

# Embedding reaction systems into link-calculus

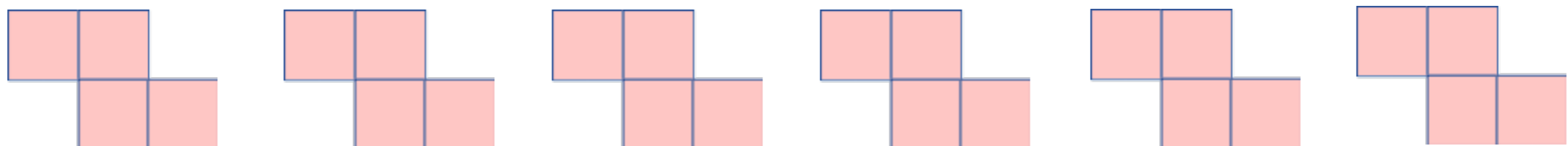
**Linda Brodo (Sassari)**

joint work with

**Roberto Bruni (Pisa)**

**Moreno Falaschi (Siena)**

SECOND INTERNATIONAL WORKSHOP ON REACTION SYSTEMS  
JUNE 5-7, 2019 TORUŃ, POLAND



# Roadmap

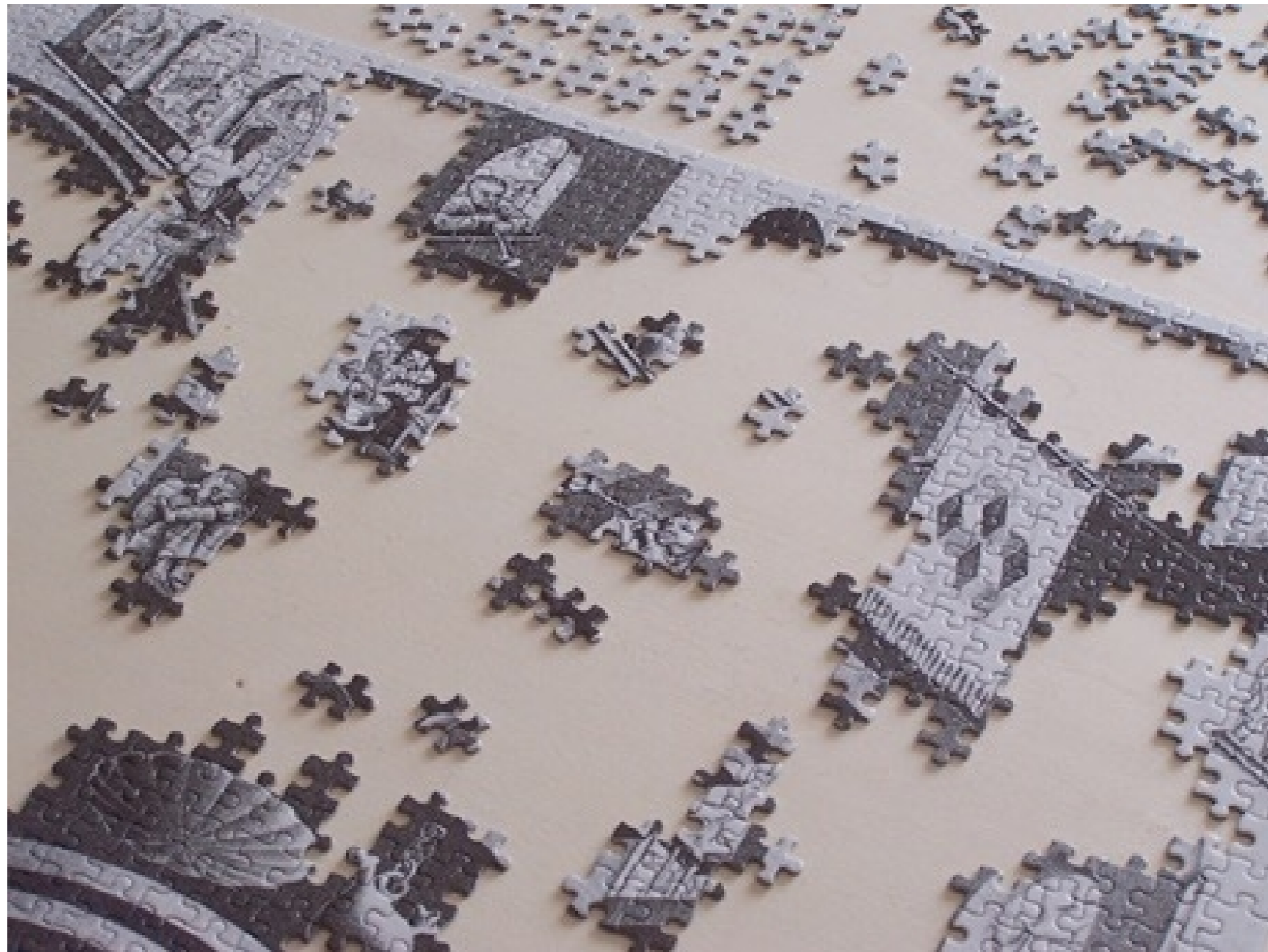
- ✓ **An open multi-party calculus**  
(joint work with Roberto Bruni and Chiara Bodei -Univ. of Pisa-)
- ✓ Encoding reactions
- ✓ Encoding entities
- ✓ Encoding contexts
- ✓ Enhancing expressivity for reaction systems
- ✓ Conclusion and future work

# Interaction

An interaction is an action  
by which  
(communicating) processes  
can influence each other.

# Multiparty interaction

An interaction is multiparty when it involves two or more processes



# Open interaction

An interaction is open when  
the number of involved processes is not fixed



# Notation

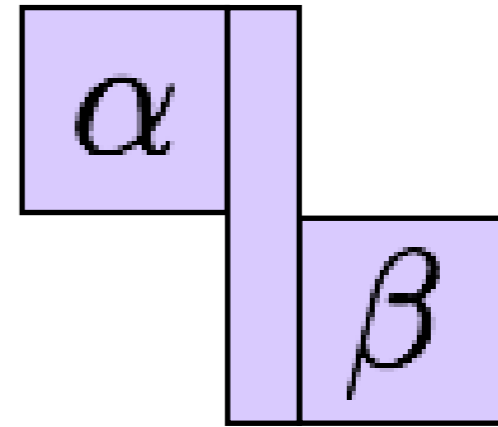
$a$  interaction over a

$\tau$  silent interaction

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

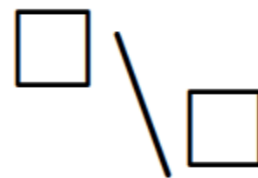
# Link

$\alpha \setminus \beta$  From  $\alpha$  to  $\beta$



Valid:

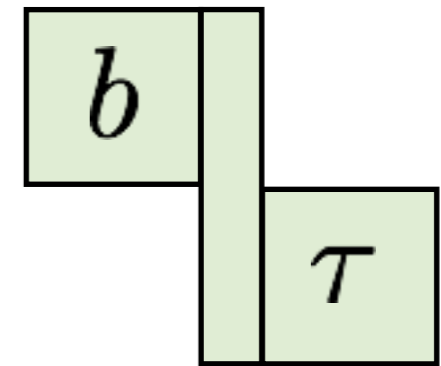
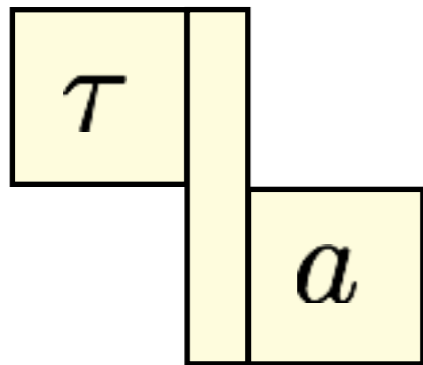
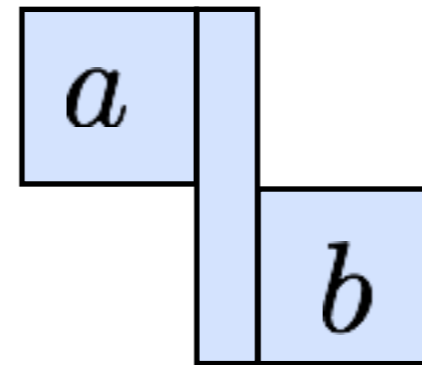
if it is **virtual**



if it is **solid**

$$\alpha, \beta \neq \square$$

# Example: three party





# Link chain

$$\alpha_1 \setminus \beta_1 \quad \alpha_2 \setminus \beta_2 \quad \dots \quad \alpha_n \setminus \beta_n$$

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

such that:

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

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

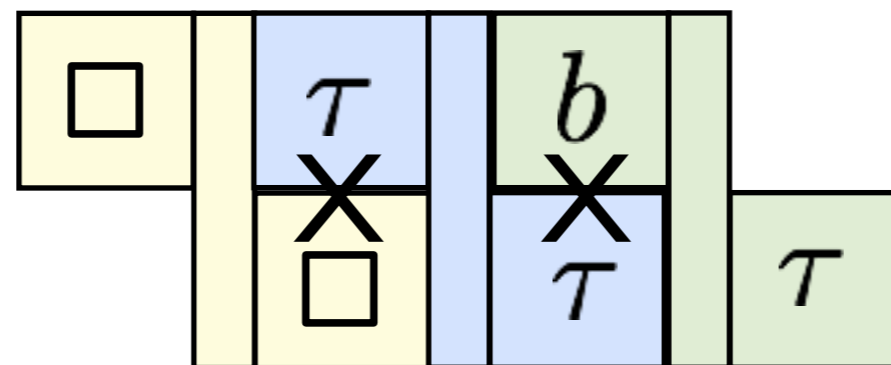
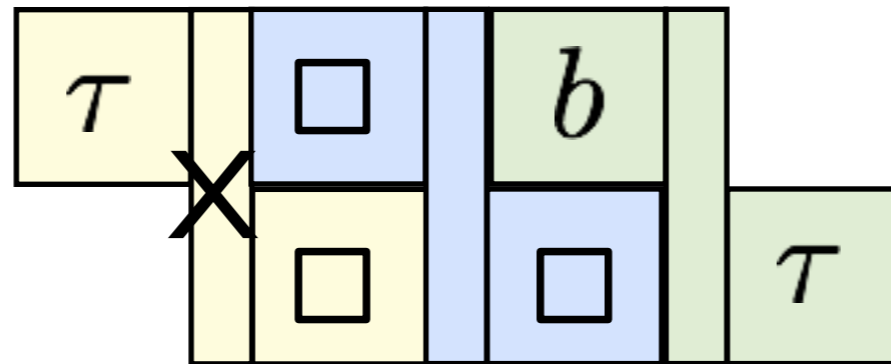
# Link chain: terminology

$$\alpha_1 \setminus \beta_1 \quad \alpha_2 \setminus \beta_2 \quad \dots \quad \alpha_n \setminus \beta_n$$

Solid:

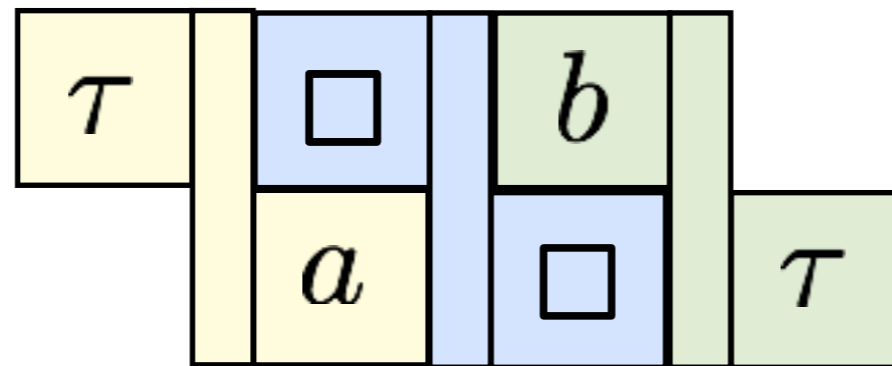
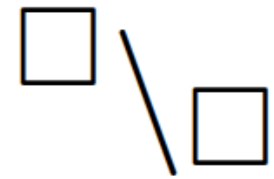
if all its links are so

# Counter-examples

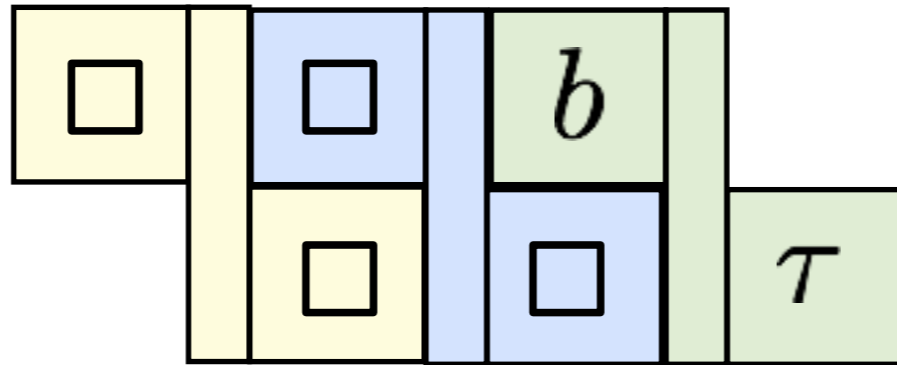
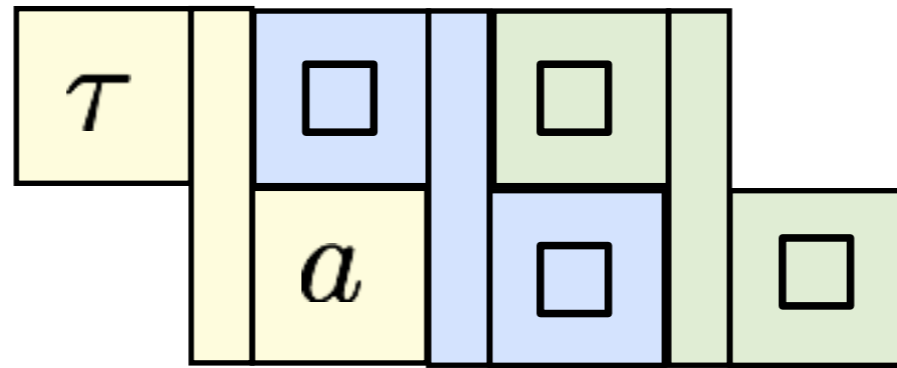


# Examples: non solid

Virtual links  
can be read as missing pieces of the puzzle



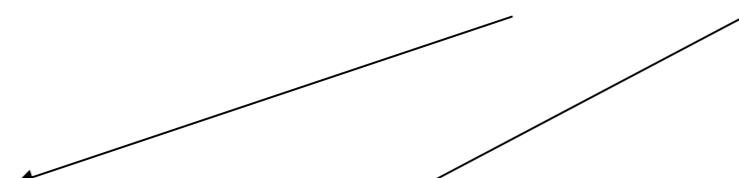
# Examples: merge



# Merge

$$s = l_1 \dots l_n \quad s' = l'_1 \dots l'_n$$

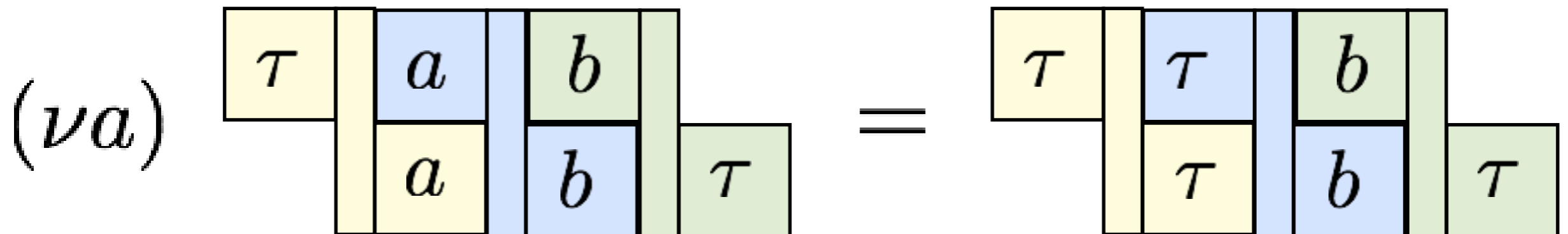
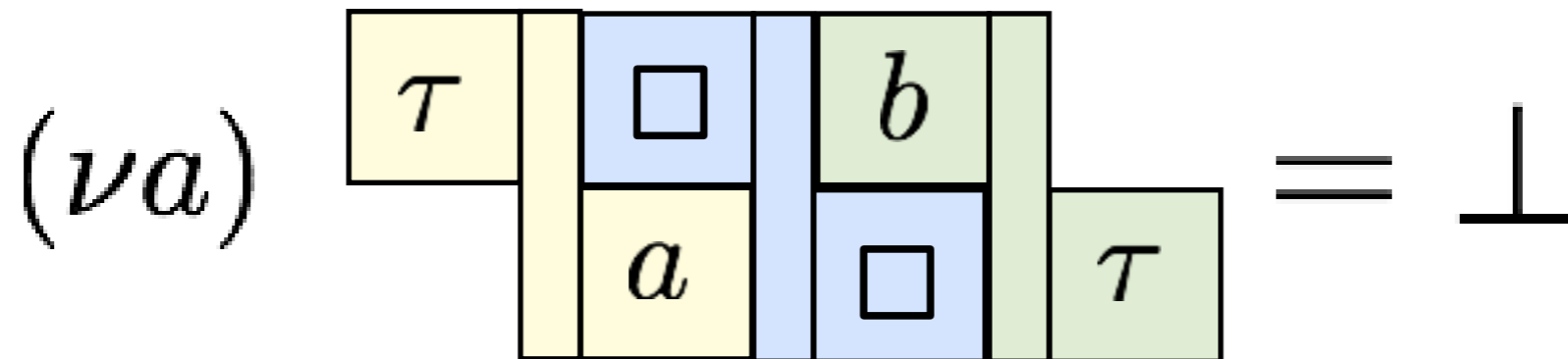
$$s \bullet s' \triangleq (l_1 \bullet l'_1) \dots (l_n \bullet l'_n)$$


$$\alpha \setminus_{\beta} \bullet \alpha' \setminus_{\beta'} \triangleq (\alpha \bullet \alpha') \setminus_{(\beta \bullet \beta')}$$

$$\alpha \bullet \beta \triangleq \begin{cases} \alpha & \text{if } \beta = \square \\ \beta & \text{if } \alpha = \square \end{cases}$$

The result is undefined if the outcome is not valid

# Examples: restriction



# Restriction

$$(\nu a)s \triangleq \begin{cases} ((\nu a)\ell_1) \dots ((\nu a)\ell_n) & \text{if } a \text{ is } \textit{matched} \text{ in } s \\ \perp & \text{otherwise} \end{cases}$$

$$(\nu a)^\alpha \setminus \beta \triangleq ((\nu a)\alpha) \setminus ((\nu a)\beta)$$

$$(\nu a)\alpha \triangleq \begin{cases} \tau & \text{if } \alpha = a \\ \alpha & \text{otherwise} \end{cases}$$



# Equivalence relation over link chains (the black tie)

$$s \square \backslash \square \quad \blacktriangleright \quad s$$

$$s_1 \square \backslash \square \backslash \square s_2 \quad \blacktriangleright \quad s_1 \square \backslash \square s_2$$

$$\square \backslash \square s \quad \blacktriangleright \quad s$$

$$s_1^\alpha \backslash a \backslash \beta s_2 \quad \blacktriangleright \quad s_1^\alpha \backslash \square \backslash a \backslash \beta s_2$$

# link-calculus syntax

$$P, Q ::= 0 \mid l.P \mid P + Q \mid P|Q \mid (\nu a)P \mid P[\phi] \mid A$$

null action

choice

restriction

recursion

prefix  
(link prefix)

parallel

relabelling

very closed to the CCS syntax

# (Relevant) SOS rules

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

$$\frac{s \bowtie \ell}{\ell.P \xrightarrow{s} P} \text{ (Act)}$$

$$\frac{P \xrightarrow{s} P'}{(\nu a)P \xrightarrow{(\nu a)s} (\nu a)P'} \text{ (Res)}$$

$$\frac{P \xrightarrow{s} P'}{P|Q \xrightarrow{s} P'|Q} \text{ (Lpar)}$$

$$\frac{P \xrightarrow{s} P' \quad Q \xrightarrow{s'} Q'}{P|Q \xrightarrow{s \bullet s'} P'|Q'} \text{ (Com)}$$

# Example

$$P \triangleq \tau \backslash_a . P_1 \mid (\nu b) Q, \quad Q \triangleq b \backslash_\tau . P_2 \mid a \backslash_b . \mathbf{0}$$

$$\frac{}{b \backslash_\tau . P_2 \xrightarrow{\square \backslash_\square \backslash_b \backslash_\tau} P_2} \text{ (Act)} \quad \frac{}{a \backslash_b . \mathbf{0} \xrightarrow{\square \backslash_\square \backslash_a \backslash_b \backslash_\square} \mathbf{0}} \text{ (Act)}$$


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$$\text{ (Com)}$$

$$\frac{}{\tau \backslash_a . P_1 \xrightarrow{\tau \backslash_\square \backslash_a \backslash_\square \backslash_\square} P_1} \text{ (Act)} \quad \frac{Q \xrightarrow{\square \backslash_\square \backslash_a \backslash_b \backslash_\tau} P_2 \mid \mathbf{0}}{(\nu b) Q \xrightarrow{\square \backslash_\square \backslash_a \backslash_\tau \backslash_\tau} (\nu b) (P_2 \mid \mathbf{0})} \text{ (Res)}$$


---


$$\text{ (Com)}$$

$$P \xrightarrow{\tau \backslash_\square \backslash_a \backslash_\tau \backslash_\tau} P_1 \mid (\nu b) (P_2 \mid \mathbf{0})$$

# Bibliography

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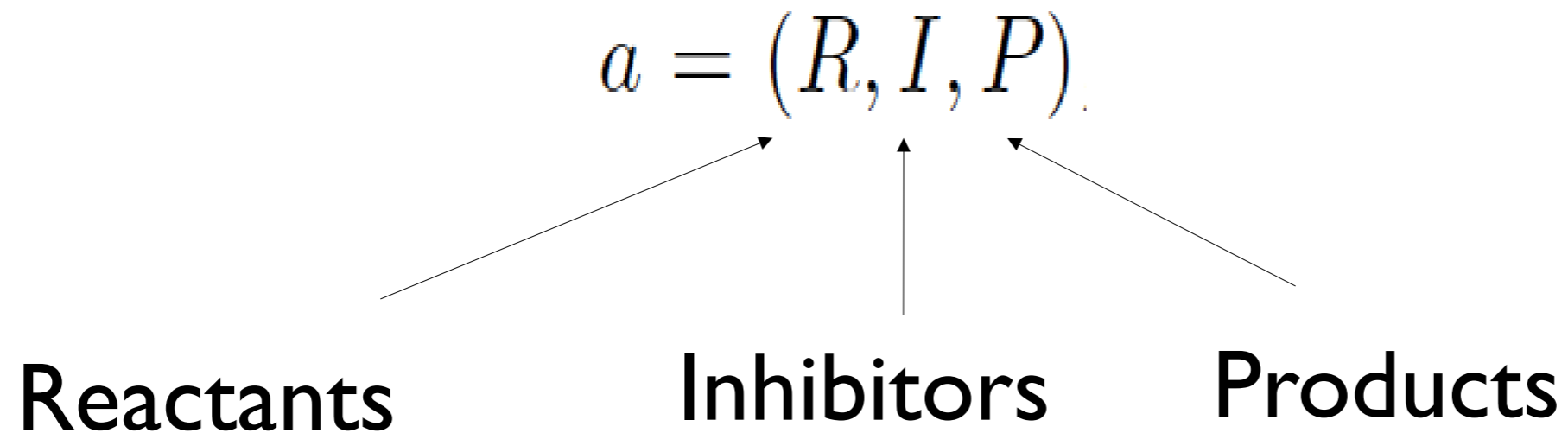
The link-calculus homepage:  
<http://linkcalculus.di.unipi.it>

# Roadmap

- ✓ An open multi-party calculus
- ✓ Encoding reaction systems
- ✓ Encoding entities
- ✓ Encoding contexts
- ✓ Enhancing expressivity for reaction systems
- ✓ Conclusion and future work

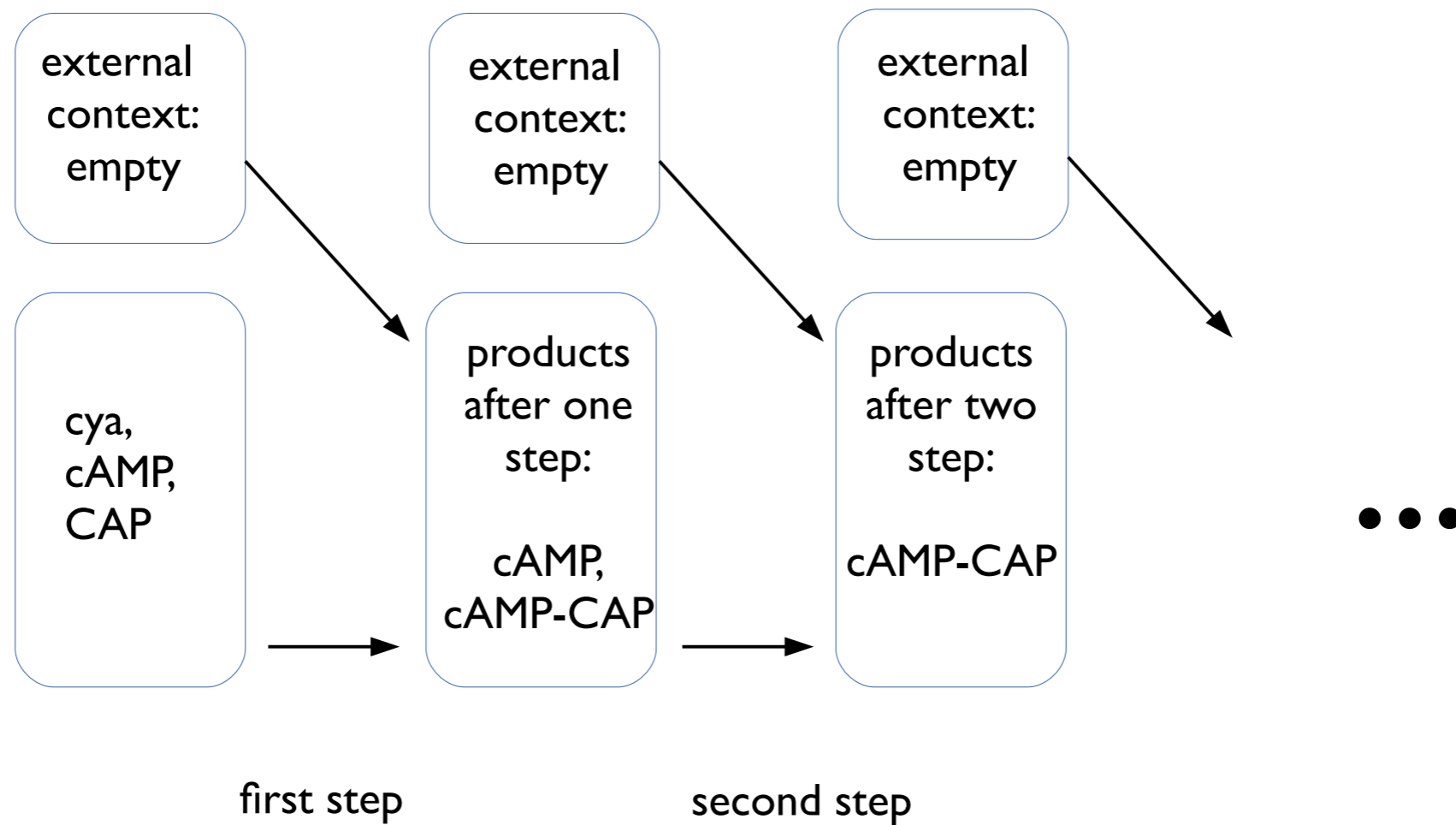
# Reaction Systems

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



$(\{cAMP, CAP\}, \{glucose\}, \{cAMP-CAP\})$

# Reaction Systems



always are applied  
(when possible)  
all together

$(\{cya\}, \{\dots\}, \{cAMP\})$

$(\{cAMP, CAP\}, \{glucose\}, \{cAMP-CAP\})$



# 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  $v = \ell_1 \dots \ell_n$

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

# Encoding reaction systems:

usage of the names

entities assume different behaviours:

reaction  
systems

a

present

acting as reagent or inhibitor

a

absent

a

products

link-  
calculus

a

$\bar{a}$

$\tilde{a}$

# Encoding reactions

(when applicable)

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

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

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

encoding the two reactions as link-calculus processes

reaction 1  $P_1 \triangleq \tau \backslash_{cya_i} \square \backslash_{cya_o} \square \backslash_{cAMP_i} \widetilde{cAMP}_o \backslash_{r_2} \cdot P_1 + \dots$

reaction 2

$P_2 \triangleq r_2 \backslash_{cAMP_i} \square \backslash_{cAMP_o} \square \backslash_{CAP_i} \square \backslash_{CAP_o} \square \backslash_{glucose_i} \overline{glucose}_o \backslash_{cAMP-CAP_i} \widetilde{cAMP-CAP}_o \backslash_{\tau} \cdot P_2$   
 $+ \dots$

# Encoding reactions

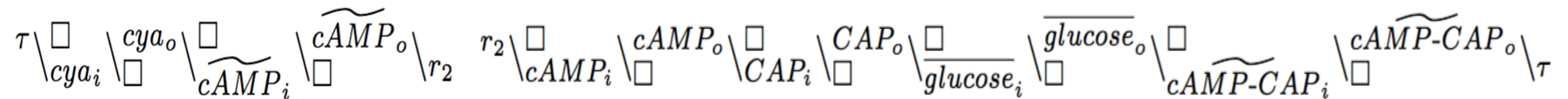
when the reaction is not applicable, we still execute the process encoding the reaction

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

$$\begin{aligned} P_2 &\triangleq \dots + \\ &r_2 \left[ \frac{\square}{glucose_i} \right] \left[ \frac{glucose_o}{\square} \right] \tau.P_2 \\ &+ \\ &r_2 \left[ \frac{\square}{cAMP_i} \right] \left[ \frac{\overline{cAMP}_o}{\square} \right] \tau.P_2 \\ &+ \\ &r_2 \left[ \frac{\square}{CAP_i} \right] \left[ \frac{\overline{CAP}_o}{\square} \right] \tau.P_2 \end{aligned}$$

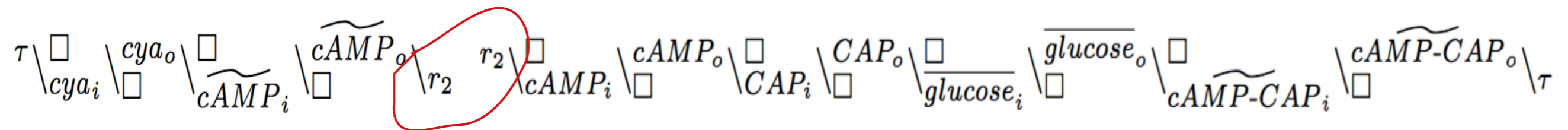
# Encoding reactions

the link chain prefixes of the two reactions can be linked



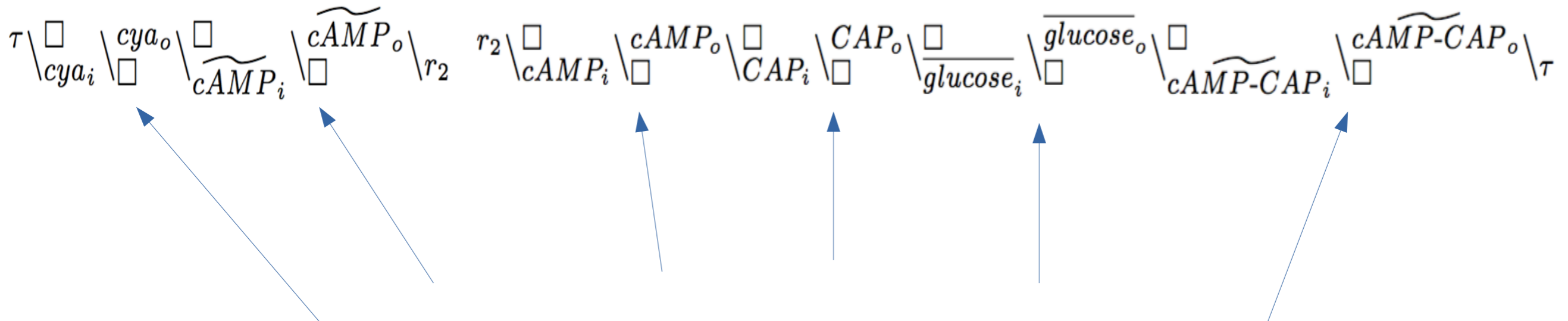
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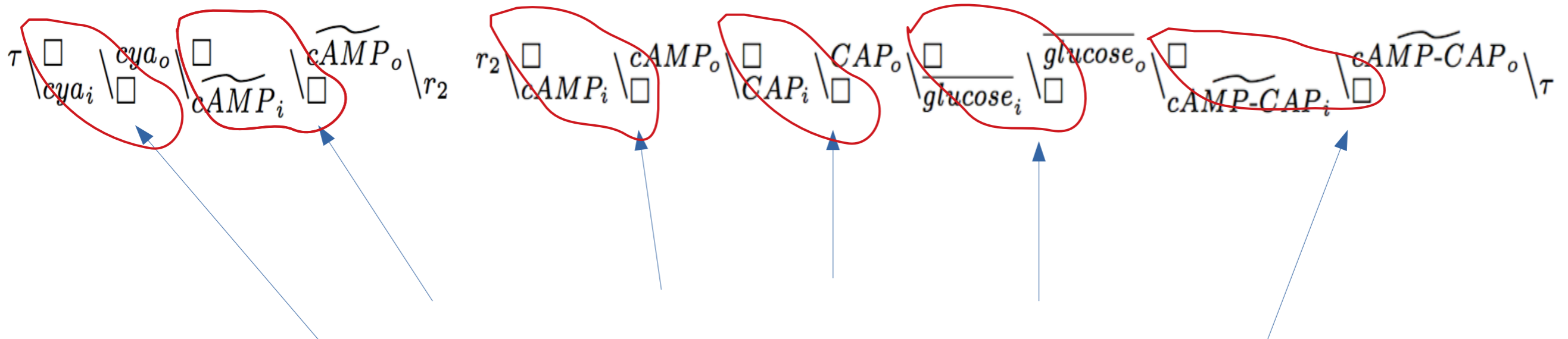
the link chain prefixes of the two reactions can be linked  
(forming a sort of communication backbone):



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

# Encoding reactions

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# Enconding entities

When the entity is present or produced

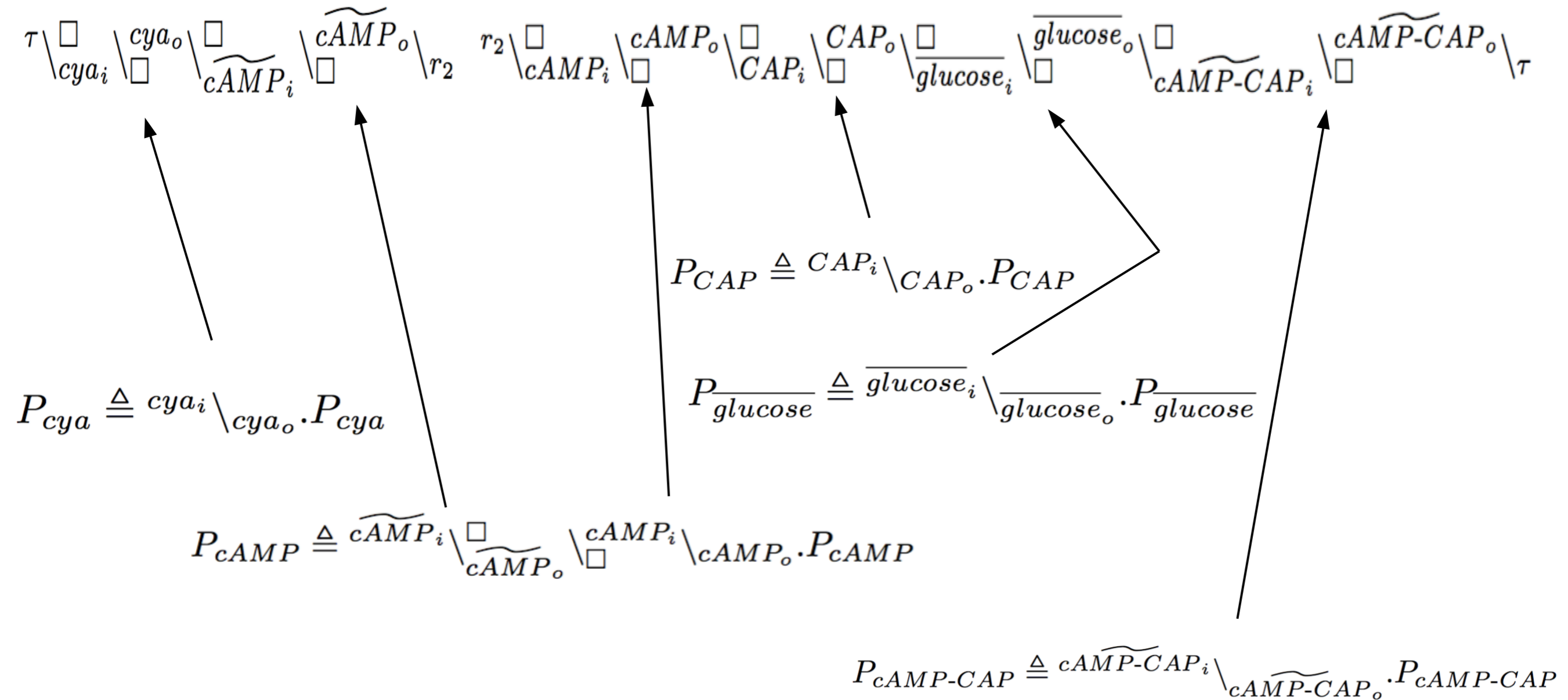
$$P_{cya} \triangleq \sum_{h,k \geq 0} (cya_i \setminus \square_{cya_o} \setminus \square)^h (c\tilde{y}a_i \setminus \square_{c\tilde{y}a_o} \setminus \square)^k \cdot P_{cya} \\ + \\ \sum_{h \geq 0} (cya_i \setminus \square_{cya_o} \setminus \square)^h \cdot \overline{P_{cya}}$$

# Enconding entities

When the entity is absent or produced

$$\begin{aligned} \overline{P_{cya}} &\triangleq \sum_{h,k \geq 0} (\overline{cya}_i \setminus \frac{\square}{cya}_o \setminus \square)^h (c\tilde{y}a_i \setminus \frac{\square}{c\tilde{y}a}_o \setminus \square)^k \cdot P_{cya} \\ &+ \\ &\sum_{h \geq 0} (\overline{cya}_i \setminus \frac{\square}{cya}_o \setminus \square)^h \cdot \overline{P_{cya}} \end{aligned}$$

# The encoding: reactions + entities



encoding the entities

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# Encoding reaction systems:

(more) usage of the names

entities assume different roles:

reaction  
systems

link-  
calculus

...

a provided by the context  $\hat{a}$

a not provided by the context  $\underline{a}$   
(absence)

# Adding contexts

how a context behaves

$$Cxt_{cya}^n \triangleq \left\{ \begin{array}{l} cxt_j \sqcap_{\hat{c}y a_i} \sqcap_{c\hat{y} a_o} cxt_{j+1} \cdot Cxt_{cya}^{n+1} \\ cxt_j \sqcap_{\underline{c}y a_i} \sqcap_{\underline{c}y a_o} cxt_{j+1} \cdot Cxt_{cya}^{n+1} \end{array} \right.$$

$$Cxt_{cya} \triangleq Cxt_{cya}^1$$

# Make contexts synchronise with entities

$$\begin{aligned}
 P_{cya} &\triangleq \sum_{h,k \geq 0} (cya_i \sqcup_{cya_o} \sqcup) ^h \hat{c}y a_i \sqcup_{\hat{c}y a_o} \sqcup (c\tilde{y} a_i \sqcup_{c\tilde{y} a_o} \sqcup) ^k \cdot P_{cya} \\
 &+ \\
 &\sum_{h \geq 0, k \geq 1} (cya_i \sqcup_{cya_o} \sqcup) ^h \underline{c}y a_i \sqcup_{\underline{c}y a_o} \sqcup (c\tilde{y} a_i \sqcup_{c\tilde{y} a_o} \sqcup) ^k \cdot P_{cya} \\
 &+ \\
 &\sum_{h \geq 0} (cya_i \sqcup_{cya_o} \sqcup) ^h \underline{c}y a_i \sqcup_{\underline{c}y a_o} \cdot \overline{P_{cya}}
 \end{aligned}$$



# Make contexts synchronise with reactions

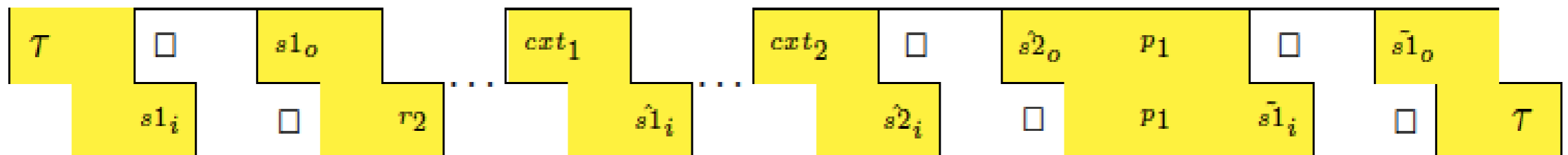
$$\begin{aligned} P_2 &\triangleq \dots + \\ & r_2 \left[ \frac{\square}{glucose_i} \right] \left[ \frac{glucose_o}{\square} \right]_{\tau} \cdot P_2 \\ & + \\ & r_2 \left[ \frac{\square}{cAMP_i} \right] \left[ \frac{\overline{cAMP}_o}{\square} \right]_{\tau} \cdot P_2 \\ & + \\ & r_2 \left[ \frac{\square}{CAP_i} \right] \left[ \frac{\overline{CAP}_o}{\square} \right]_{\tau} \cdot P_2 \end{aligned}$$

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# What we gain:

- ✓ recursive contexts
- ✓ modeling mutating entities
- ✓ **communicating reaction systems:** for example, the lac operon system (that depends on the presence or absence of the glucose) can be connected with the system producing the glucose.
- ✓ **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:

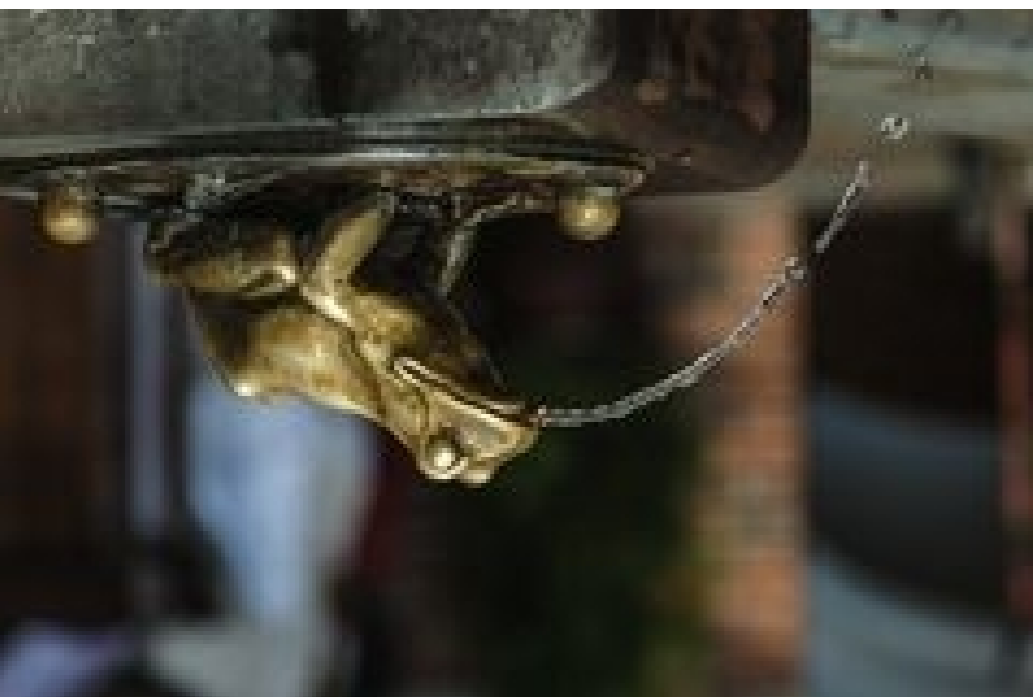
- ✓ model two communicating reaction systems;
- ✓ model a reaction system with mutating entities;
- ✓ exploit the nature of process algebra to define properties of reaction systems;
- ✓ ...

✓



**THANKS FOR YOUR  
ATTENTION!**

**questions ?... any suggestion ?**





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