

# Embedding reaction systems into link-calculus

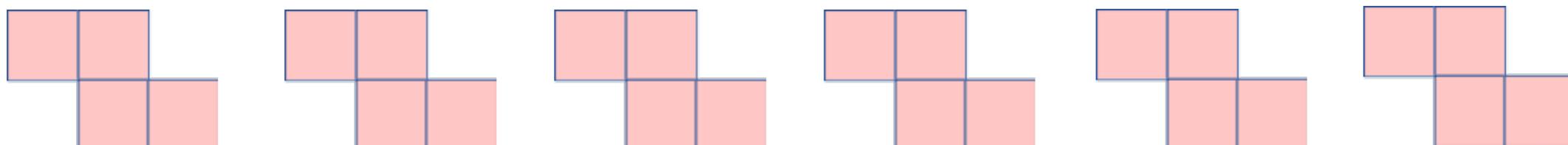
Linda Brodo (Sassari)

joint work with

Roberto Bruni (Pisa)

Moreno Falaschi (Siena)

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



# Roadmap

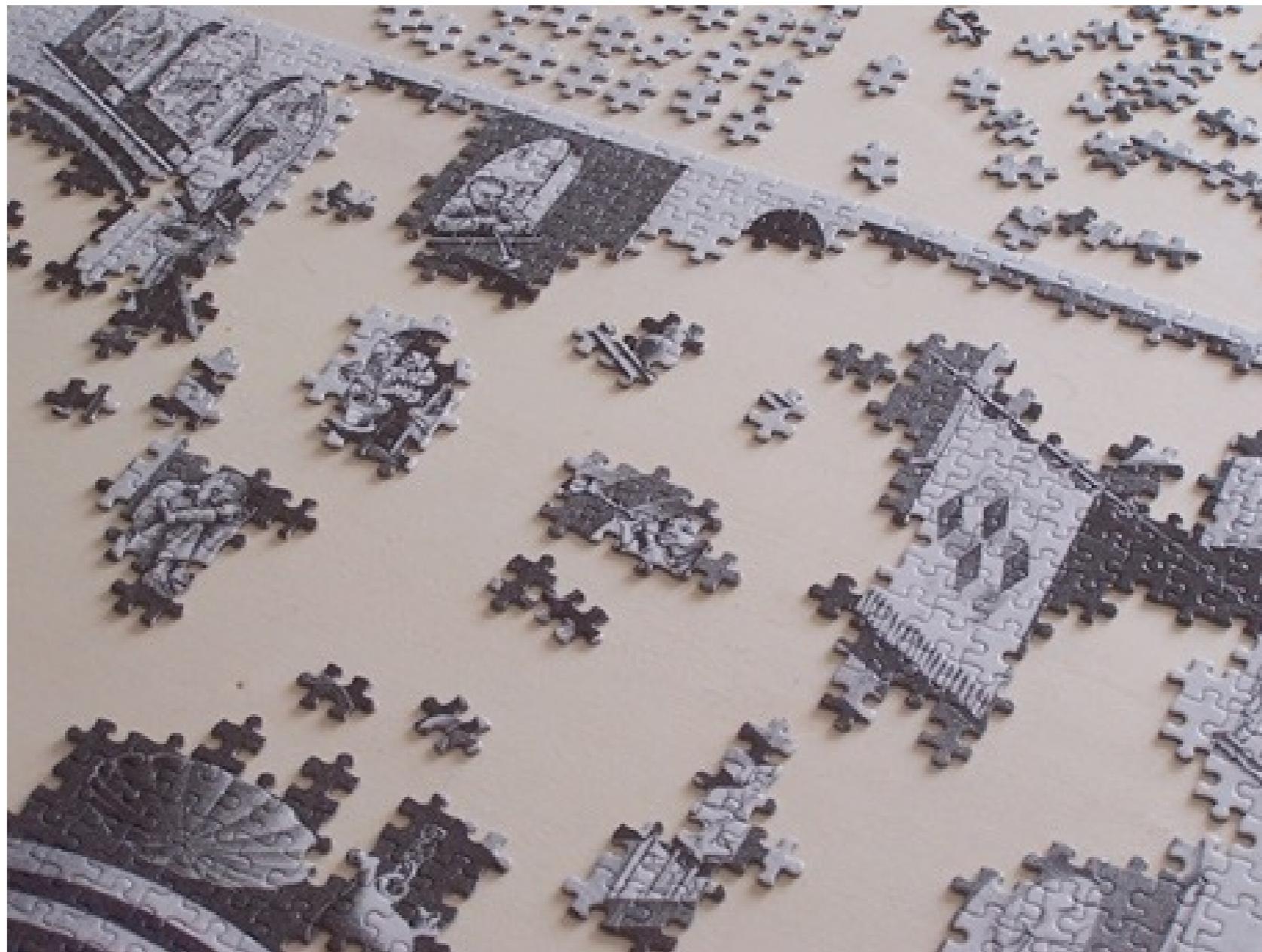
- ✓ **An open multi-party calculus**  
(joint work with Roberto Bruni and Chiara Bodei -Univ. of Pisa-)
- ✓ Encoding reactions
- ✓ Encoding entities
- ✓ Encoding contexts
- ✓ Enhancing expressivity for reaction systems
- ✓ Conclusion and future work

# Interaction

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

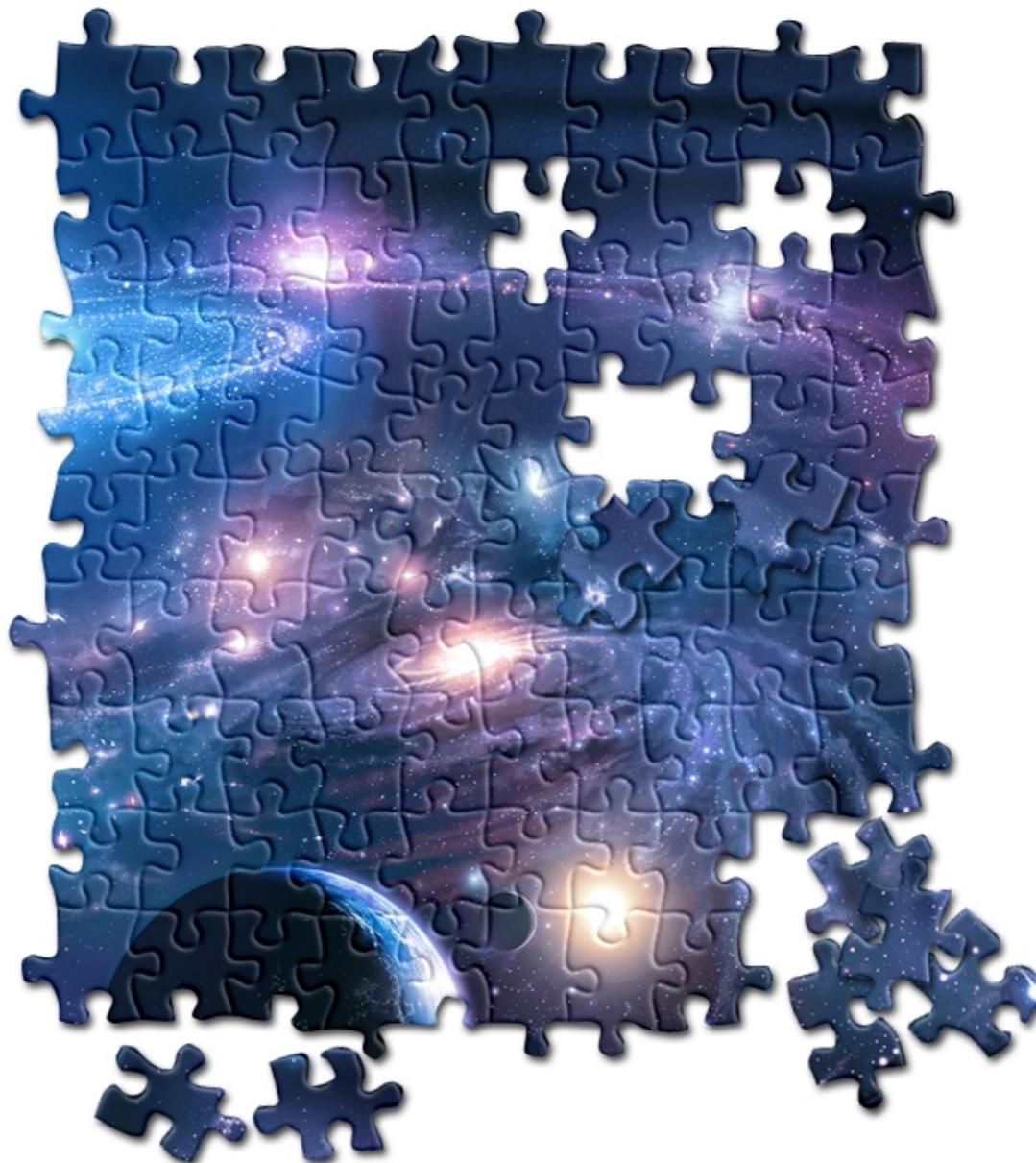
# Multiparty interaction

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

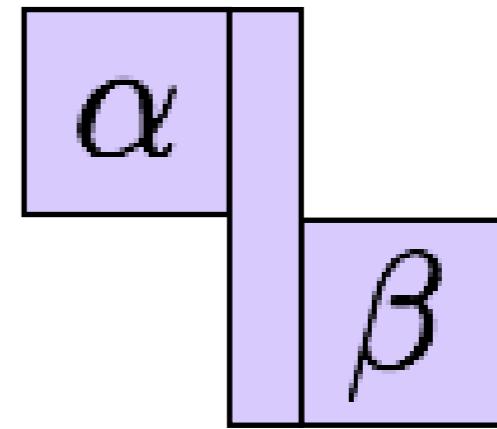
$\square$

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

# Link

$\alpha \setminus \beta$

From  $\alpha$  to  $\beta$



Valid:

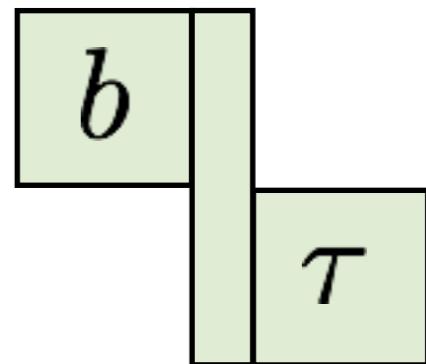
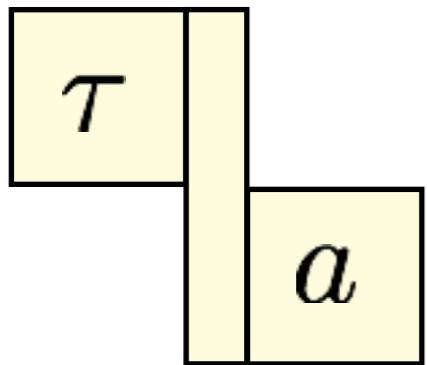
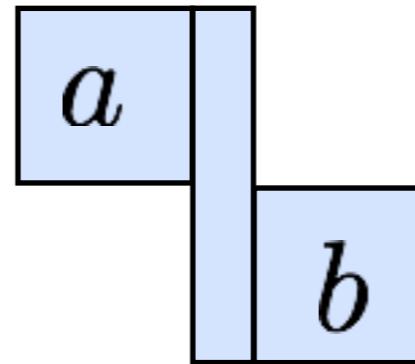
if it is **virtual**

$\square \setminus \square$

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:

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

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

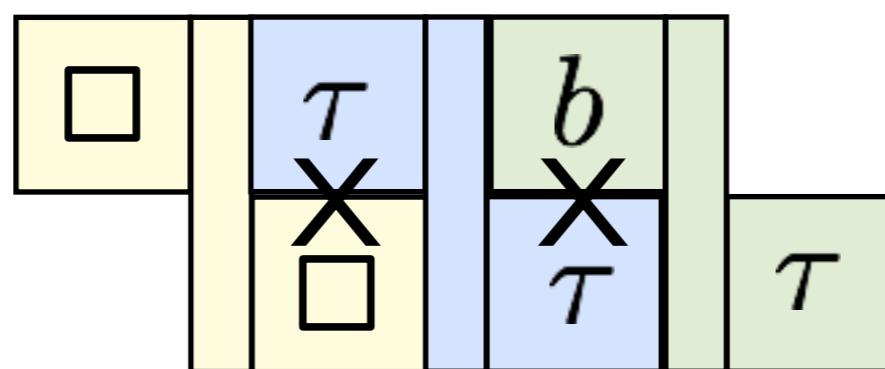
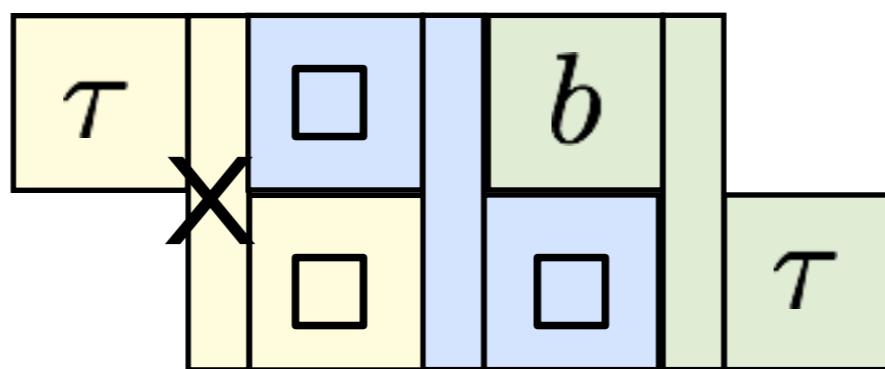
# Link chain: terminology

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

Solid:

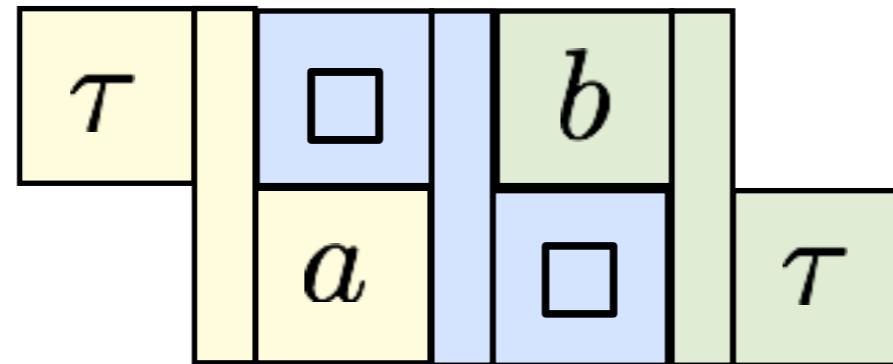
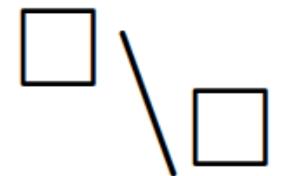
if all its links are so

# Counter-examples

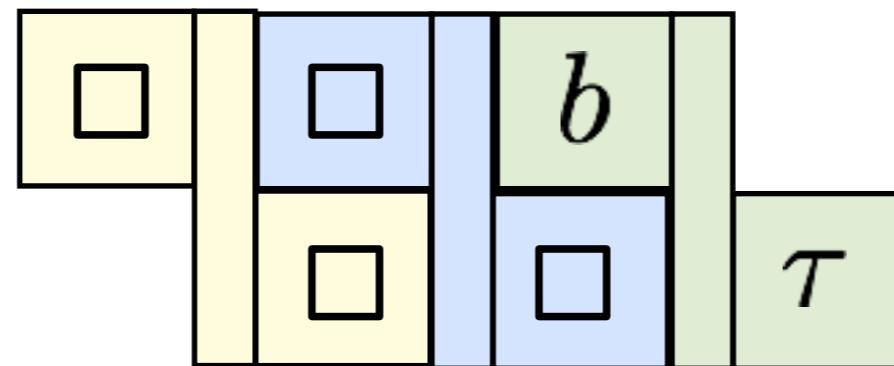
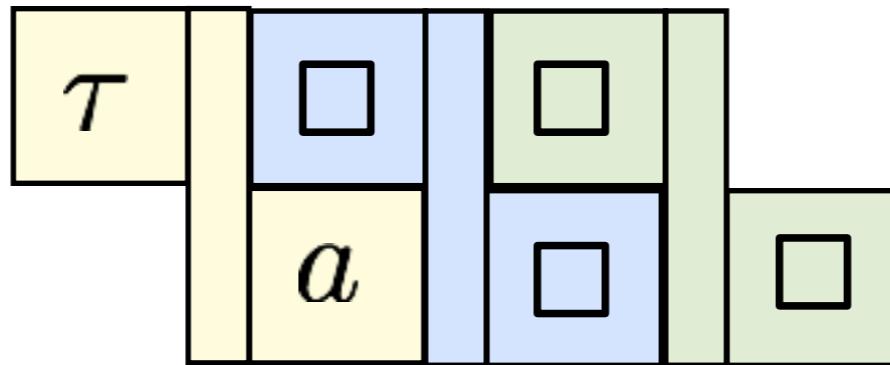


# Examples: non solid

Virtual links  
can be read as missing pieces of the puzzle



# Examples: merge



# Merge

$$s = \ell_1 \dots \ell_n$$

$$s' = \ell'_1 \dots \ell'_n$$

$$s \bullet s' \triangleq (\ell_1 \bullet \ell'_1) \dots (\ell_n \bullet \ell'_n)$$

$$\alpha \setminus \beta \bullet \alpha' \setminus \beta' \triangleq (\alpha \bullet \alpha') \setminus (\beta \bullet \beta')$$

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

The result is undefined if the outcome is not valid

# Examples: restriction

$$(\nu a) \quad \begin{array}{c} \text{---} \\ | \\ \tau \quad | \quad \square \quad | \quad b \\ | \quad | \\ a \quad \square \end{array} \quad = \quad \perp$$

$$(\nu a) \quad \begin{array}{c} \text{---} \\ | \\ \tau \quad | \quad a \quad | \quad b \\ | \quad | \\ a \quad b \end{array} \quad = \quad \begin{array}{c} \text{---} \\ | \\ \tau \quad | \quad \tau \quad | \quad b \\ | \quad | \\ \tau \quad b \end{array} \quad \tau$$

# 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)

$$s^{\square} \setminus \square \quad \blacktriangleright \quad s$$

$$\square \setminus \square s \quad \blacktriangleright \quad s$$

$$s_1^{\square} \setminus \square \setminus \square s_2 \quad \blacktriangleright \quad s_1^{\square} \setminus \square s_2$$

$$s_1^{\alpha} \setminus_a \setminus_{\beta} s_2 \quad \blacktriangleright \quad s_1^{\alpha} \setminus_a \setminus_{\square}^a \setminus_{\beta} s_2$$

# link-calculus syntax

$P, Q ::= 0 \mid \ell.P \mid P + Q \mid P Q \mid (\nu a)P \mid P[\phi] \mid A$			
null action	choice	restriction	recursion
prefix <b>(link prefix)</b>	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

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

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

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

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

# Example

$$P \triangleq \tau \setminus_a P_1 | (\nu b) Q, Q \triangleq b \setminus_\tau P_2 | a \setminus_b \mathbf{0}$$

$$\frac{\text{---} \quad \text{---}}{b \setminus_\tau P_2 \xrightarrow{\square \setminus \square \setminus^b \square \setminus_\tau} P_2} \begin{array}{c} (Act) \\ \xrightarrow{\square \setminus \square \setminus^b \square \setminus_\tau} \end{array} \quad \frac{\text{---} \quad \text{---}}{a \setminus_b \mathbf{0} \xrightarrow{\square \setminus \square \setminus^a \square \setminus_\square} \mathbf{0}} \begin{array}{c} (Act) \\ \xrightarrow{\square \setminus \square \setminus^a \square \setminus_\square} \end{array}$$


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$$\frac{\text{---} \quad \text{---}}{\tau \setminus_a P_1 \xrightarrow{\tau \setminus \square \setminus \square \setminus_\square} P_1} \begin{array}{c} (Act) \\ \xrightarrow{\tau \setminus \square \setminus \square \setminus_\square} \end{array} \quad \frac{Q \xrightarrow{\square \setminus \square \setminus^a \square \setminus^b \square \setminus_\tau} P_2 | \mathbf{0} \quad \text{---} \quad \text{---}}{(\nu b) Q \xrightarrow{\square \setminus \square \setminus^a \square \setminus_\tau} (\nu b)(P_2 | \mathbf{0})} \begin{array}{c} (Res) \\ \xrightarrow{\square \setminus \square \setminus^a \square \setminus_\tau} \end{array}$$


---


$$P \xrightarrow{\tau \setminus_a \square \setminus_\tau} P_1 | (\nu b)(P_2 | \mathbf{0})$$

# Bibliography

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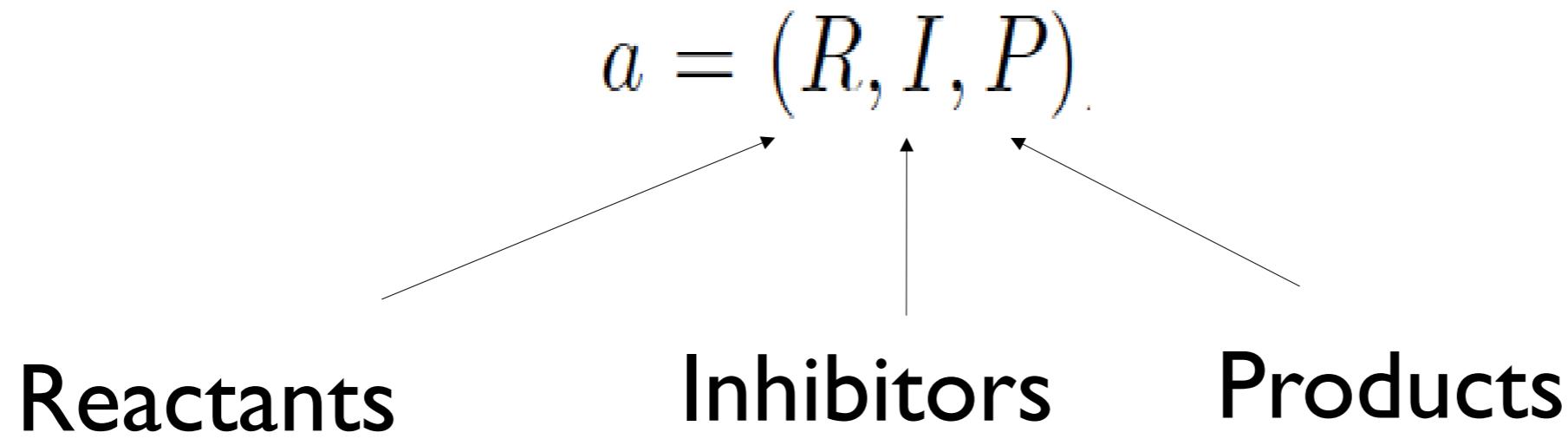
The link-calculus homepage:  
<http://linkcalculus.di.unipi.it>

# Roadmap

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

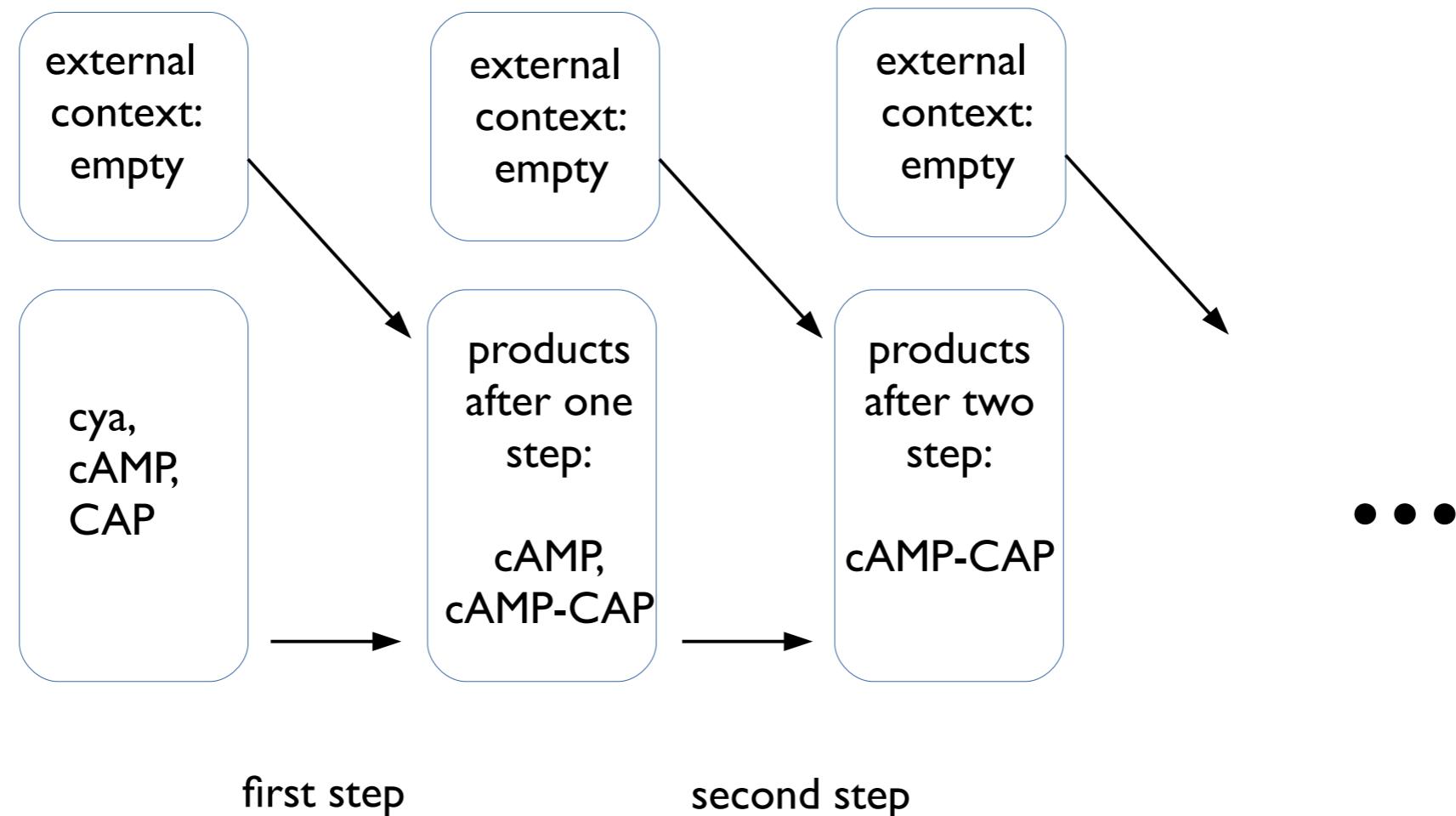
# Reaction Systems

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

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

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

# 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

$$\frac{v \blacktriangleright\!\!> v_j}{\sum_{i \in I} v_i.P_i \xrightarrow{v} P_j} \text{ (Sum)}$$

# 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

— 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  $P_1 \triangleq \tau \setminus_{cya_i} \setminus_{\square}^{cya_o} \setminus_{\square}^{cAMP_i} \setminus_{\square}^{\widetilde{cAMP}_o} \setminus_{r_2} P_1 + \dots$

reaction 2

$$P_2 \triangleq r_2 \setminus_{cAMP_i} \setminus_{\square}^{cAMP_o} \setminus_{CAP_i} \setminus_{\square}^{CAP_o} \setminus_{\square}^{\overline{glucose}_i} \setminus_{\square}^{\overline{glucose}_o} \setminus_{\square}^{cAMP-CAP_i} \setminus_{\square}^{\widetilde{cAMP-CAP}_o} \setminus_{\tau} P_2 + \dots$$

# Encoding reactions

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

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

$$P_2 \triangleq \dots +$$

$$r_2 \frac{\square}{glucose_i} \frac{glucose_o}{\square} \backslash_{\tau} P_2$$

+

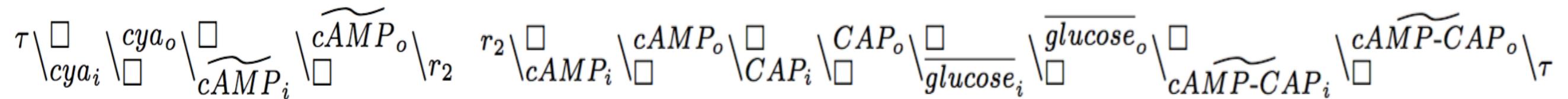
$$r_2 \frac{\square}{\overline{cAMP}_i} \frac{\overline{cAMP}_o}{\square} \backslash_{\tau} P_2$$

+

$$r_2 \frac{\square}{\overline{CAP}_i} \frac{\overline{CAP}_o}{\square} \backslash_{\tau} P_2$$

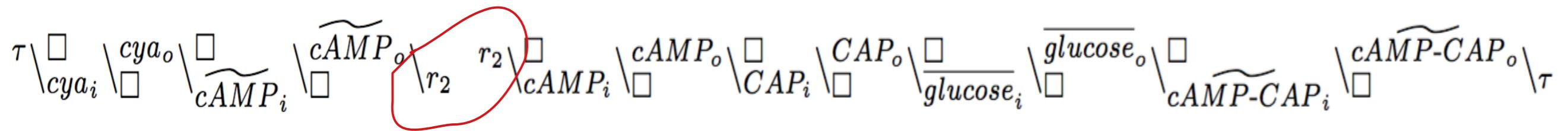
# Encoding reactions

the link chain prefixes of the two reactions can be linked



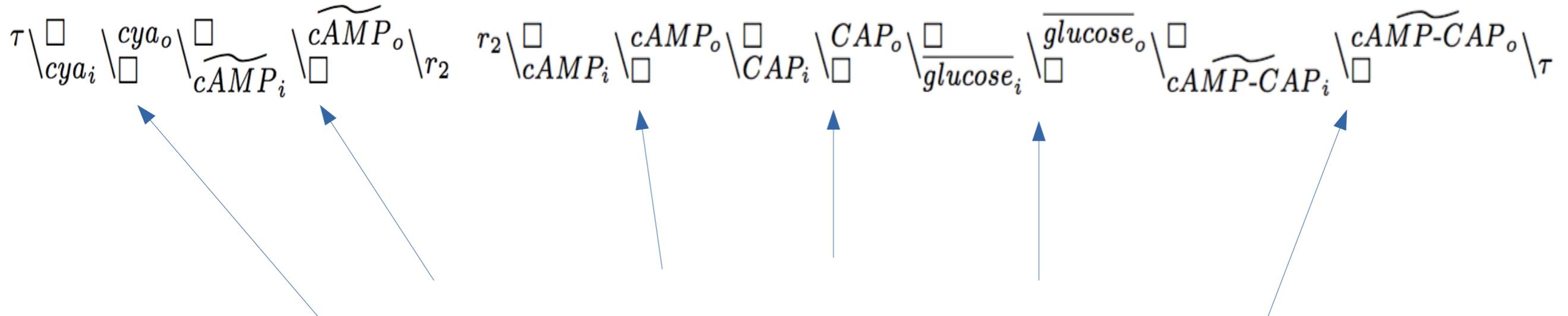
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# Encoding reactions

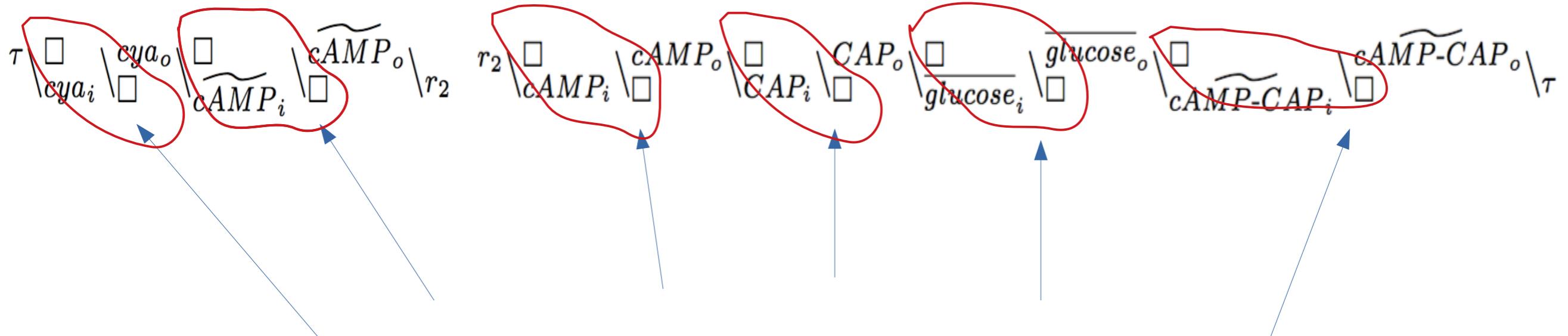
the link chain prefixes of the two reactions can be linked  
(*forming a sort of communication backbone*):



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

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

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# Enconding entities

When the entity is present or produced

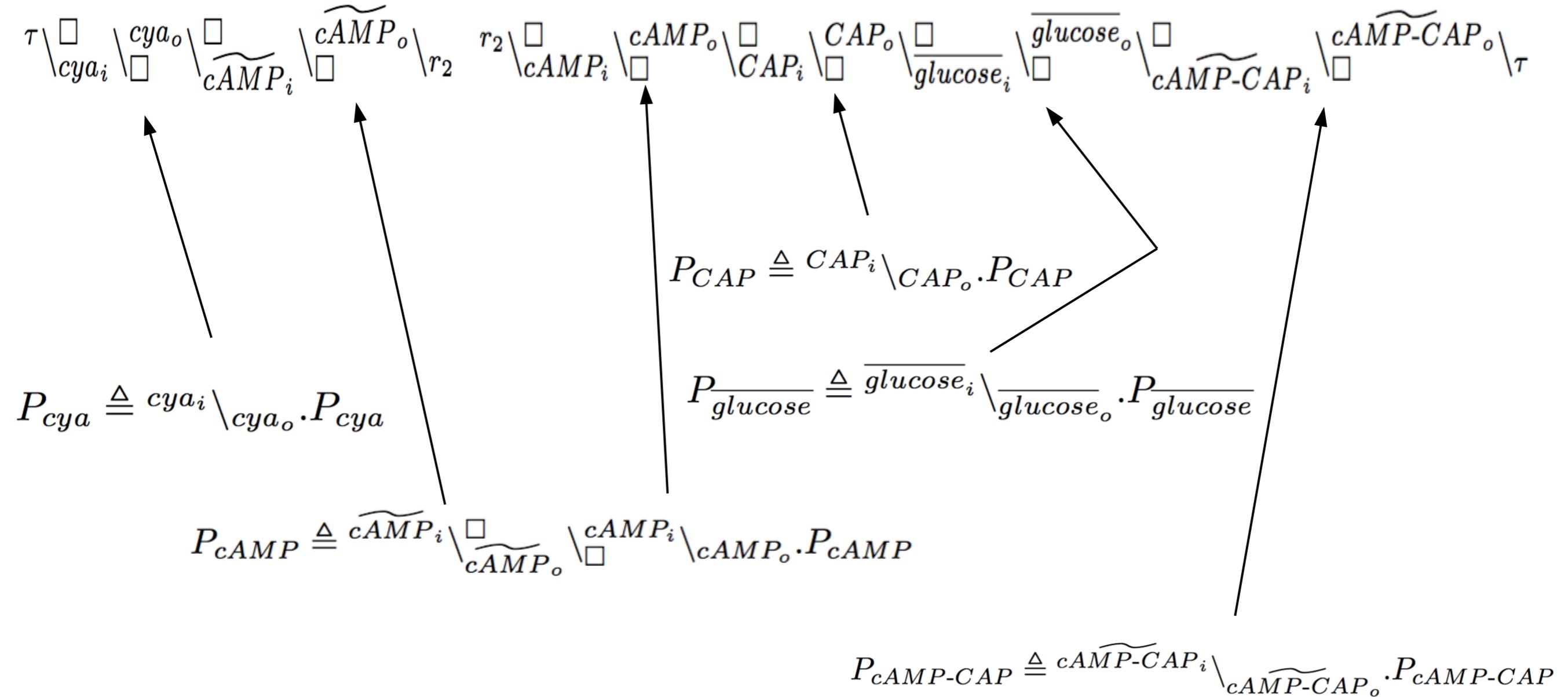
$$\begin{aligned} P_{cya} \triangleq & \sum_{h,k \geq 0} (cya_i \setminus_{cya_o} \square)^h (\tilde{cya}_i \setminus_{\tilde{cya}_o} \square)^k . P_{cya} \\ & + \\ & \sum_{h \geq 0} (cya_i \setminus_{cya_o} \square)^h . \overline{P_{cya}} \end{aligned}$$

# Enconding entities

When the entity is absent or produced

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

# 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

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

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

# Make contexts synchronise with entities

$$\begin{aligned} P_{cya} \triangleq & \sum_{h,k \geq 0} (cya_i \setminus \square_{cya_o} \setminus \square)^h \underbrace{c\hat{y}a_i \setminus \square_{c\hat{y}a_o}}_{c\hat{y}a_i \setminus \underline{cya}_o} \setminus \square (c\tilde{y}a_i \setminus \square_{c\tilde{y}a_o} \setminus \square)^k . P_{cya} \\ & + \\ & \sum_{h \geq 0, k \geq 1} (cya_i \setminus \square_{cya_o} \setminus \square)^h \underbrace{\underline{cya}_i \setminus \square_{\underline{cya}_o}}_{c\hat{y}a_i \setminus \underline{cya}_o} \setminus \square (c\tilde{y}a_i \setminus \square_{c\tilde{y}a_o} \setminus \square)^k . P_{cya} \\ & + \\ & \sum_{h \geq 0} (cya_i \setminus \square_{cya_o} \setminus \square)^h \underbrace{\underline{cya}_i \setminus \underline{cya}_o}_{\overline{P_{cya}}} . \overline{P_{cya}} \end{aligned}$$

# Make contexts synchronise with reactions

$$P_2 \triangleq \dots +$$

$$r_2 \frac{\square}{\cancel{glucose}_i} \frac{\cancel{glucose}_o}{\square} \backslash_{\tau} P_2$$

+

$$r_2 \frac{\square}{\cancel{cAMP}_i} \frac{\cancel{cAMP}_o}{\square} \backslash_{\tau} P_2$$

+

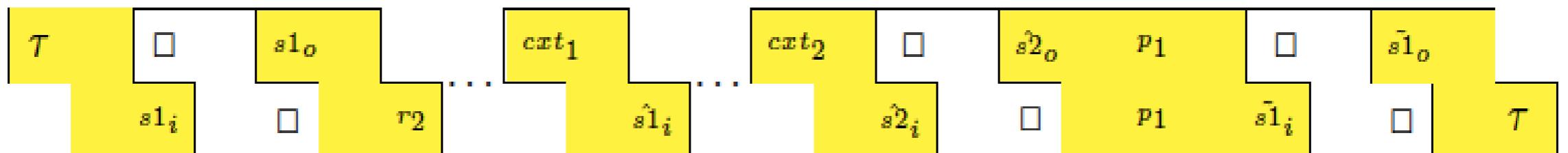
$$r_2 \frac{\square}{\cancel{CAP}_i} \frac{\cancel{CAP}_o}{\square} \backslash_{\tau} cxt_1 \cdot P_2$$

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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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