Tailoring the shape calculus towards quantitative analysis

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PaCo meeting
University of Camerino
September 15th 2010
Shape calculus - main features

- Non-deterministic timed calculus representing physical entities moving in 3D
- Processes = 3D shapes + dynamic behaviour
- Processes can move, collide and possibly bind
- Behaviours are specified with a timed CCS-like process algebra with channels aka “type of binders”
- \langle a, X \rangle, X is a portion of the surface of the process’s able to bind

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- Bound processes has behaviour equal to the interleaving of the component processes.

- Compound processes can split weakly (no reaction) or split strongly (reaction) dividing in as many pieces as the reaction products.

- Without communication (i.e. binding) collisions are considered elastic.
Shapes in Shape Calculus

Shape Syntax

\[ S ::= \sigma \mid S \langle X \rangle S \text{ where } \sigma \in \text{Basic and } X \subseteq \mathbb{R}^3 \text{ is a non-empty set of points. The set } X \text{ is intended to be the common surface on which the two shapes are attached.} \]

Examples of compound shapes in 2D

(a) \quad (b) \quad (c) \quad (d)
Shape example

Representation of enzymatic reaction in Shape Calculus

Shape approximation
Time evolution and velocity update

- 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 $t_i = t_{i-1} + \min(\Delta, Ftc(t_{i-1}), Ftr(t_{i-1}))$

- The updating of the velocities is represented by a function $\text{steer}: \mathbb{T} \rightarrow \text{Shapes} \hookrightarrow \mathbb{V}$ gives the velocity vector $\text{steer}_t S$ to assign to shape $S$ at time $t$
Collision Detection

First time of contact

(a) Interpenetration

(b) First time of contact

(c) $t' < \Delta$
Collision Response

Elastic and inelastic collision (one dimensional case)

\[ \mathbf{v}(S_0) = 1\text{ cm/s} \quad \mathbf{v}(S_1) = -1\text{ cm/s} \]

\[ m(S_0) = 2g \quad m(S_1) = 1g \]

\[ \mathbf{v}(S_0) = -\frac{1}{3}\text{ cm/s} \quad \mathbf{v}(S_1) = \frac{5}{3}\text{ cm/s} \]

\[ \mathbf{v}(S_0 \langle X \cap Y \rangle S_1) = \frac{1}{3}\text{ cm/s} \]
Shapes behaviours

Set $\mathcal{B}$ of *shapes’ behaviours* grammar

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

where $\langle \alpha, X \rangle \in \mathcal{C}$, $L$ is a non-empty subset of $\mathcal{C}$ whose channels are pairwise incompatible, $t \in \mathbb{T}$ and $K$ is a process name in $\mathcal{K}$.

Set 3DP of *3D processes* grammar

$$P ::= S[B] \mid P \langle a, X \rangle P, \text{ where } S \in \text{Shapes}, B \in \mathcal{B}, a \in \Lambda \text{ and } X \subseteq \mathbb{R}^3$$

intersection between the surface active sites that are bound

Modelling Hexokinase in Shape Calculus

$$S_h[\text{HEX}] \text{ where } \text{HEX} = \langle \text{atp}, X_{\text{ha}} \rangle . \text{HA} + \langle \text{glc}, Y_{\text{hg}} \rangle . \text{HG}$$
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Modelling HEX, ATP and Glucose behaviours

$\text{HEX} = \langle \text{atp}, X_{ha} \rangle . \text{HA} + \langle \text{glc}, X_{hg} \rangle . \text{HG},$

$\text{HA} =$
$\omega(\text{atp}, X_{ha}).\text{HEX} + \epsilon(t_h).\langle \text{glc}, X_{hg} \rangle . \rho(\{\langle \text{atp}, X_{ha} \rangle, \langle \text{glc}, Y_{hg} \rangle \}).\text{HEX},$

$\text{HG} =$
$\omega(\text{glc}, X_{hg}).\text{HEX} + \epsilon(t_h).\langle \text{atp}, X_{ha} \rangle . \rho(\{\langle \text{atp}, X_{ha} \rangle, \langle \text{glc}, Y_{hg} \rangle \}).\text{HEX},$

where $X_{ha}, Y_{hg}$ are the surfaces of contact.

$\text{ATP} = \langle \overline{\text{atp}}, X_{ah} \rangle . (\epsilon(t_a) . \rho(\{\langle \overline{\text{atp}}, X_{ah} \rangle \}).\text{ADP} + \omega(\text{atp}, X_{ah}).\text{ATP})$
Towards quantitative analysis

- Shape Calculus can represent a great variety of scenarios.
- Soon it will be integrated with our tool BIOSHAPE for analyse biological phenomena.
- Providing formal verification techniques for the Shape Calculus is the next step.
- The objective is to find the right abstractions to apply existing quantitative model checking or quantitative equivalence checking techniques.
For instance...

- probabilistic timed automata could be useful to describe in more detail the behaviour of the processes and their interactions

- hybrid automata could be used to specify schemes of motion to be associated to certain classes of processes

- Suitable logic languages for specifying the properties must also be identified
Logic(s) for...

- verifying that certain 3D configurations are reached
- verifying that a certain molecule concentration is achieved
- verifying occurrence of certain oscillatory behaviours
- verifying that with a certain probability a reaction can occur
- ...

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In the end...

...thanks for your attention! :)

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