Modelling and Verification of Spatiality: The Shape Calculus

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Explicitly Spatial Models and Languages

- For modeling Distributed Systems with a known spatial distribution and/or moving components, e.g. protocols for mobile systems with positions/trajectories
- For modelling Biological Systems:
  - **Spatiality**: proximity, affinity, crowding, co-localization, perception, . . .
  - **Shape/Geometry**: the shape usually determines the function
  - **Movement**: biological entities can move with different patterns (Brownian motion, chemical gradient-guided, . . .)

Which Space Representation?

- Topological space
  - Compartments, no explicit coordinates - Interactions occur among entities in the same compartment
  - e.g. Membrane Computing (1998), Bio Ambients (2004), Brane Calculi (2004)
- Discrete Grid space
  - 2D or 3D cells, discrete coordinates - Interactions by proximity of cells, discrete movements
  - e.g. Cellular Automata (1940s), Spatial P Systems (2010)
- Continuous Geometrical space
  - 3D positions, with continuous coordinates - Interactions can be defined in different ways, using geometrical information
  - e.g. Real-space Process Algebra (Spatio-temporal ACP, 1993!), Space-π (2008), 3π(2012), Shape Calculus (2010)

*Examples mainly Bio-oriented languages

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Challenging Features

The area is relatively new, there is a lot of room for working :-)

- Representation of Space and Time
- Expression of (Complex) Movements
- Space-driven Interactions vs Classical communication
- Shapes, Bonds, Re-shaping, Growth, Reversibility of Reactions
- How to deal with collisions
- Modelling and Simulation, what about Verification?

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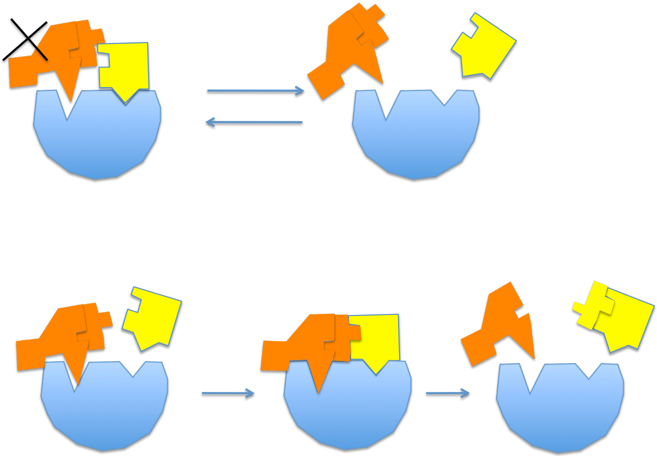
What we have done so far...

- We defined a process calculus with a very rich set of features: the Shape Calculus
- Shape Calculus models are stub code for entities in a simulator
- We retain the possibility of formal **verification**, e.g. by abstract interpretation
- We can combine **simulation** (with a less effort of coding) with **verification**

Scenario we want to model



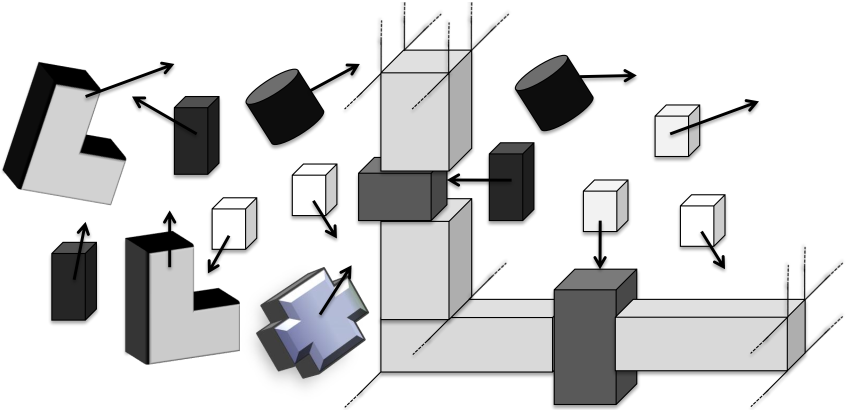
Shape Calculus

- Spatial 3D, Deterministically Timed, Individual-based
- Shape-based $\rightarrow$ modelled entities have a 3D **geometrical** shape, a position and a velocity with which they move
- Entities can interact $\rightarrow$ bindings (collision-driven) and splittings (driven by internal behaviour)

† E. Bartocci, F. Corradini, M. R. Di Berardini, E. Merelli, and L. Tesei, *Shape Calculus. A Spatial Mobile Calculus for 3D Shapes*, Scientific Annals of Computer Science **20** (2010), pp. 1-31.

† E. Bartocci, D. R. Cacciagrano, M. R. Di Berardini, E. Merelli, and L. Tesei, *Shape Calculus: Timed Operational Semantics and Well-Formedness*, Scientific Annals of Computer Science **20** (2010), pp. 32-52.

Shape Calculus: Scenario



What is a 3D spatial process, geometrically?

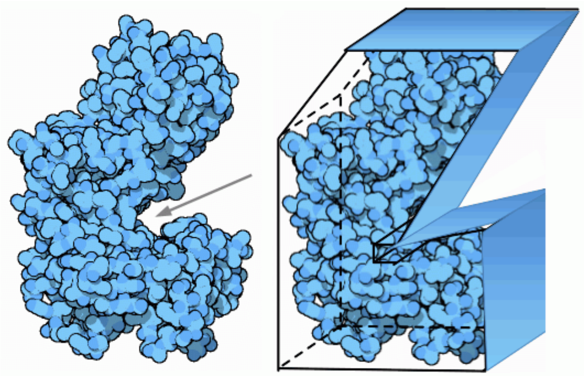
In most of the languages with explicit space, a process is a point $\vec{p} \in \mathbb{R}^3$

- Real space, but no dimension
- Interactions can depend only on distance (e.g. in Space-π or in spatio-temporal ACP)

In Shape Calculus, a process is a set of points $V \subseteq \mathbb{R}^3$

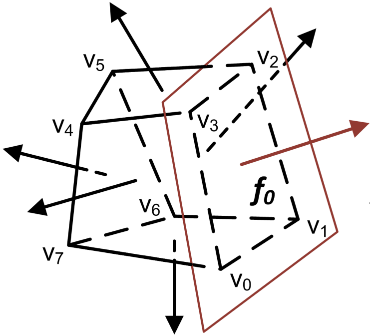
- A "physical body" is associated to the process, its **shape**
- Interactions can depend on distance, but also on the shape and on the 3D orientation of the process

Shape Approximation



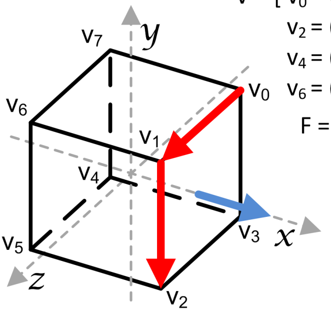
Basic Shapes, Shape Calculus Approach

- We take only *convex polyhedra* as basic shapes
- A convex polyhedron is determined by the planes of its faces and their outward normals $\rightarrow$ it is defined by its *features*



Basic Shapes

- We are interested in the features, which can be communication channels, more than in the internal points
- Basic shapes are represented as *Indexed face set*, i.e. as point tuples (faces)



$$V = [\ v_0 = (1\ \ 1\ \ {-1})\quad v_1 = (1\ \ 1\ \ 1)$$
$$v_2 = (1\ {-1}\ \ 1)\quad v_3 = (1\ {-1}\ {-1})$$
$$v_4 = ({-1}\ {-1}\ {-1})\quad v_5 = ({-1}\ {-1}\ 1)$$
$$v_6 = ({-1}\ \ 1\ \ 1)\quad v_7 = ({-1}\ \ 1\ {-1})\ ]$$

$$F = \{\ f_0 = [v_0,v_1,v_2,v_3],$$
$$f_1 = [v_3,v_4,v_7,v_0],$$
$$f_2 = [v_0,v_7,v_6,v_1],$$
$$f_3 = [v_1,v_6,v_5,v_2],$$
$$f_4 = [v_2,v_5,v_4,v_3],$$
$$f_5 = [v_4,v_5,v_6,v_7]\ \}$$

Shape Syntax

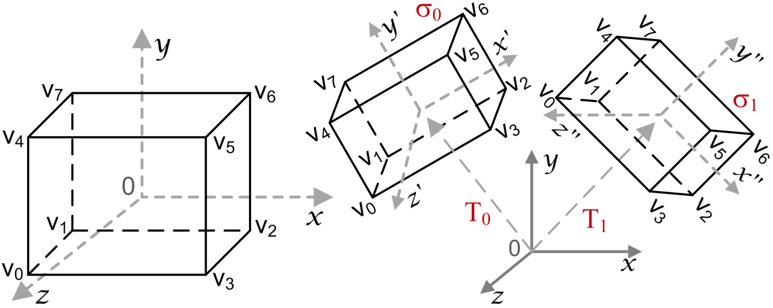
$$S ::= \sigma \mid S \langle \varphi_1, \varphi_2 \rangle S$$

$\sigma \in$ Basic, φ_1, φ_2 are two features, one for each of the shapes, W is an IFS, ω is the angular velocity (quaternion) and *s* is a **name** identifying univocally the shape

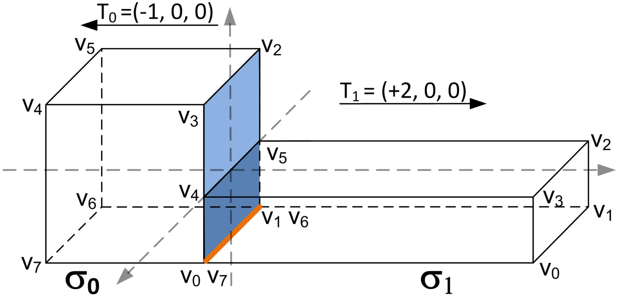
$$\sigma = \langle W, m, \mathbf{v}, \omega, s, T \rangle$$

- *W* is the *template* shape, with coordinates expressed in the *local frame*
- *W* is moved to the *reference frame* by the **affine transformation** T associated to the shape (similar to 3π)

IFSs and shapes

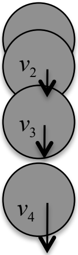


Compound Shapes



- Two faces touch: $s_0.f_0 = [s_0.v_0, s_0.v_1, s_0.v_2, s_0.v_3]$, $s_1.f_1 = [s_1.v_4, s_1.v_5, s_1.v_6, s_1.v_7]$
- The compound shape is $S_1 = \sigma_0\langle\{s_0.f_0, s_1.f_1\}\rangle\sigma_1$

Movement



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

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

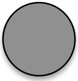
$$v_2 = Move(S,t_1) = [0,-0.49,0]\, m/s$$

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

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

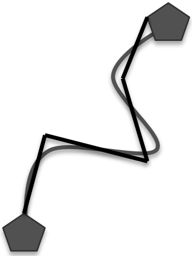
$$t_i = t_{i-1} + \Delta$$

$$\Delta = 0.05 s$$

$S =$ 

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

(a)



(b)

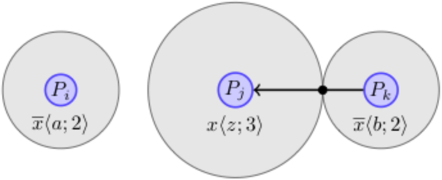
Time evolution and velocity update

- Time domain is continuous, divided into **small** discrete time steps Δ
- At each step the velocity and rotation of each entity is changed by the Move function

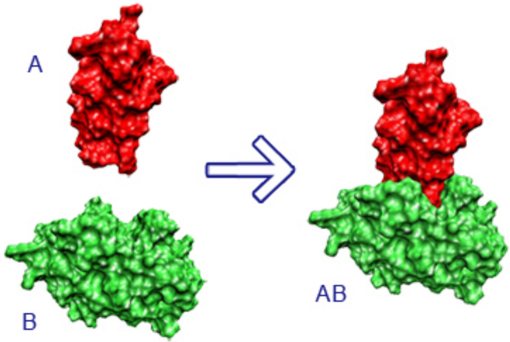
Spatial-dependent communication

In languages with no shapes, communication:

- Can depend on distance
- Can be synchronous, checking distances at regular time steps (Space-π)
- Can be asynchronous, with spherical propagation of messages (Spatio-temporal ACP)
- Classical communication can be re-obtained, allowing infinite distance

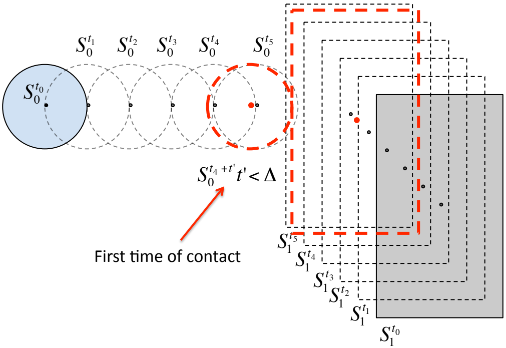


Interactions of 3D processes: binding and splitting



In Shape Calculus, Communication is synchronous and only local (collision-driven)

Collision Detection



- FTOC can be determined in each Δ interval, if any
- In case of collision the time delay step is reduced from Δ to FTOC
- Collision(s) are detected and may trigger **interactions**

Behaviours

Behaviour Syntax

$$B ::= \text{nil} \mid \langle \alpha, \{\varphi_1, \ldots, \varphi_n\}\rangle.B \mid \epsilon(t).B \mid B + B \mid K \mid$$

$$\omega(a, \{\varphi_1, \ldots, \varphi_n\}).B \mid \rho(L).B$$

where $\varphi_1, \ldots, \varphi_n$ are feature representations and
$L = \{\langle a, \{\varphi_1, \ldots, \varphi_n\}\rangle \mid \langle a, \{\varphi_1, \ldots, \varphi_n\}\rangle$ is a channel$\}$.

- **Spatial channels** can be open on several features of the shape, even disjoint
- Communication is possible only between compatible spatial channels that are **colliding**

SOS rules for Behaviours

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

$$\textsc{Str}_1 \frac{L = \{\langle \alpha, X \rangle\}}{\rho(L).B \xrightarrow{\rho(\alpha,X)} B} \qquad \textsc{Str}_2 \frac{L = \{\langle \alpha, X \rangle\} \cup L' \quad L' \neq \emptyset}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L').B}$$

$$\textsc{Str}_3 \frac{B \xrightarrow{\rho(\alpha,X)} B'}{\rho(L).B \xrightarrow{\rho(\alpha,X)} \rho(L).B'}$$

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

$$\textsc{Sum}_t \frac{B_1 \overset{t}{\rightsquigarrow} B_1' \quad B_2 \overset{t}{\rightsquigarrow} B_2'}{B_1 + B_2 \overset{t}{\rightsquigarrow} B_1' + B_2'} \qquad \textsc{Del}_t \frac{t' \geq t}{\epsilon(t').B \overset{t}{\rightsquigarrow} \epsilon(t'-t).B} \qquad \textsc{Del}_c \frac{B \overset{t}{\rightsquigarrow} B'}{\epsilon(t').B \overset{t+t'}{\rightsquigarrow} B'}$$

3D processes

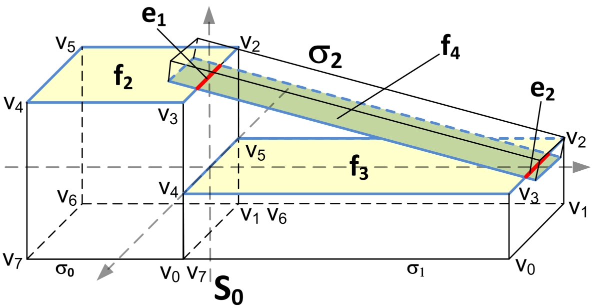
3D Process Syntax

$$P ::= S[B] \mid P \langle a, \{\varphi_1, \varphi_2\} \rangle P$$

where a is the name of the channel and φ_1, φ_2 are features belonging to the shapes associated with the compound 3D processes.

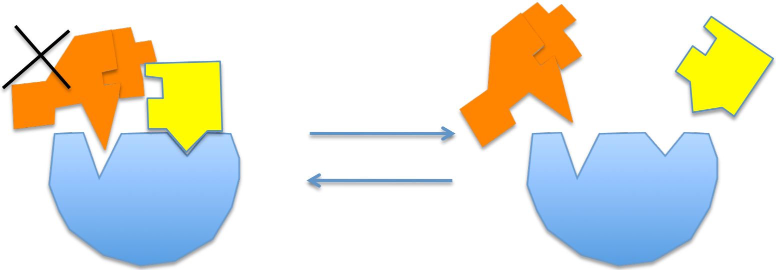
- **Composition by glueing**, after a collision on compatible active channels on surfaces
- Composed process behaviour is the **interleaving** of the components' behaviours

Binding



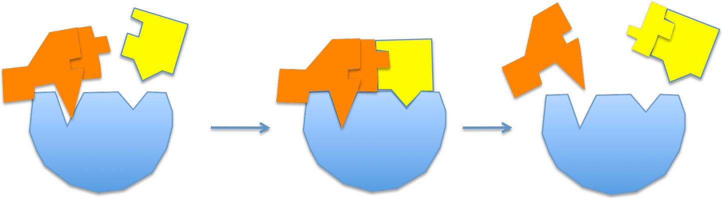
- Non-deterministically, one of the two possible bonds is chosen (s_2 is the name of σ_2):
  - $S_0[B_0]\langle a, \{s_0.e_1, s_2.f_4\}\rangle\sigma_2[B_1]$
  - $S_0[B_0]\langle a, \{s_1.e_2, s_2.f_4\}\rangle\sigma_2[B_1]$

Weak Split - $\omega(C)$



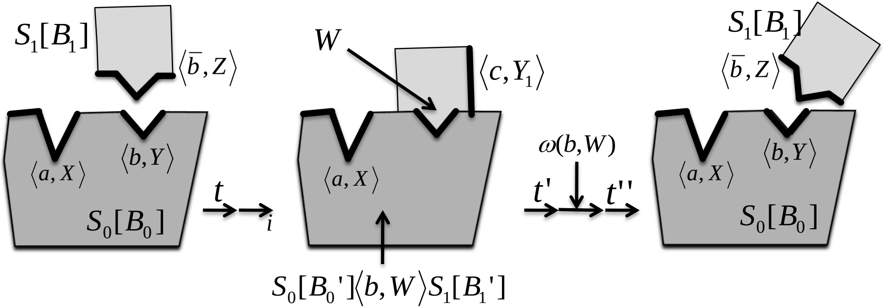
A bond on a channel C can be released non-deterministically

Strong Splitting $\rho(L)$



A subset L of bonds must split at the same time
A “re-shaping” is obtained by rearrangement of bonds

Binding and Splitting



SOS rules for 3D processes

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

$$\text{BASIC}_c \frac{B \xrightarrow{\langle \alpha, X \rangle} B' \quad Y = \text{global}(X, \mathcal{R}(S))}{S[B] \xrightarrow{\langle \alpha, Y \rangle} S[B']}$$

$$\text{BASIC}_s \frac{B \xrightarrow{\rho(\alpha, X)} B' \quad Y = \text{global}(X, \mathcal{R}(S))}{S[B] \xrightarrow{\rho(\alpha, Y)} S[B']}$$

$$\text{COMP}_s \frac{P \xrightarrow{\rho(\alpha, Y)} P'}{P \langle a, X \rangle Q \xrightarrow{\rho(\alpha, Y)} P' \langle a, X \rangle Q}$$

$$\text{COMP}_c \frac{P \xrightarrow{\langle \alpha, Y \rangle} P' \quad Y \subseteq \mathcal{B}(P \langle a, X \rangle Q)}{P \langle a, X \rangle Q \xrightarrow{\langle \alpha, Y \rangle} P' \langle a, X \rangle Q}$$

Network of 3D processes

The set of networks of 3D processes is generated by:

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

Functional and Temporal semantics of the networks

$$\textsc{Empty}_t \frac{}{\mathrm{Nil} \xrightarrow{t} \mathrm{Nil}} \qquad \textsc{Par}_t \frac{N \xrightarrow{t} N' \quad M \xrightarrow{t} M'}{N \parallel M \xrightarrow{t} N' \parallel M'} \qquad \textsc{Par}_{a1} \frac{N \xrightarrow{\nu} N'}{N \parallel N \xrightarrow{\nu} N' \parallel M}$$

- $P \xrightarrow{\nu} Q$ for $\nu \in \{\omega, \rho\}$
- $P \xrightarrow{\kappa} Q$ for every collision response
- $P \xrightarrow{t} Q$ iff $P \overset{t}{\rightsquigarrow} Q$ and either $P \overset{\rho}{\not\rightarrow}$ or $P \not\searrow$

Simulation and Verification

- The evolution of a given network can be **simulated**
- Algorithms and data structures can be imported from computational geometry
- Sources of randomness: movement function (e.g. Brownian motion)
- Sources of non-determinism: alternative choices among spatial channels, weak splits, multiple collision response
- Verification?

Verification by Abstract Interpretation

- Approach: 3D Networks are abstracted and abstract fixpoint semantics is executed
- The abstract domain and the abstract operators should guarantee termination
- First (huge) abstraction done on movement, shape and time
- Untimed and Unspatial safety properties can be checked!

†Federico Buti, Massimo Callisto De Donato, Flavio Corradini, Maria Rita Di Berardini, Emanuela Merelli, Luca Tesei: *Towards Abstraction-Based Verification of Shape Calculus*. Electr. Notes Theor. Comput. Sci. **284**: 23-34 (2012)

Concrete Set and abstraction

- $(\wp(\mathbb{N}), \subseteq, \cup, \cap, \{\}, \mathbb{N})$
- 3D processes "instances" *collapse* to a single abstract process
- A network is abstracted to a set of abstract processes
- $\epsilon(t)$ delays are collapsed to $\epsilon(\cdot)$, bindings possible at any time

Abstraction Function

$\alpha_S(\sigma)$	$=$	$\langle V, m, \odot, \odot\rangle$
$\alpha_S(S\langle X\rangle S)$	$=$	$\alpha_S(S)\langle\odot\rangle\alpha_S(S)$
$\alpha_B(\text{nil})$	$=$	$\text{nil}^\sharp$
$\alpha_B(\langle a, X\rangle.B)$	$=$	$\langle a, X\rangle.\alpha_B(B)$
$\alpha_B(B_1 + B_2)$	$=$	$\alpha_B(B_1) + \alpha_B(B_2)$
$\alpha_B(\omega(a, X).B)$	$=$	$\omega(a, X).\alpha_B(B)$
$\alpha_B(\rho(a, X).B)$	$=$	$\rho(a, X).\alpha_B(B)$
$\alpha_B(\epsilon(t).B)$	$=$	$\epsilon(\cdot).\alpha_B(B)$
$\alpha_B(\rho(L).B)$	$=$	$\rho(L).\alpha_B(B)$
$\alpha_P(S[B])$	$=$	$\alpha_S(S)[\alpha_B(B)]$
$\alpha_P(P\langle a, X\rangle Q)$	$=$	$\alpha_P(P)\langle a, \odot\rangle\alpha_P(Q)$
$\alpha_P(\Vert_{i\in I} P_i)$	$=$	$\bigcup_{i\in I}\{\alpha(P_i)\}$

Abstract Set and concretization

- $(\wp(3DP^\sharp), \subseteq, \cup, \cap, \{\}, 3DP^\sharp)$
- Every abstract set is concretized considering all the possible values of velocity, position and cardinality
- Velocity of shapes is limited to a *maximal velocity* v_{max}.
- From a compounded abstract shape a set of concrete compounded shapes is generated
- Each set differs in its cardinality and in the number of concrete instances of each abstract 3D process
- The cardinality can be zero

Concretization Function

$\gamma_S(\sigma^\sharp)$	$=$	$\{\sigma = \langle V, m, p, v\rangle \mid p \in \mathbb{P}, 0 \leq \|v\| \leq v_{max}\}$
$\gamma_S(S^\sharp\langle\odot\rangle T^\sharp)$	$=$	$\{S\langle Y\rangle T \mid S \in \gamma_S(S^\sharp), T \in \gamma_S(T^\sharp),$ $Y \subseteq \mathcal{B}(S) \cap \mathcal{B}(T), Y \neq \emptyset\}$
$\gamma_B(\mathrm{nil}^\sharp)$	$=$	$\{\mathrm{nil}\}$
$\gamma_B(\langle a, X\rangle.B^\sharp)$	$=$	$\{\langle a, X\rangle.B \mid B \in \gamma_B(B^\sharp)\}$
$\gamma_B(B_1^\sharp + B_2^\sharp)$	$=$	$\{B_1 + B_2 \mid B_1 \in \gamma_B(B_1^\sharp), B_2 \in \gamma_B(B_2^\sharp)\}$
$\gamma_B(\omega(a, X).B^\sharp)$	$=$	$\{\omega(a).B \mid B \in \gamma_B(B^\sharp)\}$
$\gamma_B(\rho(a, X).B^\sharp)$	$=$	$\{\rho(a, X).B \mid B \in \gamma_B(B^\sharp)\}$
$\gamma_B(\epsilon(\cdot).B^\sharp)$	$=$	$\{\epsilon(t).B \mid t \in \mathbb{T}, B \in \gamma_B(B^\sharp)\}$
$\gamma_B(\rho(L).B^\sharp)$	$=$	$\{\rho(L).B \mid B \in \gamma_B(B^\sharp)\}$
$\gamma_P(S^\sharp[B^\sharp])$	$=$	$\{S[B] \mid S \in \gamma_S(S^\sharp), B \in \gamma_B(B^\sharp)\}$
$\gamma_P(P^\sharp\langle a^\sharp, \odot\rangle Q^\sharp)$	$=$	$\{P\langle a, X\rangle Q \mid P \in \gamma_P(P^\sharp), Q \in \gamma_P(Q^\sharp),$ $X \subseteq \mathcal{B}(\mathrm{shape}(P)) \cap \mathcal{B}(\mathrm{shape}(Q)), X \neq \emptyset\}$
$\gamma_P(\{P_1^\sharp, \ldots, P_n^\sharp\})$	$=$	$\wp\{N \in \mathbb{N} \mid N = (\|_{i=1}^n (\|_{P\in U} P)), U \in \wp(\gamma_P(P_i^\sharp)),\ U \text{ finite}\}$

Abstract semantics

$$\textsc{Del}_a^\sharp \frac{B^\sharp \xrightarrow{\mu}_\sharp B'^\sharp}{\epsilon(\cdot).B^\sharp \xrightarrow{\mu}_\sharp B'^\sharp} \qquad \textsc{Del}_t^\sharp \frac{}{\epsilon(\cdot).B^\sharp \overset{t}{\rightsquigarrow}_\sharp \epsilon(\cdot).B^\sharp} \qquad \textsc{Del}_c^\sharp \frac{B^\sharp \overset{t}{\rightsquigarrow}_\sharp B'^\sharp}{\epsilon(\cdot).B^\sharp \overset{t'}{\rightsquigarrow}_\sharp B'^\sharp}$$

$$\textsc{Comp}_t^\sharp \frac{P^\sharp \overset{t}{\rightsquigarrow}_\sharp P'^\sharp \quad Q^\sharp \overset{t}{\rightsquigarrow}_\sharp Q'^\sharp}{P^\sharp \langle a, \odot\rangle\, Q^\sharp \overset{t}{\rightsquigarrow}_\sharp P'^\sharp \langle a, \odot\rangle\, Q'^\sharp} \qquad \textsc{Comp}_c^\sharp \frac{P^\sharp \xrightarrow{\langle a,\odot\rangle}_\sharp P'^\sharp}{P\, \langle a, \odot\rangle\, Q^\sharp \xrightarrow{\langle a,\odot\rangle}_\sharp P'^\sharp \langle a, \odot\rangle\, Q^\sharp}$$

$$\textsc{Basic}_c^\sharp \frac{B^\sharp \xrightarrow{\langle a,X\rangle}_\sharp B'^\sharp}{S^\sharp[B^\sharp] \xrightarrow{\langle a,\odot\rangle}_\sharp S^\sharp[B'^\sharp]} \qquad \textsc{Basic}_s^\sharp \frac{B^\sharp \xrightarrow{\langle a,X\rangle}_\sharp B'^\sharp}{S^\sharp[B^\sharp] \xrightarrow{\rho(\alpha,\odot)}_\sharp S^\sharp[B'^\sharp]}$$

$$\textsc{StrSync}^\sharp \frac{P^\sharp \xrightarrow{\rho(\alpha,\odot)}_\sharp P'^\sharp \quad Q^\sharp \xrightarrow{\rho(\overline{\alpha},\odot)}_\sharp Q'^\sharp \quad \alpha \in \{a, \overline{a}\}}{P^\sharp \langle a, \odot\rangle\, Q^\sharp \overset{\rho(a,\odot)}{\Rightarrow} P'^\sharp \langle a, \odot\rangle\, Q'^\sharp}$$

Verification of Safety Properties

- Given a network N we calculate the least fixpoint of the abstract semantics:
  - $F \uparrow^0 (N) = \alpha(\{N\})$
  - $F \uparrow^n (N) = \bigcup_{M^\sharp \in \{N^\sharp \mid F\uparrow^{n-1}(N) \xrightarrow{x}_\sharp N^\sharp,\ x \in \{\omega,\rho,\kappa,t\}\}} M^\sharp$
- "If an abstract 3D process is not present in $F \uparrow^\omega (N)$, then a concrete corresponding 3D process can never appear in the evolution of N"
- To fix - termination is not guaranteed: infinite polymers can be created
- Next Refinement: retain **time** to verify quantitative timed safety properties like "a certain abstract 3D process will never be produced before 20 time units"

Future Work and Open Questions

- Systematize, compare and complete the existing different approaches to spatial features:
  - Deterministic Time vs Stochastic Time (through abstraction?)
  - Probabilistic Behaviours, where probability may depend on the geometrical features
- Make a clear hierarchy of spatial calculi, relating them by abstractions and/or encodings
- Investigate relationships of spatial calculi with hybrid systems for which reachability is semi-decidable
- Can the movement function be less abstract, e.g. expressed by an appropriate transition relation?
- Is there any suitable equivalence for spatial calculi at different levels of abstractions?
- Can other verification techniques be applied for (fully detailed) spatial calculi?

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Thank you!


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