-formed 3D network. Several technical proofs of the results are omitted in this paper, but they can be found in the extended version [1]. On top of this formal framework, we intend to define abstractions of the semantics in order to be able to prove, statically, properties of a given 3D network. Moreover, we intend to add information to the basic calculus, for instance by equipping any process with a steer component, rather than having an abstract function for movements.

## References


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