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CNRS LIX-École Polytechnique de Paris

Enhancing "Reaction Systems": a process algebraic approach

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joint work with

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Roadmap

- ✔ A new kind of interaction (subsuming CCS)
- ✔ Encoding reaction systems
- ✔ Conclusion and future work

Interactions are not always binary, think at biological systems or contracts !

Notation

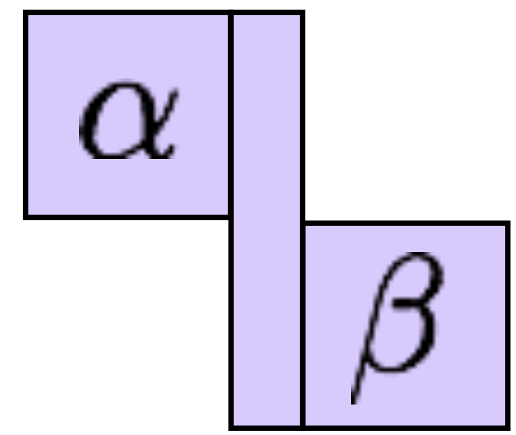
a interaction over channel a

τ silent interaction

$\square$ free “slot”, accepting
any interaction (only in labels)

Link

$^{\alpha}\backslash_{\beta}$ From α to β



Valid:

if it is **virtual** $^{\square}\backslash_{\square}$

if it is **solid** $\alpha, \beta \neq \square$

Link chain

$$\alpha_1 \backslash_{\beta_1} \; \alpha_2 \backslash_{\beta_2} \; \cdots \; \alpha_n \backslash_{\beta_n}$$

$\mathcal{C}$ is the set of channel names

such that:

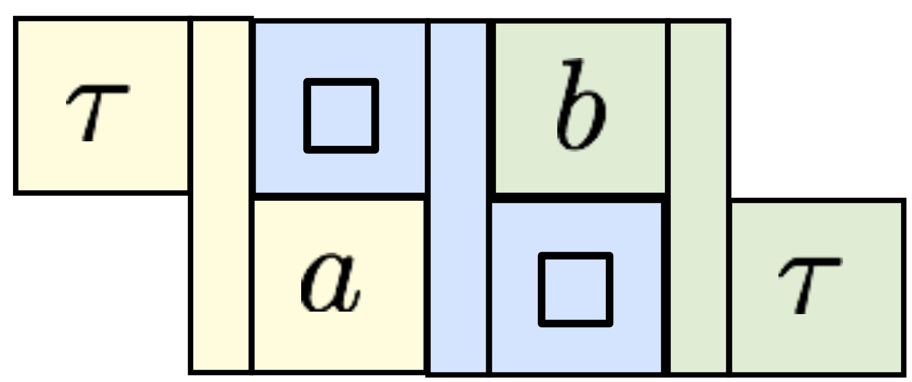
$$\beta_i, \alpha_{i+1} \in \mathcal{C} \quad \text{implies } \beta_i = \alpha_{i+1}$$

$$\beta_i = \tau \quad \text{iff } \alpha_{i+1} = \tau$$

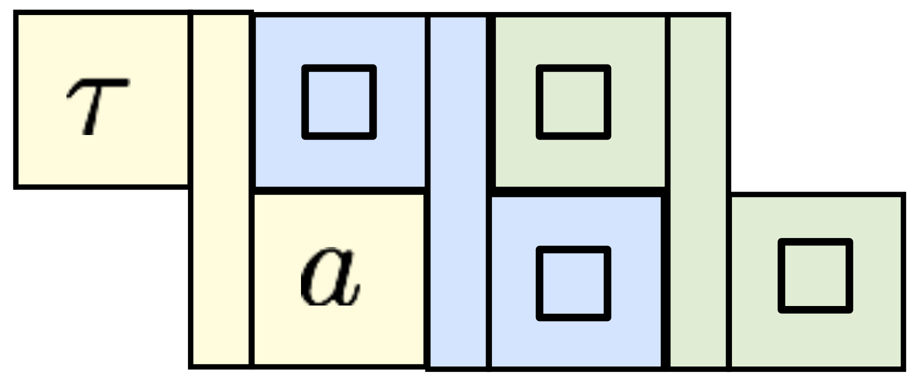
Examples: non solid

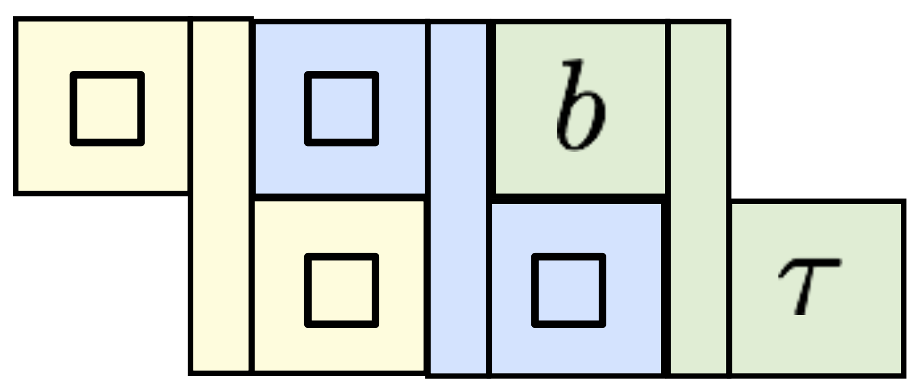
Virtual links
can be read as missing pieces of the puzzle

$\Box \backslash \Box$

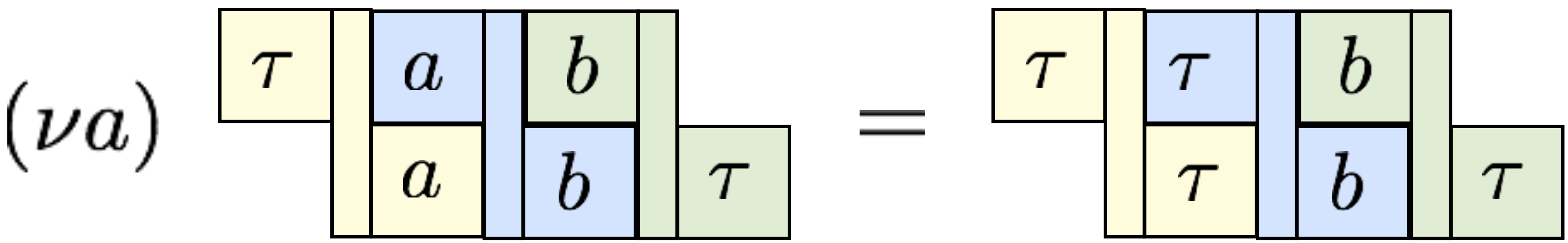


Examples: merge





Examples: restriction



Equivalence relation over link chains

(the black tie)

$$s^{\square}\backslash_{\square} \quad \bowtie \quad s \qquad\qquad s_1{}^{\square}\backslash^{\square}_{\square}\backslash_{\square} s_2 \quad \bowtie \quad s_1{}^{\square}\backslash_{\square} s_2$$

$${}^{\square}\backslash_{\square} s \quad \bowtie \quad s \qquad\qquad s_1{}^{\alpha}\backslash^{a}_{a}\backslash_{\beta} s_2 \quad \bowtie \quad s_1{}^{\alpha}\backslash^{\square}_{a}\backslash^{a}_{\square}\backslash_{\beta} s_2$$

link-calculus syntax

$$P, Q \;::=\; \mathbf{0} \mid \ell.P \mid P + Q \mid P|Q \mid (\nu\, a)P \mid P[\phi] \mid A$$

null action

prefix
(link prefix)

choice

parallel

restriction

relabelling

recursion

(Relevant) SOS rules

the length of the link chains
(of a transition) is decided
by the semantics

$$\frac{s \bowtie \ell}{\ell.P \xrightarrow{s} P}\ (Act) \qquad \frac{P \xrightarrow{s} P'}{(\nu\, a)P \xrightarrow{(\nu\, a)s} (\nu\, a)P'}\ (Res)$$

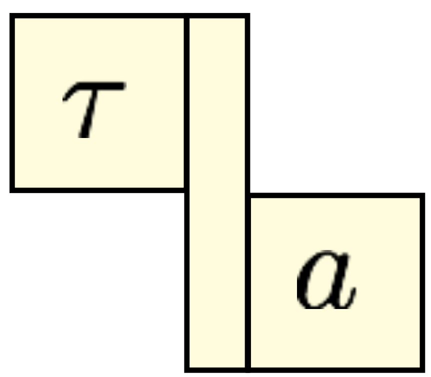
$$\frac{P \xrightarrow{s} P'}{P|Q \xrightarrow{s} P'|Q}\ (Lpar) \qquad \frac{P \xrightarrow{s} P' \qquad Q \xrightarrow{s'} Q'}{P|Q \xrightarrow{s \bullet s'} P'|Q'}\ (Com)$$

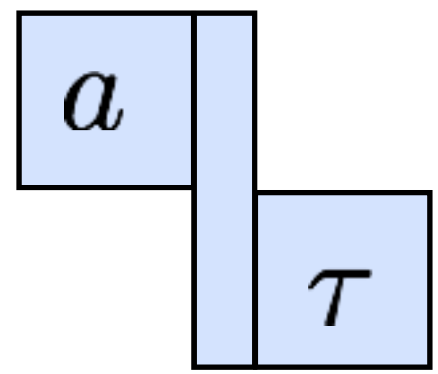
Example

$$P \triangleq {}^{\tau}\backslash_{a}.P_1|(\nu\, b)Q \text{ , } Q \triangleq {}^{b}\backslash_{\tau}.P_2|{}^{a}\backslash_{b}.\mathbf{0}$$

$$\dfrac{\dfrac{}{{}^{\tau}\backslash_{a}.P_1 \xrightarrow{{}^{\tau}\backslash^{\square}_{a}\backslash^{\square}_{\square}\backslash_{\square}} P_1}\,(Act) \qquad \dfrac{\dfrac{\dfrac{}{{}^{b}\backslash_{\tau}.P_2 \xrightarrow{\square\backslash^{\square}_{\square}\backslash^{b}_{\square}\backslash_{\tau}} P_2}\,(Act) \quad \dfrac{}{{}^{a}\backslash_{b}.\mathbf{0} \xrightarrow{\square\backslash^{a}_{\square}\backslash^{\square}_{b}\backslash_{\square}} \mathbf{0}}\,(Act)}{Q \xrightarrow{\square\backslash^{a}_{\square}\backslash^{b}_{b}\backslash_{\tau}} P_2|\mathbf{0}}\,(Com)}{(\nu\, b)Q \xrightarrow{\square\backslash^{a}_{\square}\backslash^{\tau}_{\tau}\backslash_{\tau}} (\nu\, b)(P_2|\mathbf{0})}\,(Res)}{P \xrightarrow{{}^{\tau}\backslash^{a}_{a}\backslash^{\tau}_{\tau}\backslash_{\tau}} P_1|(\nu\, b)(P_2|\mathbf{0})}\,(Com)$$

Examples: CCS-like





The process algebra of linked interactions includes CCS as a sub-calculus

Roadmap

- ✓ A new kind of interaction (subsuming CCS)
- ✓ Encoding reaction systems
- ✓ Conclusion and future work

Reaction Systems

A reaction system is a set of rules of the type:

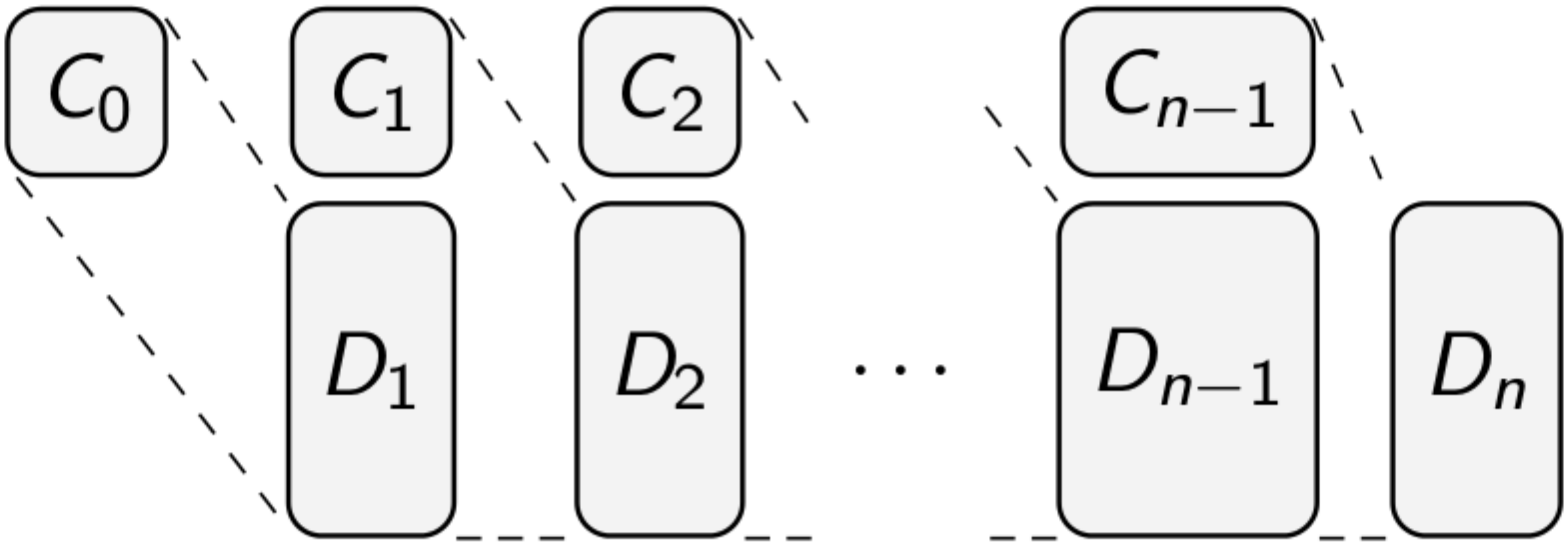
$$a = (R, I, P)$$

Reactants Inhibitors Products

$$(\{cAMP, CAP\}, \{glucose\}, \{cAMP\text{–}CAP\})$$

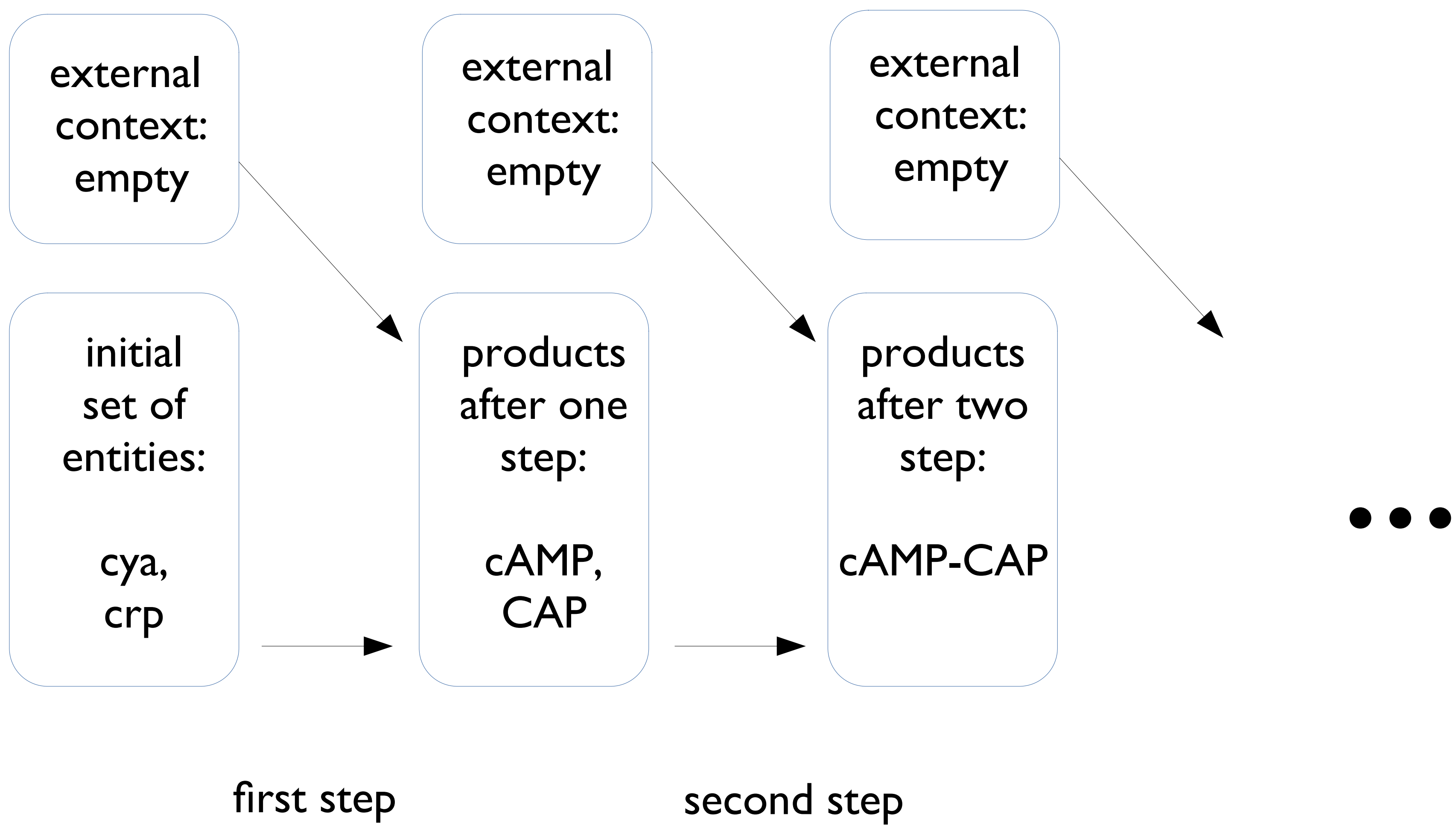
R. Brijder, A. Ehrenfeucht, M. Main, and G. Rozenberg. A tour of reaction systems. International Journal of Foundations of Computer Science, 22(07): 1499--1517, 2011.

Reaction Systems



C_i are the entities provided by the biological external context:

Reaction Systems



always are applied
(when possible)
all together

$$(\{cya\}, \{...\}, \{cAMP\})$$
$$(\{crp\}, \{...\}, \{CAP\})$$
$$(\{cAMP, CAP\}, \{glucose\}, \{cAMP\text{-}CAP\})$$

The *chained* link-calculus

Is a version of the link-calculus where prefixes are link chains.

syntax $P, Q ::= \sum_{i \in I} v_i.P_i \mid P|Q \mid (\nu\, a)P \mid P[\phi] \mid A$

link chain prefix $v = \ell_1 ... \ell_n$

relevant semantic rule $$\frac{v \bowtie v_j}{\sum_{i \in I} v_i.P_i \xrightarrow{v} P_j} \; (Sum)$$

The enconding

(Sketch of the idea)

assuming a rs with only 2 reactions, and 5 entities:

reaction 1 $(\{cya\}, \{...\}, \{cAMP\})$

reaction 2 $(\{cAMP, CAP\}, \{glucose\}, \{cAMP\text{-}CAP\})$

encoding the two reactions

reaction 1 $P_1 \triangleq \tau \backslash^{\Box}_{cya} \backslash^{cya}_{\Box} \backslash^{\Box}_{\widetilde{cAMP}} \backslash^{\widetilde{cAMP}}_{\Box} \backslash_{r_2}.P_1 + \ \ldots$

reaction 2

$$P_2 \triangleq r_2 \backslash^{\Box}_{cAMP_i} \backslash^{cAMP_o}_{\Box} \backslash^{\Box}_{CAP_i} \backslash^{CAP_o}_{\Box} \backslash^{\Box}_{\overline{glucose_i}} \backslash^{\overline{glucose_o}}_{\Box} \backslash^{\Box}_{\widetilde{cAMP\text{-}CAP_i}} \backslash^{cAMP\text{-}CAP_o}_{\Box} \backslash_{\tau}.P_2 + \ \ldots$$

The enconding

(Sketch of the idea)

the link chain prefixes of the two reactions can be linked
(*forming a sort of communication backbone*):

$$\tau \backslash^{\square}_{cya_i} \backslash^{cya_o}_{\square} \backslash^{\square}_{\widetilde{cAMP}_i} \backslash^{\widetilde{cAMP}_o}_{\square} \backslash r_2 \quad r_2 \backslash^{\square}_{cAMP_i} \backslash^{cAMP_o}_{\square} \backslash^{\square}_{CAP_i} \backslash^{CAP_o}_{\square} \backslash^{\square}_{\overline{glucose}_i} \backslash^{\overline{glucose}_o}_{\square} \backslash^{\square}_{\widetilde{cAMP\text{-}CAP}_i} \backslash^{\widetilde{cAMP\text{-}CAP}_o}_{\square} \backslash \tau$$

what is still missing is the contribution of the single entities (molecules)

The enconding

(Sketch of the idea)

$$\tau\backslash^{\square}_{cya_i}\backslash^{cya_o}_{\square}\backslash^{\square}_{\widetilde{cAMP}_i}\backslash^{\widetilde{cAMP}_o}_{\square}\backslash r_2 \quad r_2\backslash^{\square}_{cAMP_i}\backslash^{cAMP_o}_{\square}\backslash^{\square}_{CAP_i}\backslash^{CAP_o}_{\square}\backslash^{\square}_{\overline{glucose}_i}\backslash^{\overline{glucose}_o}_{\square}\backslash^{\square}_{\widetilde{cAMP\text{-}CAP}_i}\backslash^{\widetilde{cAMP\text{-}CAP}_o}_{\square}\backslash\tau$$

$$P_{CAP} \triangleq {}^{CAP_i}\backslash_{CAP_o}.P_{CAP}$$

$$P_{\overline{glucose}} \triangleq {}^{\overline{glucose}_i}\backslash_{\overline{glucose}_o}.P_{\overline{glucose}}$$

$$P_{cya} \triangleq {}^{cya_i}\backslash_{cya_o}.P_{cya}$$

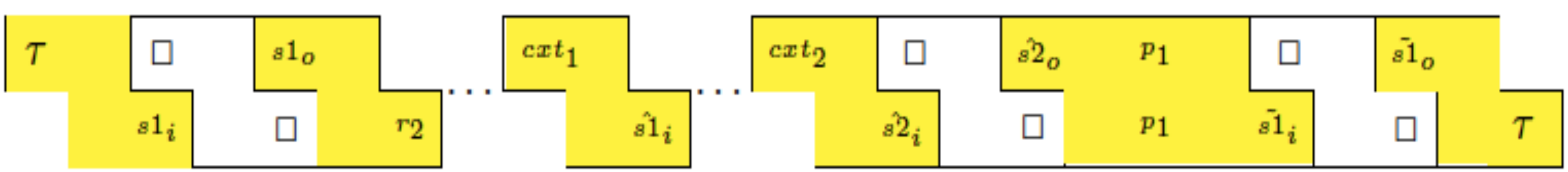
$$P_{cAMP} \triangleq {}^{\widetilde{cAMP}_i}\backslash^{\square}_{\widetilde{cAMP}_o}\backslash^{cAMP_i}_{\square}\backslash_{cAMP_o}.P_{cAMP}$$

$$P_{cAMP\text{-}CAP} \triangleq {}^{\widetilde{cAMP\text{-}CAP}_i}\backslash_{\widetilde{cAMP\text{-}CAP}_o}.P_{cAMP\text{-}CAP}$$

encoding the entities

What we gain:

- a reaction system step corresponds to a single multi-party transition
- programmable contexts
- modeling mutating entities
- communicating reaction systems: the products of a reaction system can be provided as a reagent of a second reaction system;
- modeling style: backbone + resources: the processes encoding the reactions and the context form the backbone; processes encoding entities provide the resources.



Future work

We would like to:

- ✓ optimize implementation ;
- ✓ describe mutating molecules and mutating rules
- ✓ define quantitative extensions of the calculus.

The link-calculus webpage:

- http://linkcalculus.di.unipi.it/

thanks !

questions ?