

# Graph Surfing by Reaction Systems

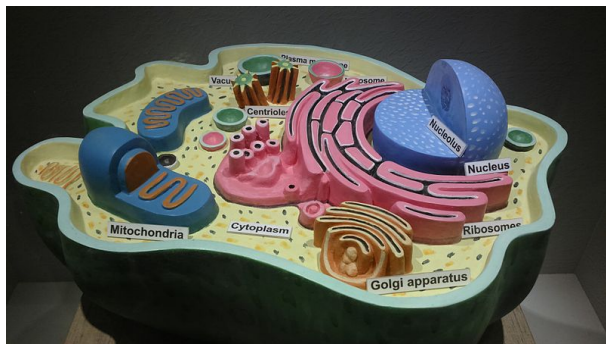
Hans-Jörg Kreowski and Grzegorz Rozenberg

set-based reaction systems introduced by  
Ehrenfeucht and Rozenberg in 2007

to model the functioning of living cells  
and as a new approach to computation

in this paper:

graph-based reaction systems  
as a new approach to graph transformation



Structure of animal cell

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Author: Royroydeb



# Reaction Systems

background

state

set

$B$

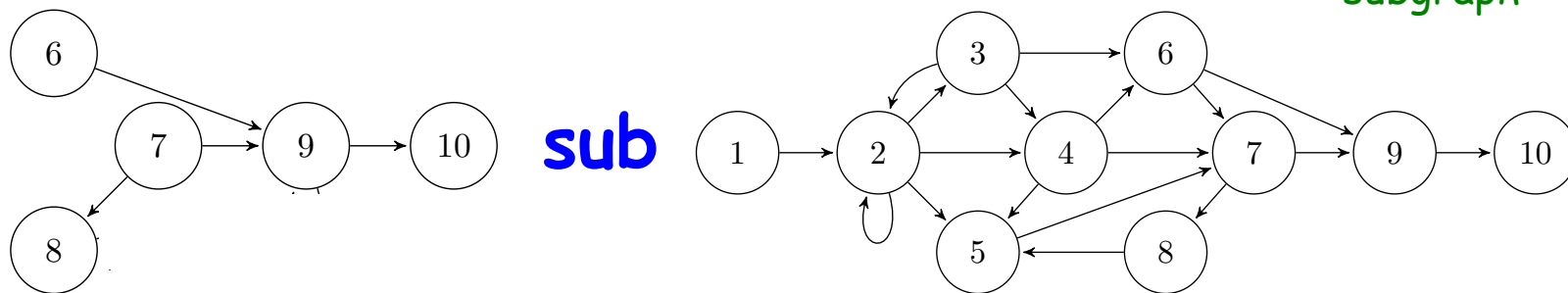
$T \subseteq B$

graph

$B$

$T \text{ sub } B$

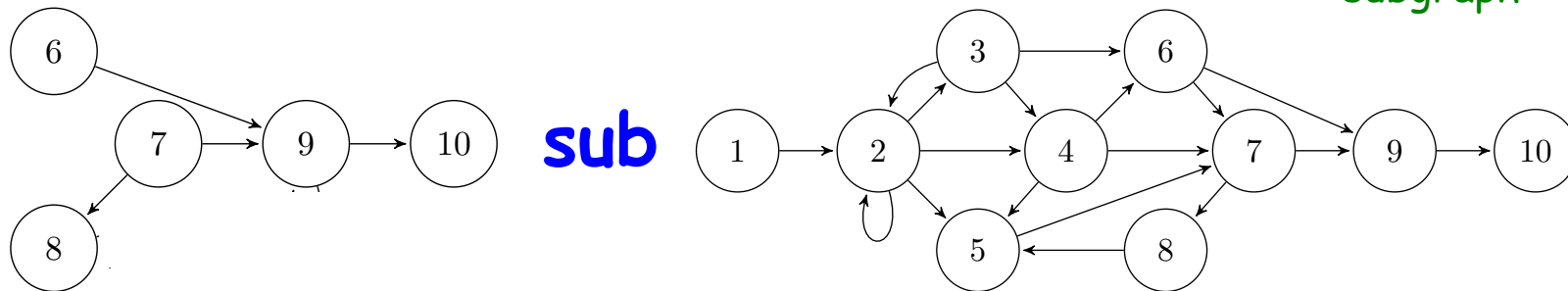
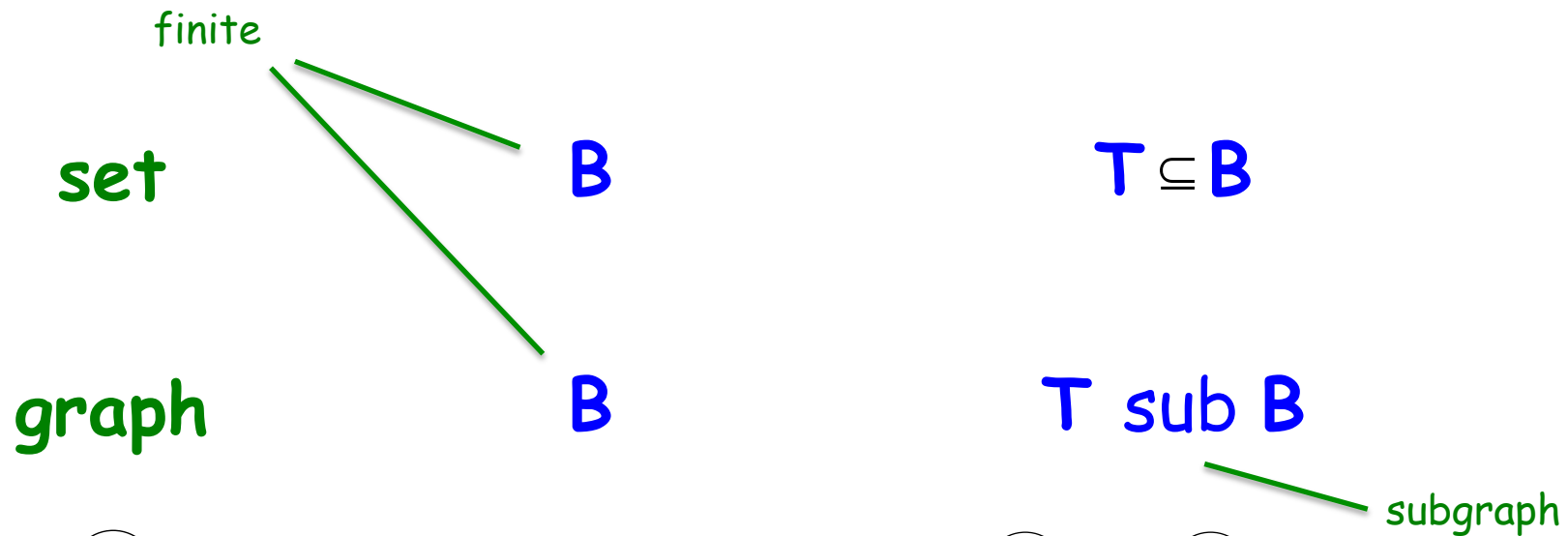
subgraph



# Reaction Systems

background

state



# Reaction Systems

reaction  $b$

reactant      inhibitor      product

set

$$R \subseteq B$$

$$I \subseteq B$$

$$P \subseteq B$$

graph

$$R \text{ sub } B$$

$$I \text{ sub } B$$

$$P \text{ sub } B$$

(?!)

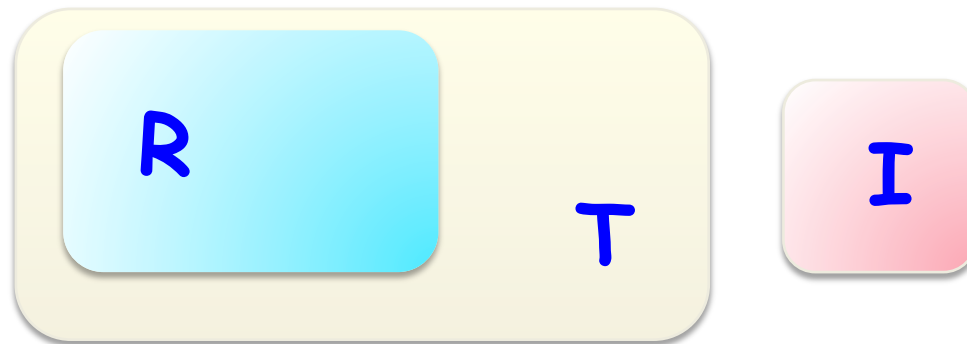


# Reaction Systems

reaction enabled on state

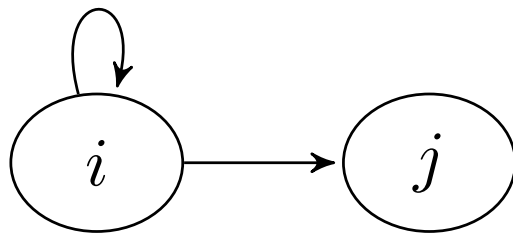
set  $R \subseteq T$  and  $I \cap T = \emptyset$

graph  $R \text{ sub } T$  and  $I \cap T = \emptyset$  (?!)

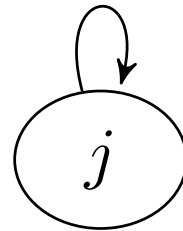


# Reaction Systems

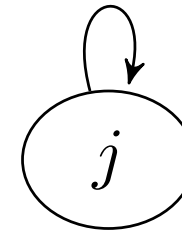
subgraph as inhibitor is inconvenient:  
for example, loop to be moved along edge  
but only if there is no loop on target



reactant



inhibitor

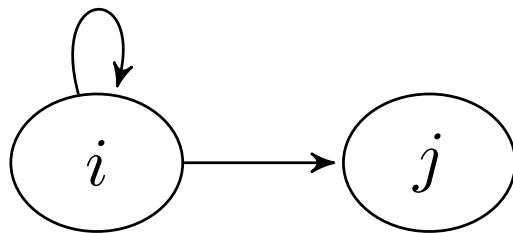


product

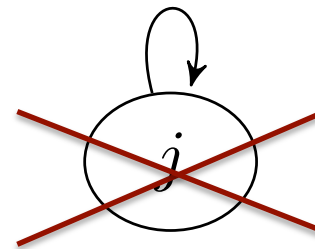


# Reaction Systems

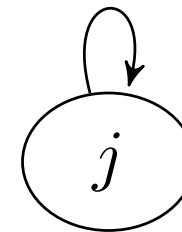
subgraph as inhibitor is inconvenient:  
for example, loop to be moved along edge  
but only if there is no loop on target



reactant



inhibitor



product

we allow to forbid an edge  
without forbidding source and target necessarily



# Reaction Systems

reaction  $b$

reactant      inhibitor      product

set

$$R \subseteq B$$

$$I \subseteq B$$

$$P \subseteq B$$

graph

$$R \text{ sub } B$$

~~$$I \text{ sub } B$$~~

$$P \text{ sub } B$$

$$I \subseteq (V_B, E_B) = U(B)$$

selector

extraction



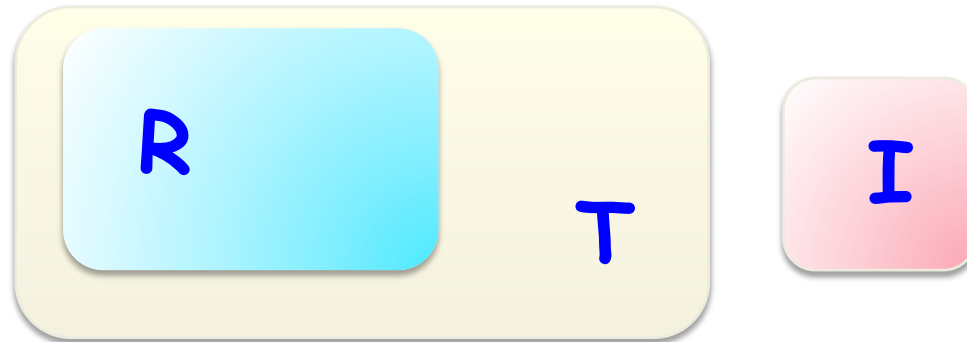


# Reaction Systems

reaction enabled on state

set  $R \subseteq T$  and  $I \cap T = \emptyset$

graph  $R \text{ sub } T$  and  $I \cap U(T) = (\emptyset, \emptyset)$



# Reaction Systems

result of reaction on state

$$\text{set/graph } \text{res}_b(T) = \begin{cases} P & \text{if } b \text{ enabled on } T \\ \emptyset & \text{otherwise} \end{cases}$$

result of set  $A$  of reactions on state

$$\text{set/graph } \text{res}_A(T) = \bigcup_{b \in A} \text{res}_b(T)$$



# Reaction Systems

$$A = ( B , A )$$

background set/graph    set of reactions

result of  $A$  on state

$$\text{res}_A(T) = \text{res}_A(T)$$



# First case study

modeling a shortest path algorithm by  
the graph-based reaction system

**SHORT**(n)

(as parallel breadth first)



# background graph of **SHORT**( $n$ )

the complete directed graph with

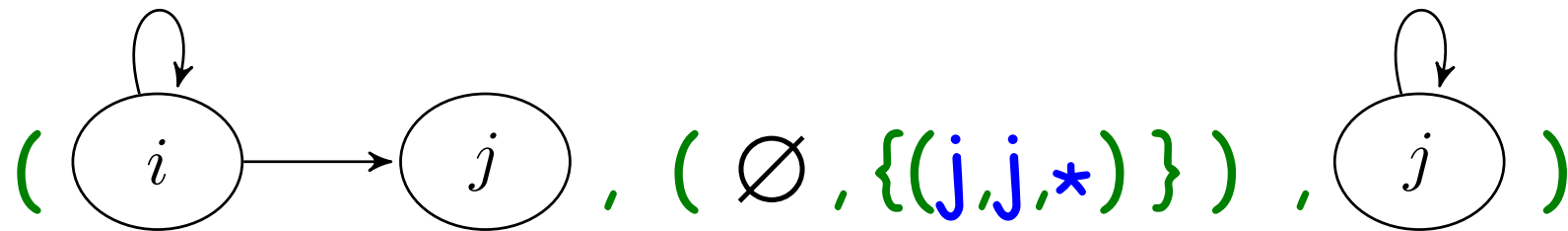
nodes  $1, 2, \dots, n$  and

edges  $(i, j, *)$  for  $i, j = 1, \dots, n$

where  $*$  is a special label invisible in drawings



reactions of **SHORT**( $n$ ) for all  $i, j = 1, \dots, n$



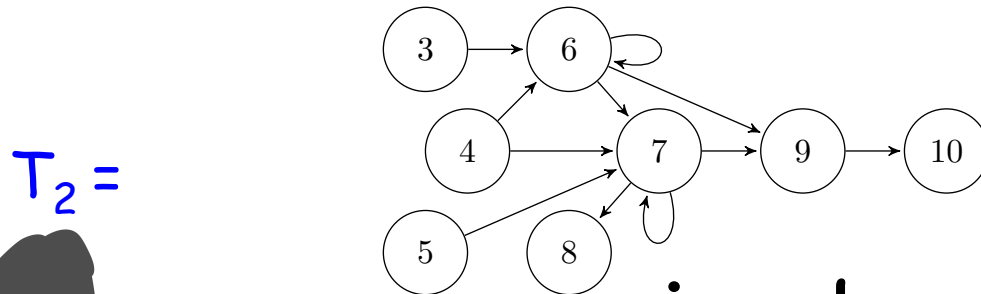
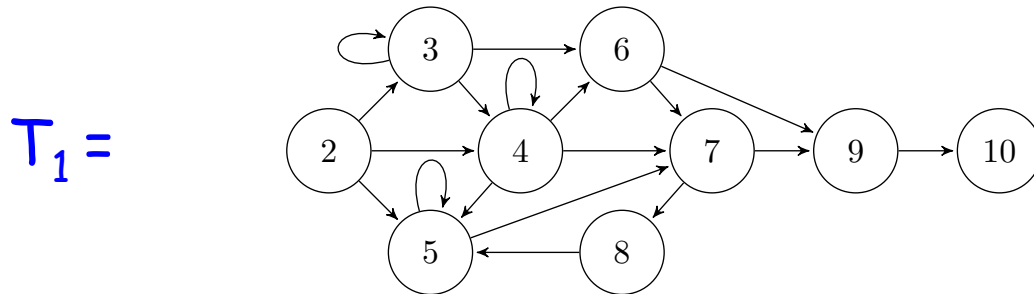
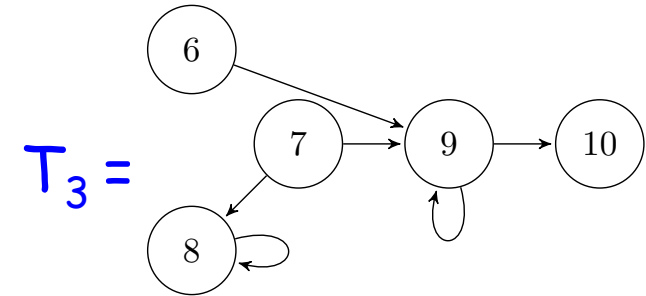
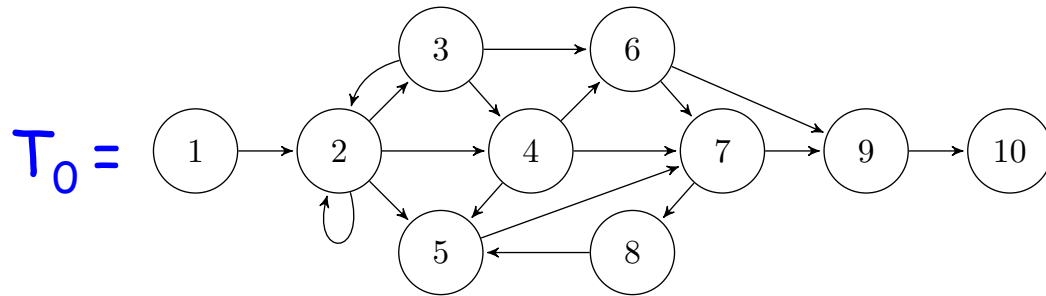
loop is moved along edge if there is no loop on target



edge is sustained if there is no loop at target



# sample sequence of states in **SHORT(10)**



given by a sequence of reactions

# Theorem

Let  $T_0$  be a state with a single loop at node  $i_0$ , and let  $T_0, \dots, T_m$  be a sequence of states in  $SHORT(n)$  such that  $T_i = \text{res}_{SHORT(n)}(T_{i-1})$  for  $i = 1, \dots, m$ .

Then the node  $j$  has a loop in  $T_k$  for some  $k$  if and only if  $k$  is the length of a shortest path from  $i_0$  to  $j$  in  $T_0$ .





# Reaction Systems

$$A = ( B , A )$$

background set/graph    set of reactions

result of  $A$  on state

$$\text{res}_A(T) = \text{res}_A(T)$$

deterministic # maximum parallel # no conflict

# nothing sustains if not (re)produced



# Reaction Systems

forcing sustainability

Let  $S$  sub  $B$ , and let  $A$  contain the (uninhibited) reactions

$(v, (\emptyset, \emptyset), v)$  for  $v \in V_S$ , and

$(e^\bullet, (\emptyset, \emptyset), e^\bullet)$  for  $e \in E_S$ .

Then  $S \cap T \subseteq \text{res}_A(T)$ .



## Second case study

modeling a finite state automaton  $F$  and  
its recognition of strings by the graph-  
based reaction system

$A(F)$

(using mainly the state graph)



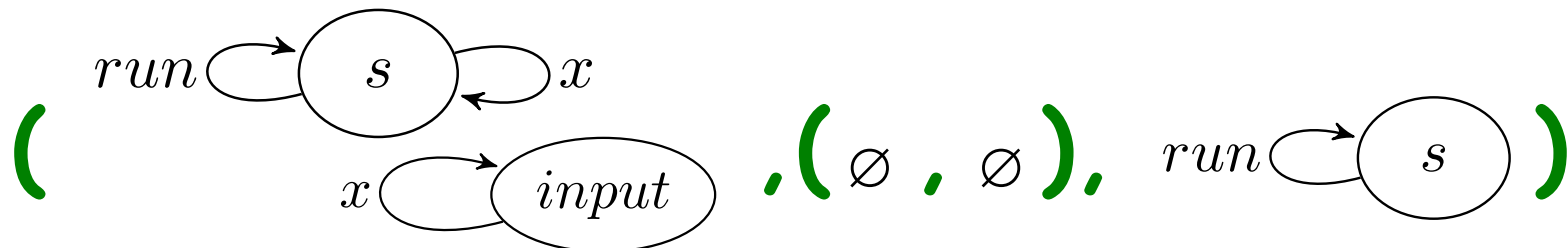
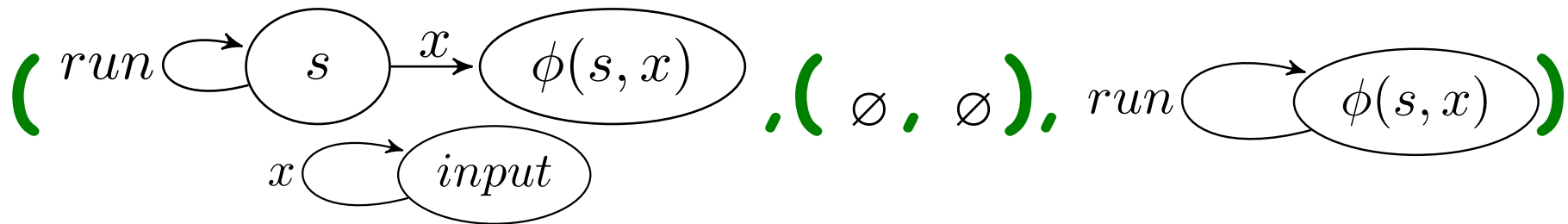
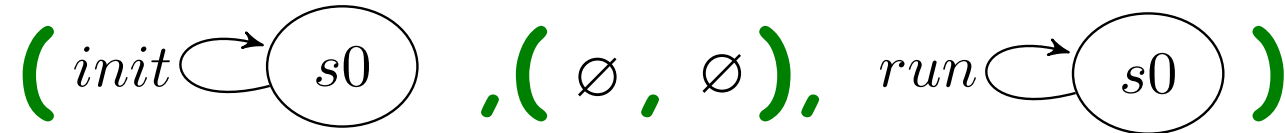
Let  $\mathcal{F} = (Q, I, \phi, s_0, F)$  be a finite state automaton.

Then the background graph of  $A(\mathcal{F})$  consists of the state graph  $gr(\mathcal{F})$  of  $\mathcal{F}$  plus a run-loop at each node plus an extra node input with an  $x$ -loop for each  $x$  in  $I$ .



$\varphi$

# The reactions of $A(\mathcal{F})$ are:

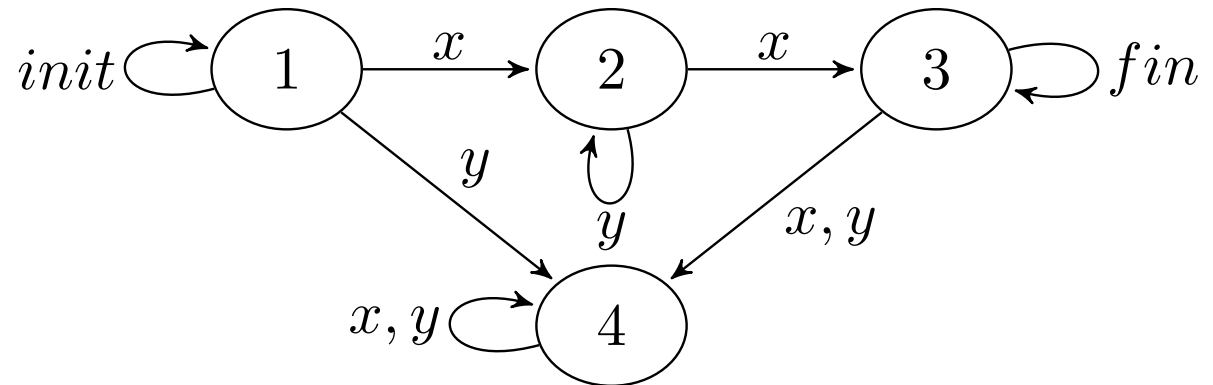


plus the reactions sustaining the state graph  $\text{gr}(\mathcal{F})$  up to the **init**-loop

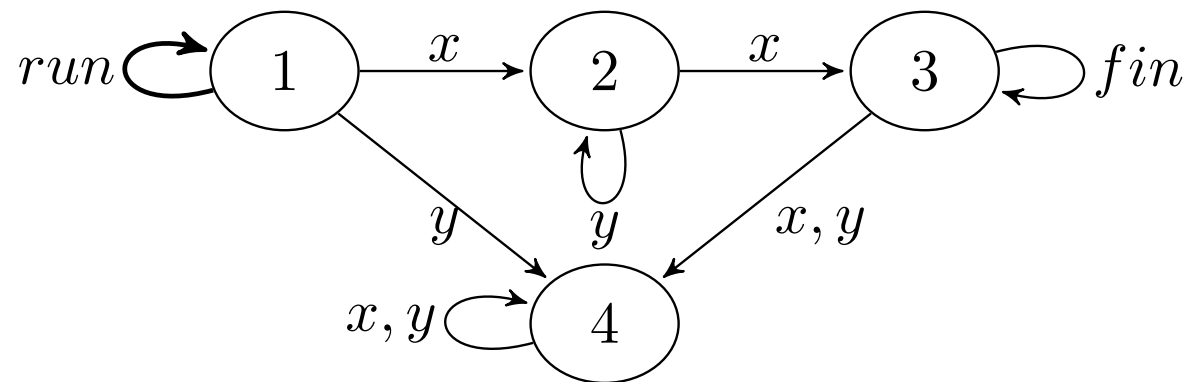


# result graphs

(0)

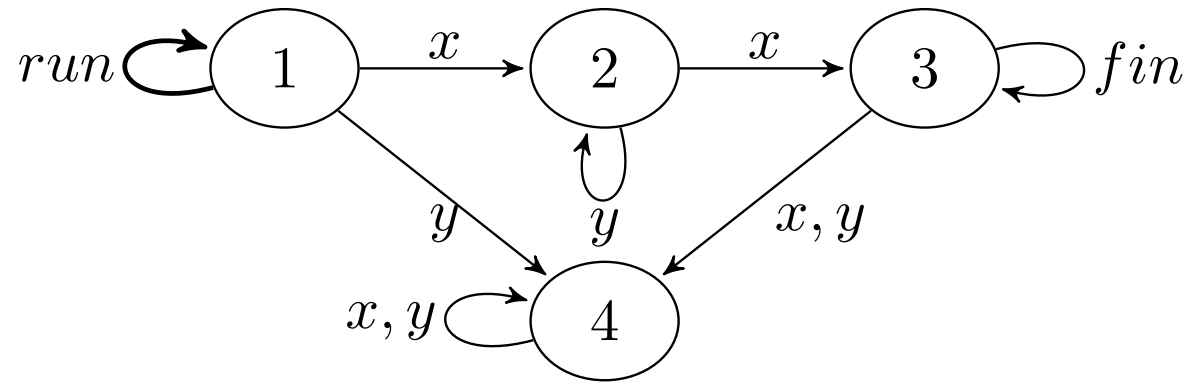


(1)

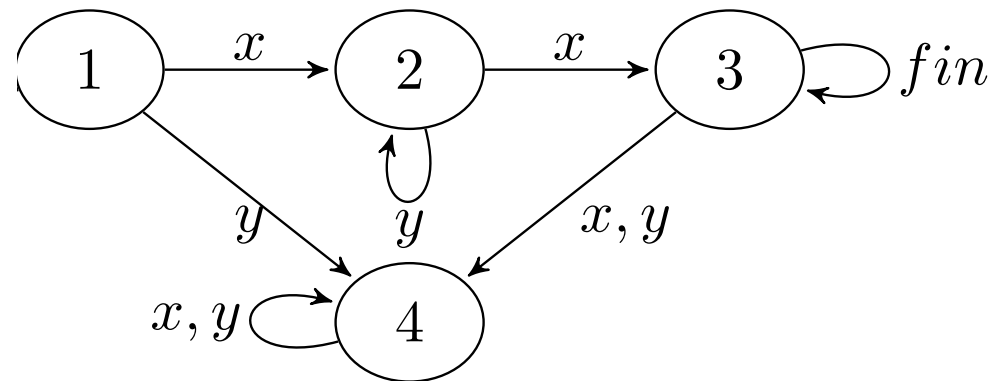


# result graphs

(1)

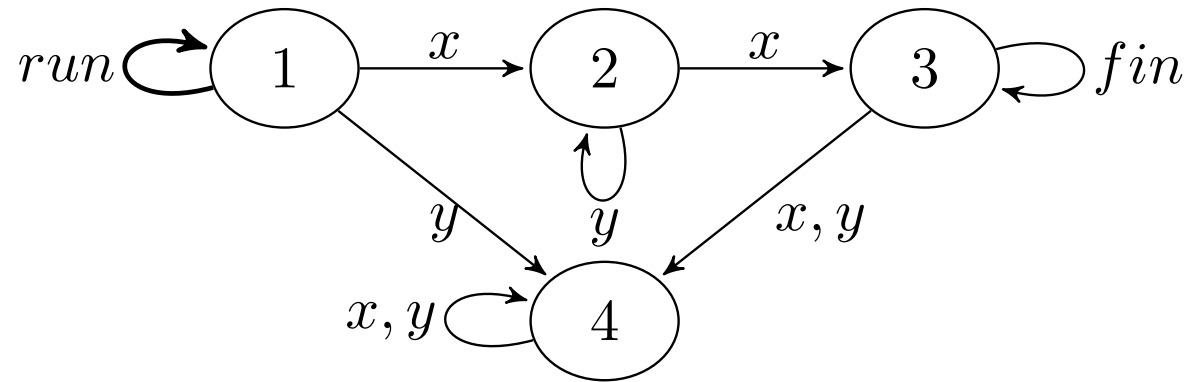


(2?)



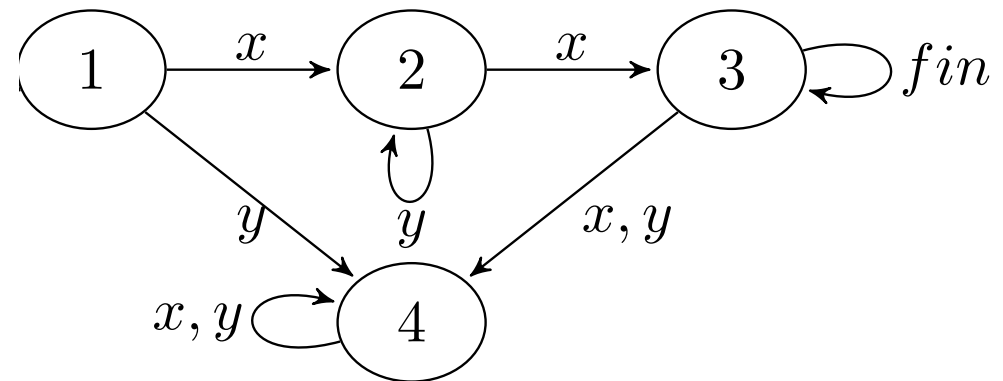
# result graphs

(1)



(2?)

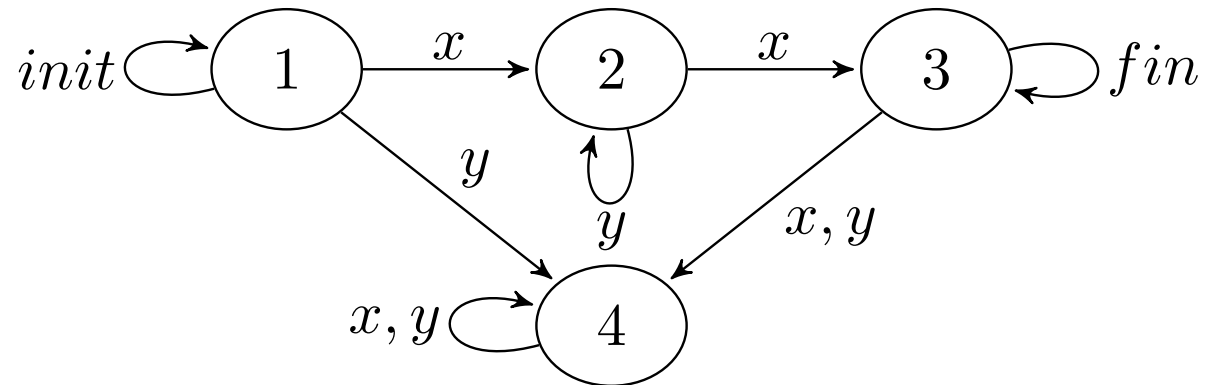
stable  
from  
here on



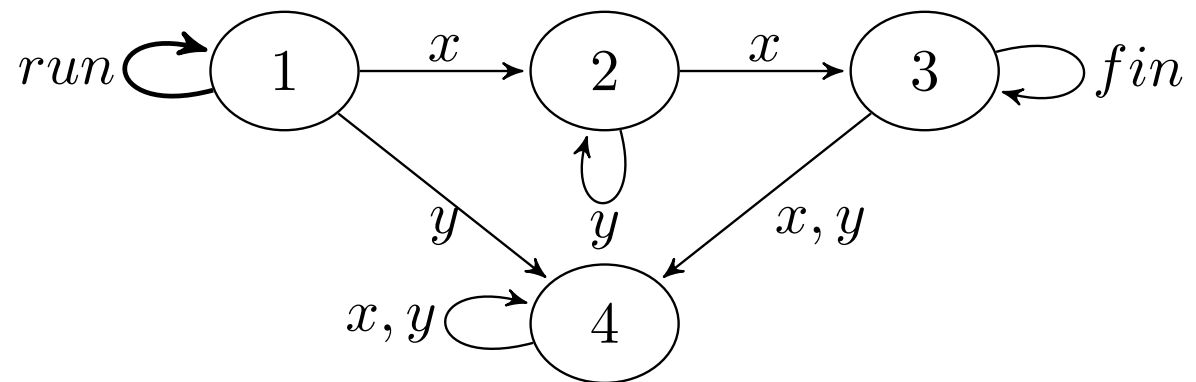


# result graphs

(0)



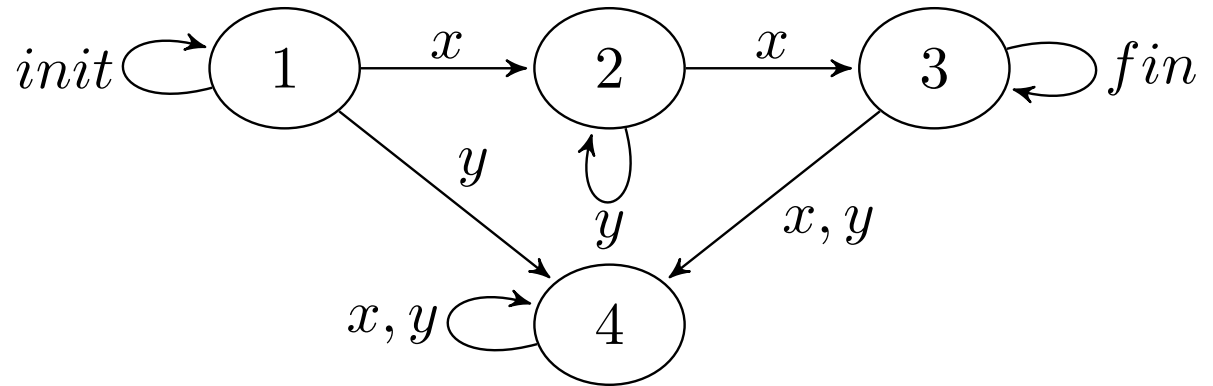
(1)



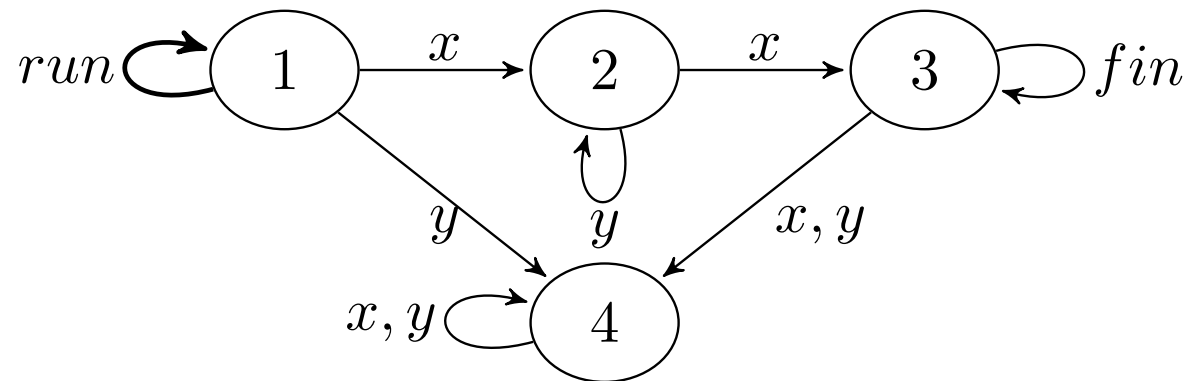
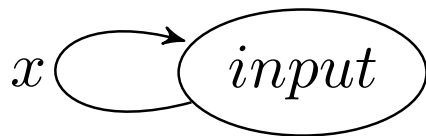
# context graphs

# result graphs

(0)



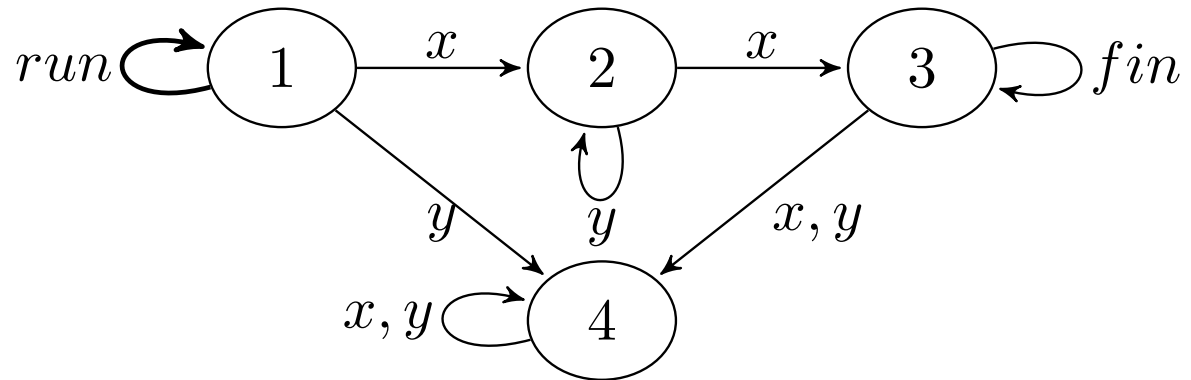
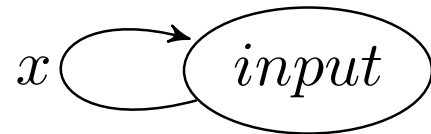
(1)



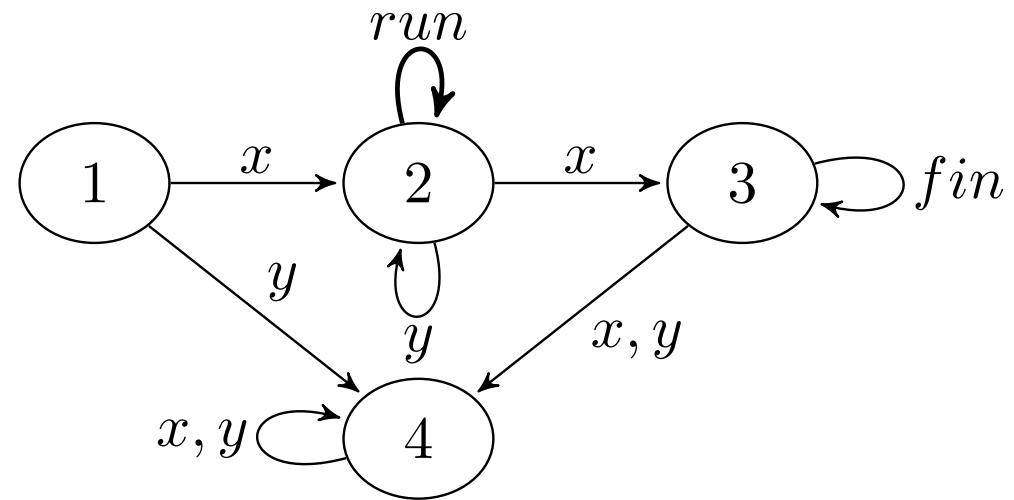
# context graphs

# result graphs

(1)



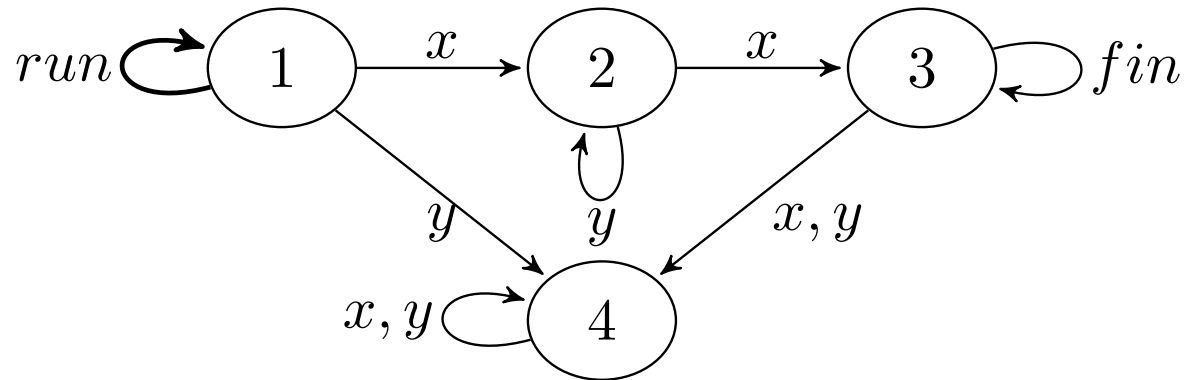
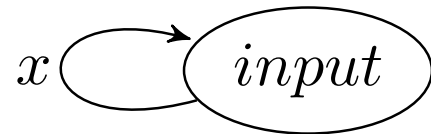
(2)



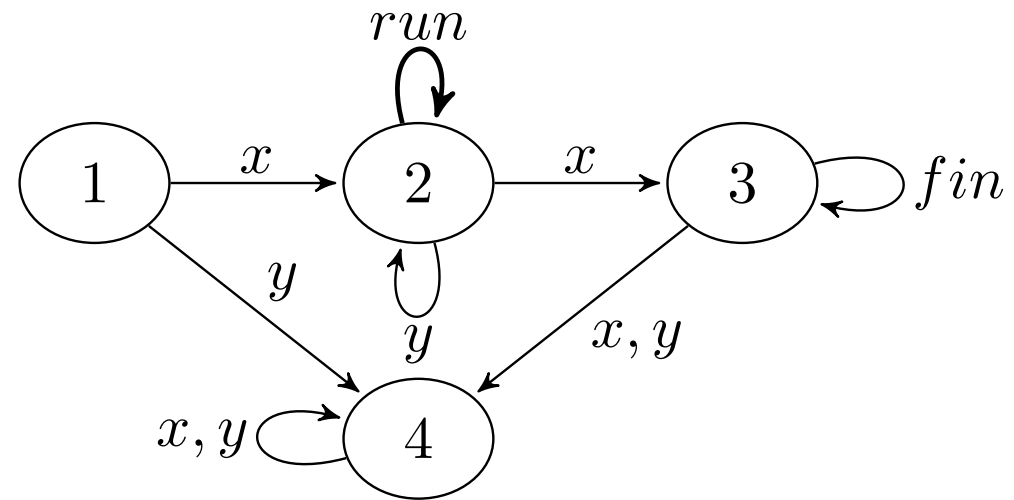
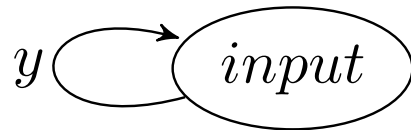
# context graphs

# result graphs

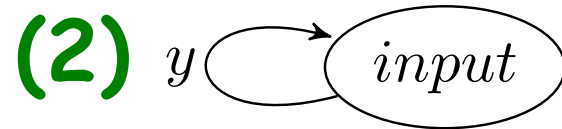
(1)



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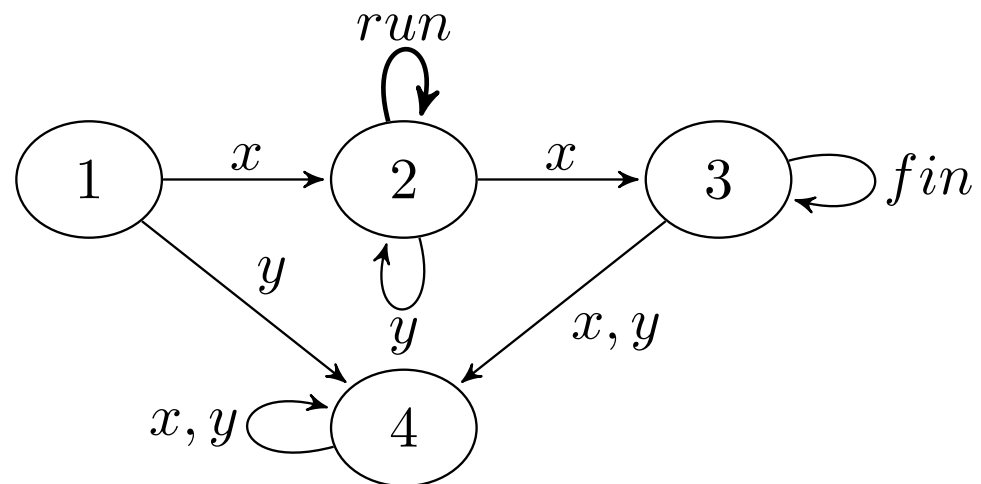
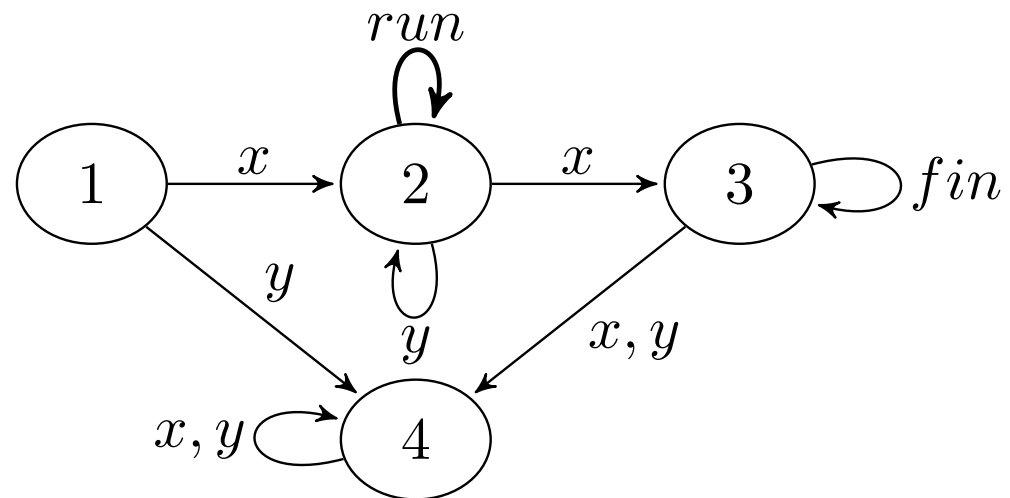
# context graphs



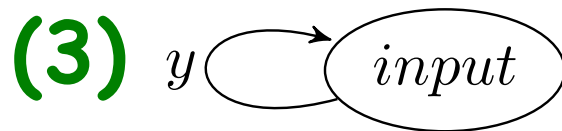
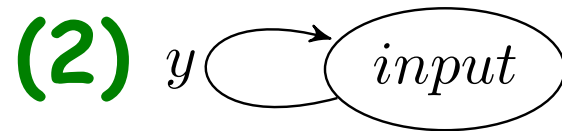
(3)



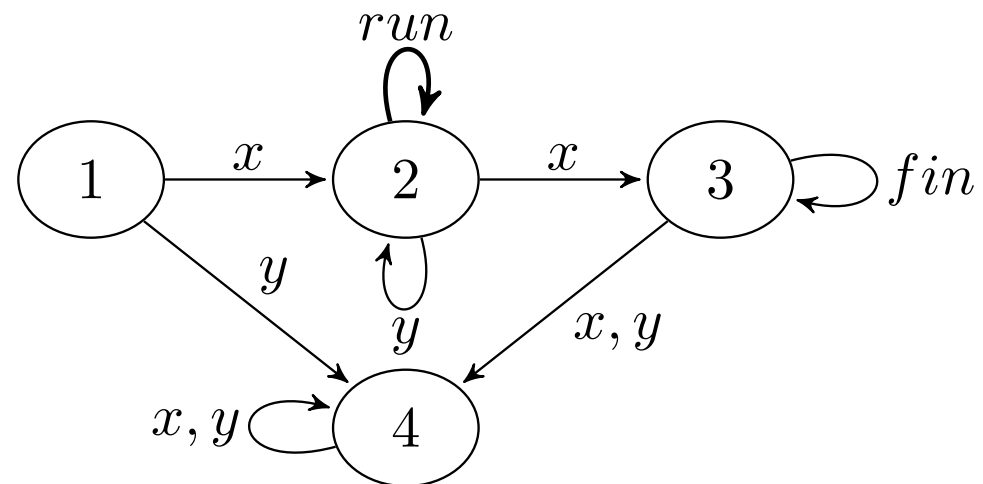
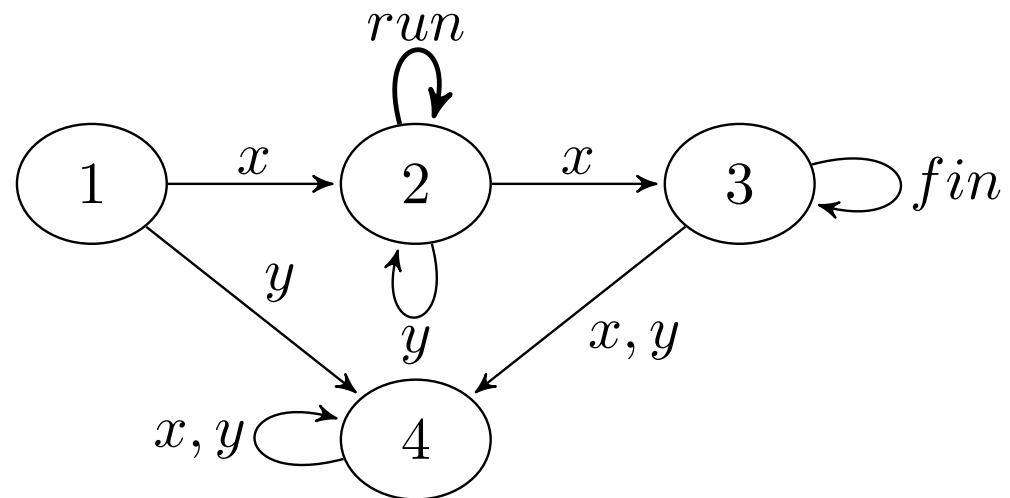
# result graphs



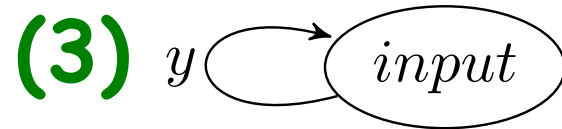
# context graphs



# result graphs



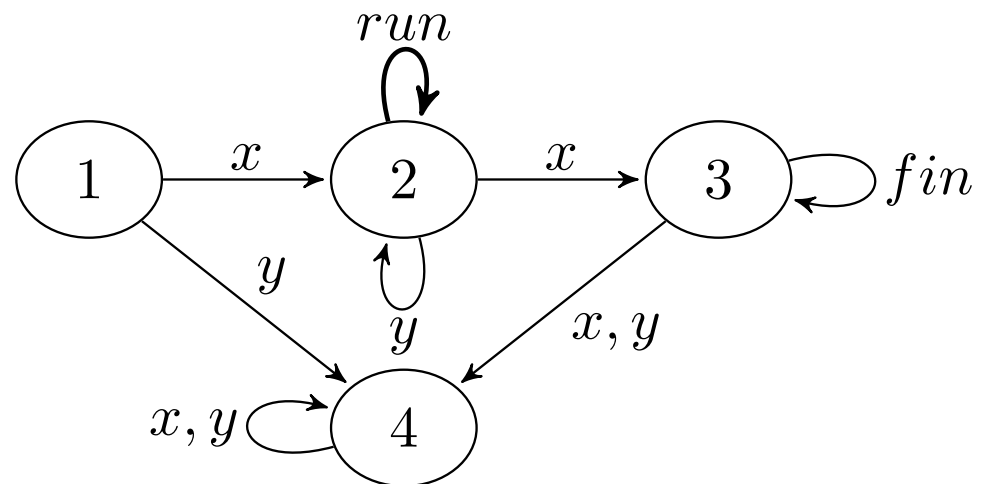
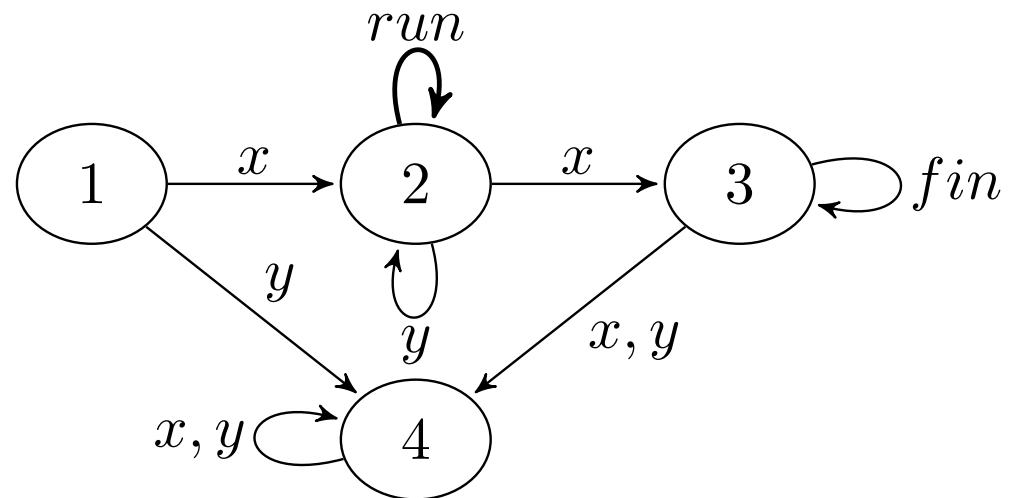
# context graphs



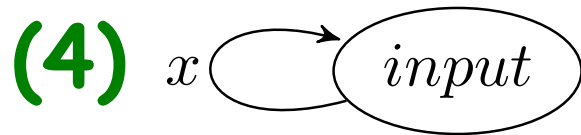
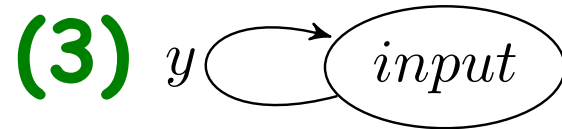
(4)



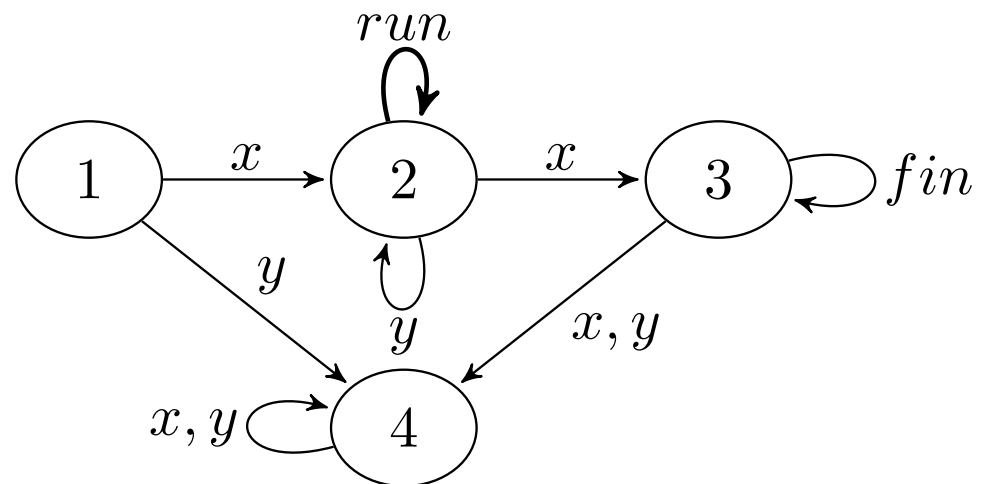
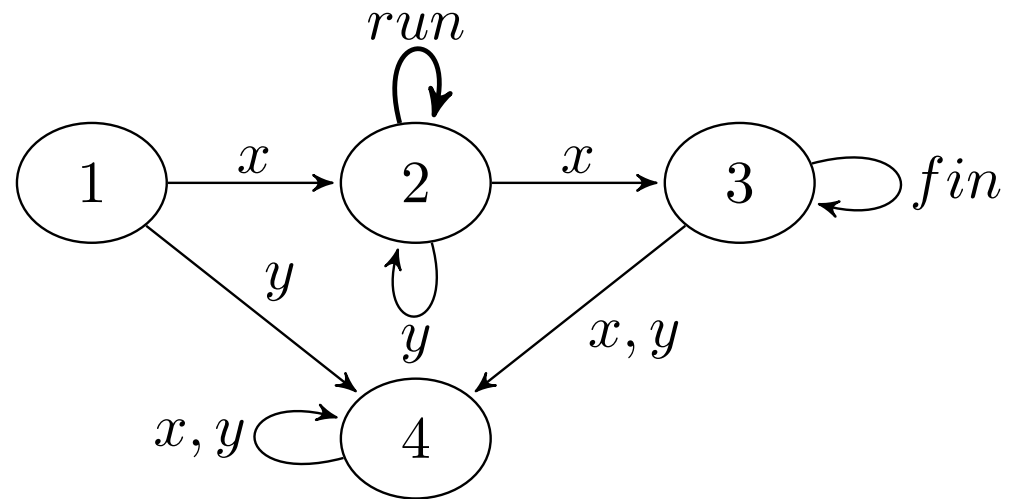
# result graphs



# context graphs

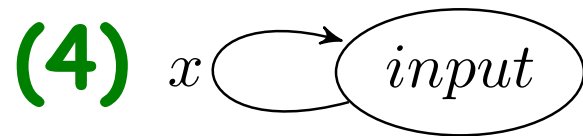


# result graphs

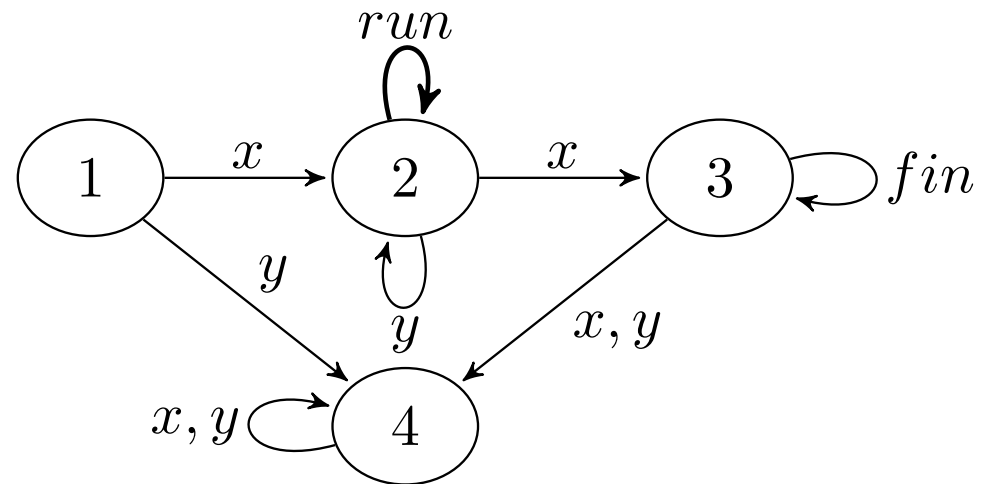




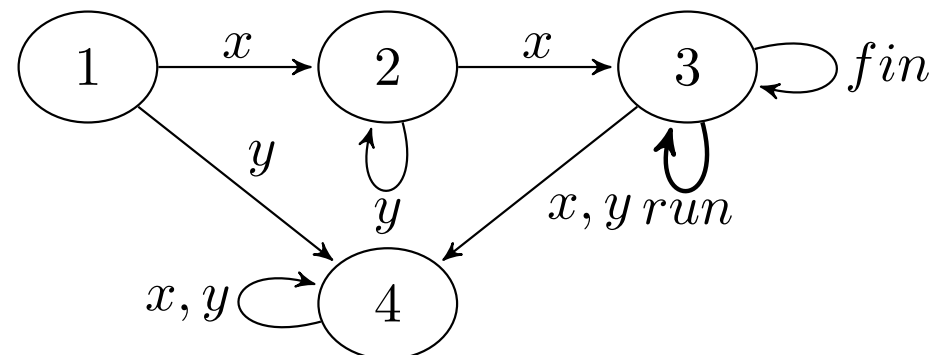
# context graphs



# result graphs



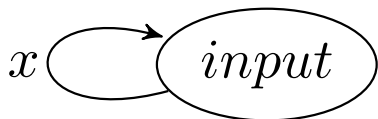
(5)



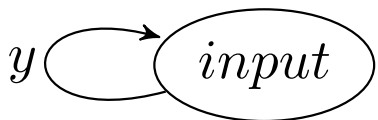
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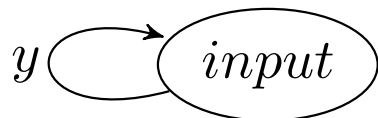
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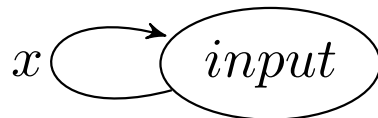
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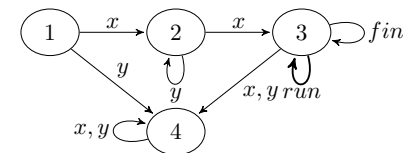
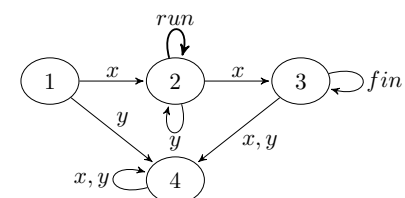
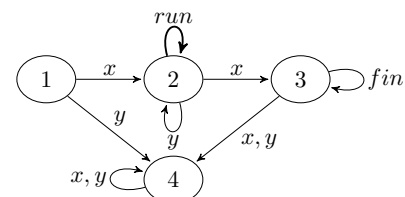
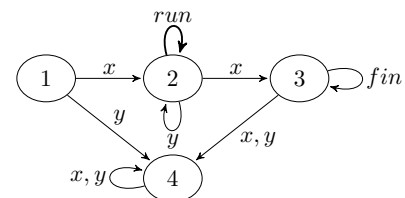
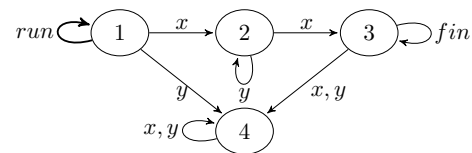
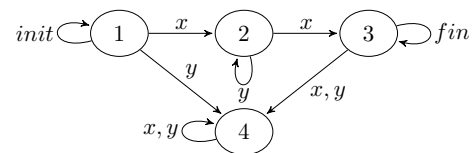
(3)



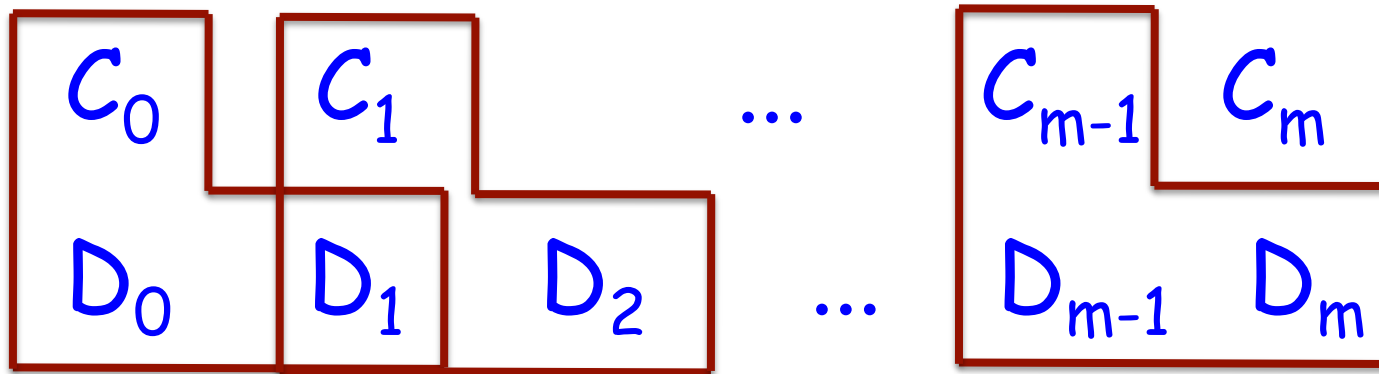
(4)



(5)



An **interactive process** is a pair  $\pi = (\gamma, \delta)$  where  $\gamma = C_0, \dots, C_m$  and  $\delta = D_0, \dots, D_m$  are two sequences of graphs for some  $m$  such that  $D_i = \text{res}_A(C_{i-1} \cup D_{i-1})$  for  $i = 1, \dots, m$ .



An interactive process is a pair  $\pi = (\gamma, \delta)$  where  $\gamma = C_0, \dots, C_m$  and  $\delta = D_0, \dots, D_m$  are two sequences of graphs for some  $m$  such that  $D_i = \text{res}_A(C_{i-1} \cup D_{i-1})$  for  $i = 1, \dots, m$ .

$\gamma$  is the **context sequence** of  $\pi$ ,  
 $\delta$  its **result sequence**, and

$\tau = T_0, \dots, T_m$  with  $T_i = C_i \cup D_i$

 for  $i = 0, \dots, m$  is its **state sequence**.

An interactive process is a pair  $\pi = (\gamma, \delta)$  where  $\gamma = C_0, \dots, C_m$  and  $\delta = D_0, \dots, D_m$  are two sequences of graphs for some  $m$  such that  $D_i = \text{res}_A(C_{i-1} \cup D_{i-1})$  for  $i = 1, \dots, m$ .

$\pi$  is the **context-independent** if  $C_i \text{ sub } D_i$  for  $i = 0, \dots, m$ . In this case,  $\delta = \tau$ , and  $\gamma = \emptyset, \dots, \emptyset$  wlog.



consider the interactive processes  $\pi(x_1 \dots x_n)$  given by context sequences of the form

$\emptyset, \text{loop}(\text{input}, x_1), \dots, \text{loop}(\text{input}, x_n), \emptyset$

for some  $n$  and  $x_i \in \Sigma$  for  $i = 1, \dots, n$ , and the state graph of  $F$  as initial result graph

then the language  $L(A(F))$  specified by  $A(F)$  contains all strings  $x_1 \dots x_n$  such that the last result graph of  $\pi(x_1 \dots x_n)$  has a node with a **run**- and a **fin**-loop



**Theorem:**  $L(A(F)) = L(F)$

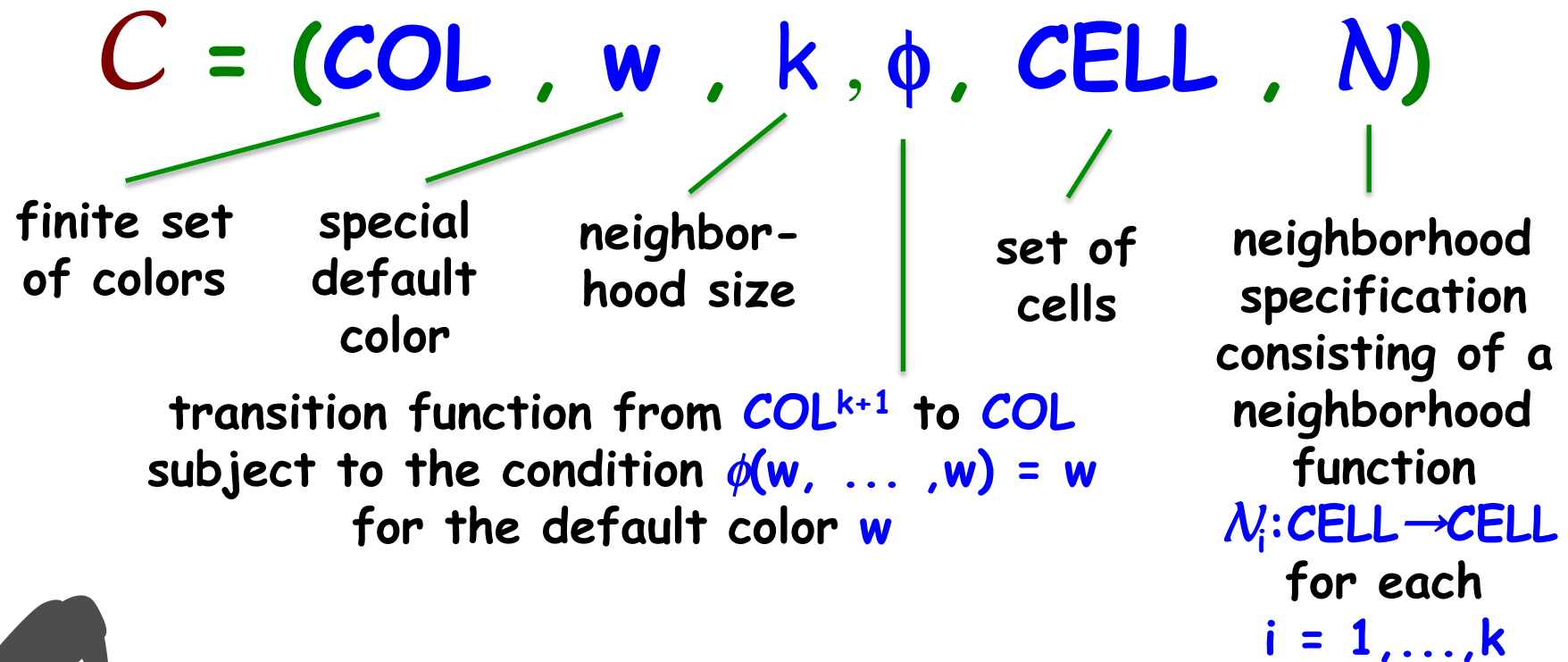
## Third case study

modeling cellular automata that form one  
of the oldest paradigms of  
massively parallel computation  
with a rich stock of  
theory and applications



# cellular automata

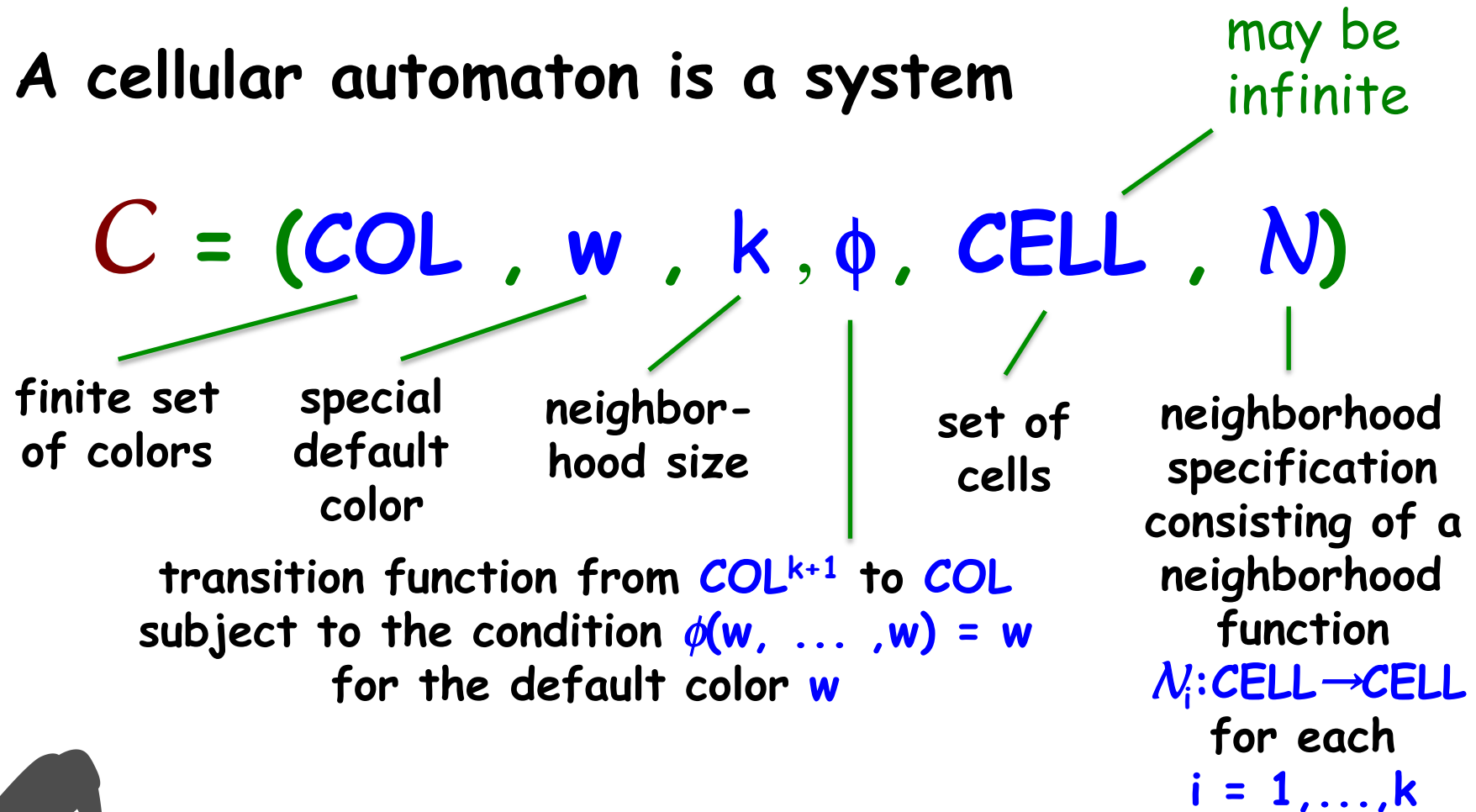
A cellular automaton is a system





# cellular automata

A cellular automaton is a system



# cellular automata

A **configuration** of  $C$  is a function

$\alpha: \text{CELL} \rightarrow \text{COL}$  such that

the set of **active cells**

$\text{act}(\alpha) = \{v \in \text{CELL} \mid \alpha(v) \neq w\}$  is finite.

$\in$

Given a configuration  $\alpha$ , one gets

a uniquely determined **successor configuration**

$\alpha' : \text{CELL} \rightarrow \text{COL}$  defined by

$\alpha'(v) = \phi(\alpha(v), \alpha(N_1(v)), \dots, \alpha(N_k(v)))$

for each  $v \in \text{CELL}$ .



# Example

transition function:

$(\text{blue}|\text{red}, c_1, \dots, c_6) \mapsto$  black in all cases

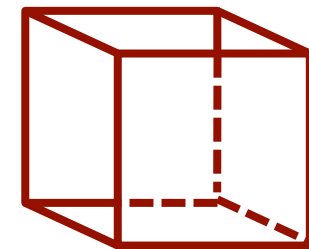
$(\text{black}, c_1, \dots, c_6) \mapsto$  blue if one  $c_i$  is red  
and the others black

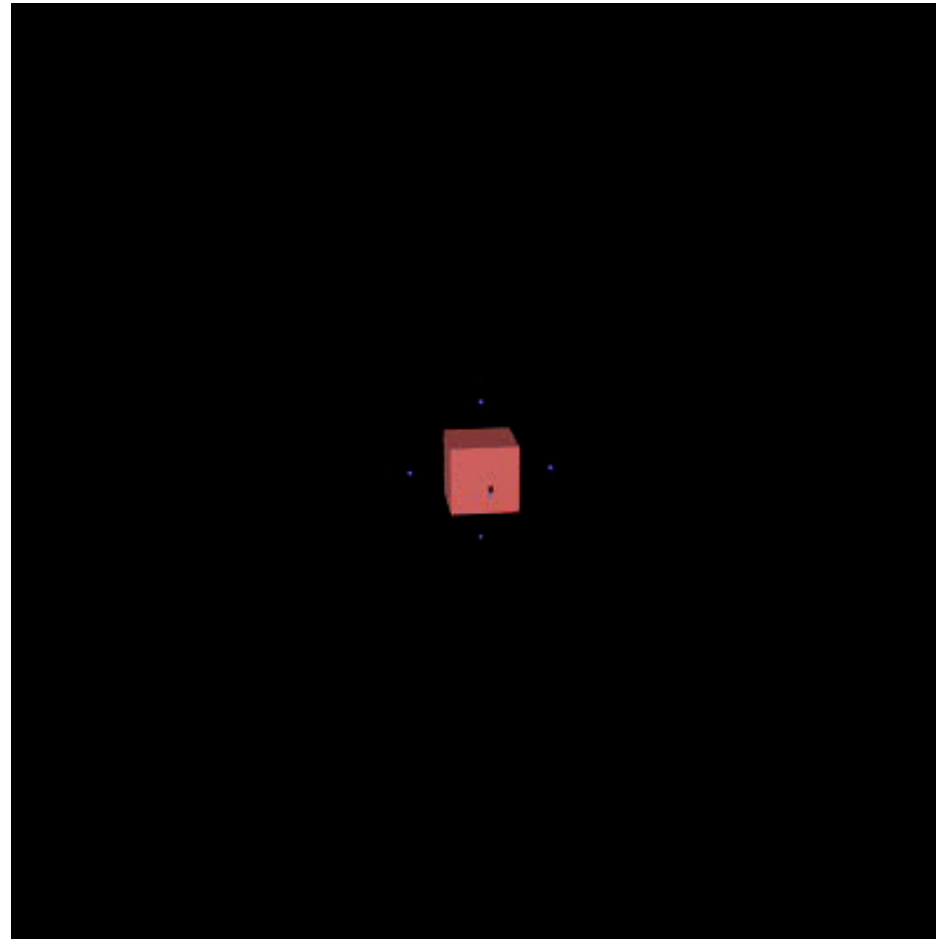
$(\text{black}, c_1, \dots, c_6) \mapsto$  red if one  $c_i$  is blue  
and the others black

$(\text{black}, c_1, \dots, c_6) \mapsto$  black in all other cases

cells: unit cubes in the Euclidean 3d space with  
integer coordinates

neighbors: the cubes that share a side





# transformation of cellular automata into graph-based reaction systems

Let  $C = (COL, w, k, \phi, CELL, N)$  be a cellular automaton. Then, for each finite subset  $Z \subseteq CELL$ , the **cells of interest**, a graph-based reaction system

$$A(C, Z) = (B(C, Z) = (V, \Sigma, E), A(C, Z))$$

is defined as follows:

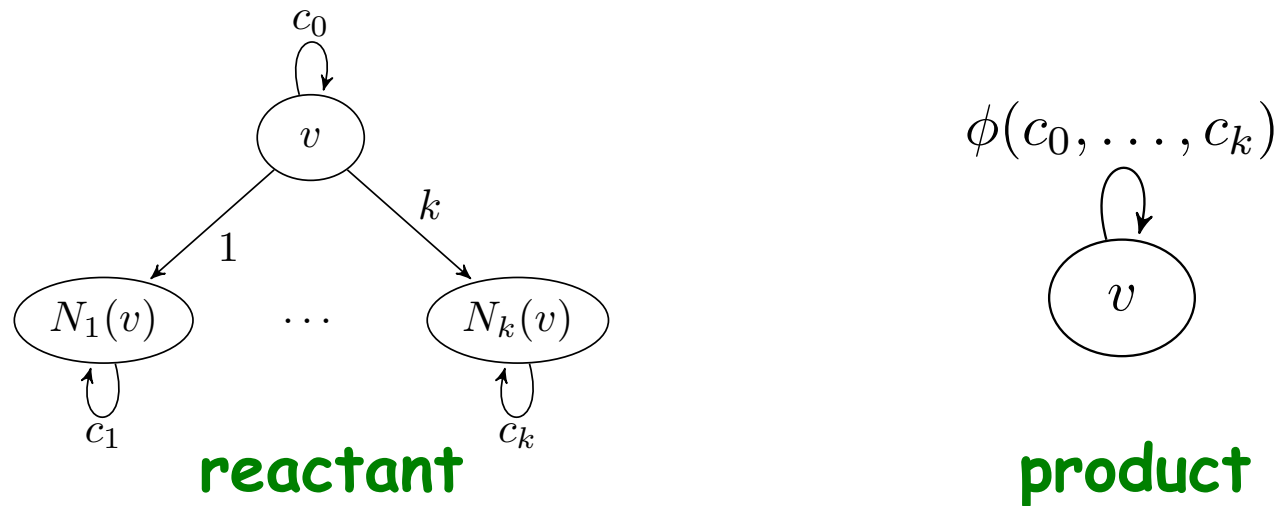
$$V = Z \cup \{N_i(v) \mid v \in Z, i = 1, \dots, k\},$$

$$\Sigma = COL \cup \{1, \dots, k\} \cup \{*\}, \text{ and}$$

$$E = \{(v, N_i(v), i) \mid v \in Z, i = 1, \dots, k\} \cup \\ \{(v, v, c) \mid v \in Z, c \in COL\} \cup \\ \{(v, v, w) \mid v \in V \setminus Z\}.$$



The set of reactions  $A(C, Z)$  consists of the following uninhibited reactions



for all  $v \in Z$  and  $c_0, \dots, c_k \in COL$   
 plus sustaining rules for the  
 neighborhood structure of all  $v \in Z$  and  
 the  $w$ -loops of all  $v \in V \setminus Z$



Let  $C = (COL, w, k, \phi, CELL, N)$  be a cellular automaton and  $A(C, Z)$  be the corresponding reaction system with respect to some finite  $Z \subseteq CELL$ .

Let  $T_{lab}$  be a **well-formed state**, i.e. all nodes, all neighborhood edges as well as one loop at each node labeled due to some labeling function  $lab: Z \rightarrow COL$  and  $w$ -loops at all  $v \in V \setminus Z$ .

**Note:** The successor state of a well-formed state is well-formed.

Let  $T_{lab0} \rightarrow \dots \rightarrow T_{labn}$  be the state sequence of the context-independent process starting in some  $T_{lab0}$



Let  $C = (COL, w, k, \phi, CELL, N)$  be a cellular automaton and  $A(C, Z)$  be the corresponding reaction system with respect to some finite  $Z \subseteq CELL$ .

For  $lab: Z \rightarrow COL$ , let  $\alpha(lab)$  be the configuration with  $\alpha(lab)(v) = lab(v)$  for  $v \in Z$  and  $\alpha(lab)(v) = w$  otherwise

Let  $\alpha(lab_0) = \alpha_0 \rightarrow \alpha_1 \rightarrow \dots \rightarrow \alpha_n$  be a computation in  $C$  subject to the condition  $act(\alpha_i) \subseteq Z$  for  $i = 1, \dots, n$ .

**Theorem:** Then  $\alpha_i = \alpha(lab_i)$  for  $i = 1, \dots, n$ .





# Discussion

graph-based reaction systems generalize  
set-based ones

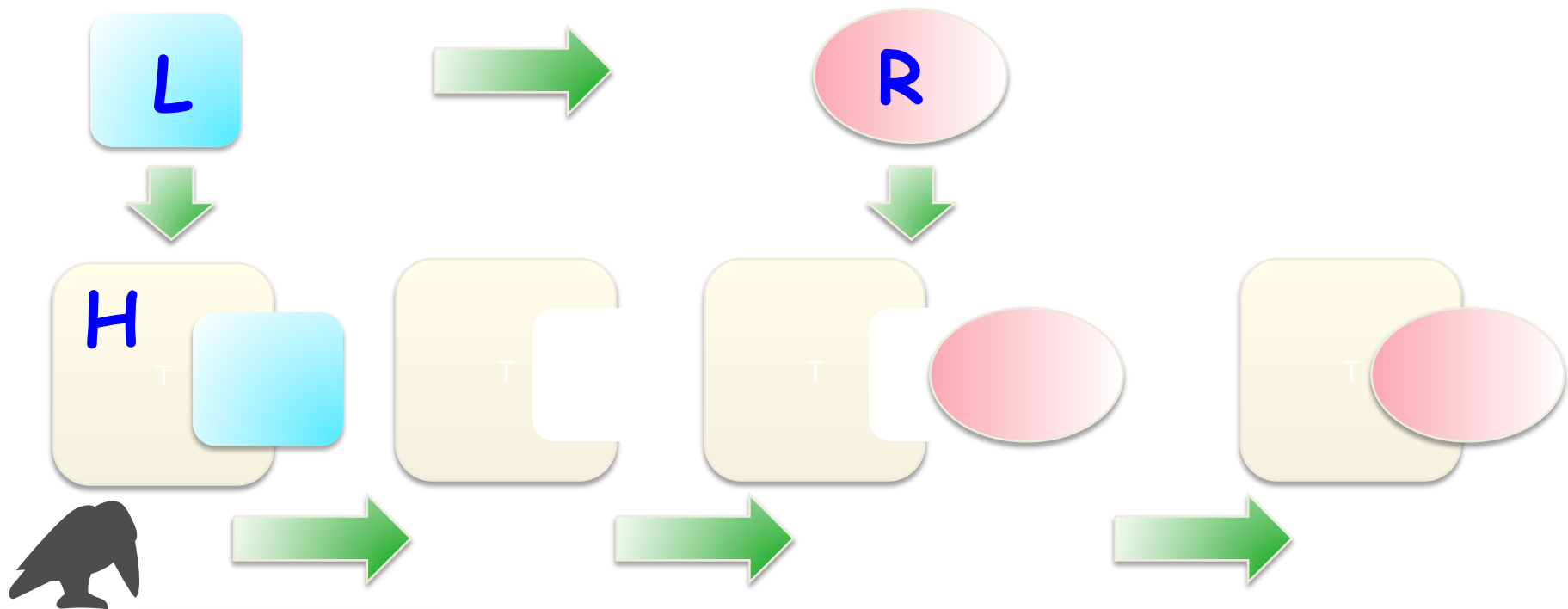
providing a graph-processing and visual level  
to the framework

the three case studies demonstrate the  
modeling capacity including the chance of  
proving correctness



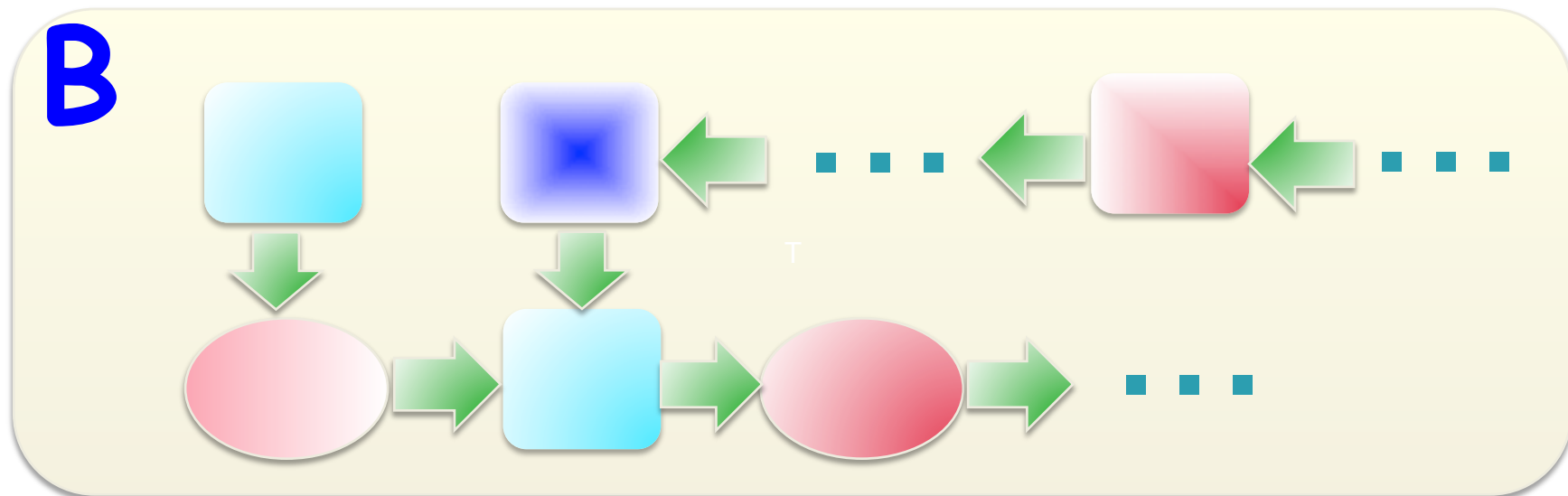
# Discussion

most known approaches to graph transformation follow the match-cut-add-paste methodology



# Discussion

in contrast to this, graph-based reaction systems provide a „surfing“ methodology



# Discussion

surfing on the background entity yields  
sequences of states

this has become a favorite research topic in the  
set case recently

we expect this to be a very promising future  
research topic in the graph case  
because graphs offer more structure than sets



thank you  
for your  
attention

