Research is the process of going up alleys to see if they are blind. Marston Bates.

Artificial Biochemistry

PolyAutomata

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www.luca.demon.co.uk/ArtificialBiochemistry.htm

Polyautomata

Polyautomata are interacting automata that can form *polymers*, or generally can *stick* to each other and then *unstick*.

new $a@r_0$ red=binders

$A_1 = !a(^{\nu}n_{r1});\ A_2(n)$

$A_2(n) = !n;\ A_3$

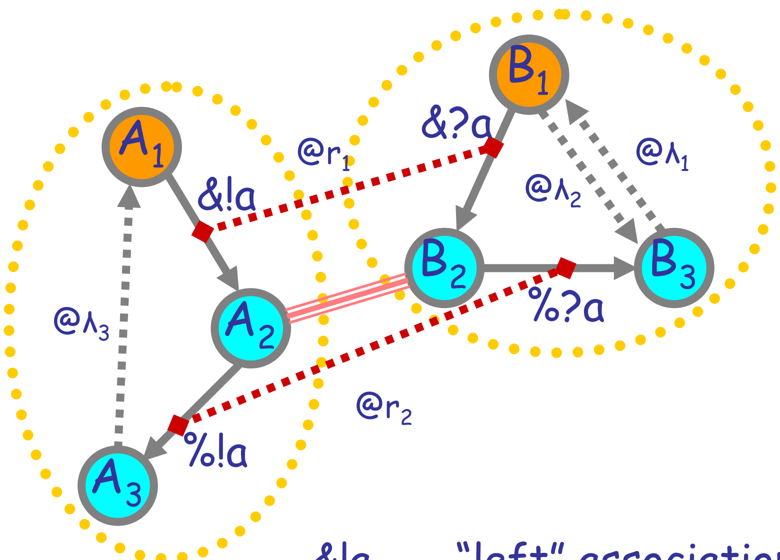
$A_3 = @\lambda_3;\ A_1$

$B_1 = ?a(n);\ B_2(n) + @\lambda_2;\ B_3$

$B_2(n) = ?n;\ B_3$

$B_3 = @\lambda_1;\ B_1$

They can be mapped to π-calculus.



&!a	"left" association	new n !a(n)
&?a	"right" association	?a(n)
%!a	"left" dissociation	!n
%?a	"right" dissociation	?n
═	exclusive association link between two specific automata	

Polyautomata Labels and Actions

Each transition label a has an associated set of one or more rates (or, in the non-stochastic case, just an integer arity >0). This is written:

$a@r_0,r_1,\ldots,r_n$ arity(a)=n (n>0)

If arity(a)=1, then r_0 is called the interaction rate. This is for *normal interaction transitions*.

If arity(a)>1, then r_0 is called the association rate and $r_1,\ldots,r_n$ are the dissociation rates. This is for *association and dissociation transitions*.

An action is of the form:

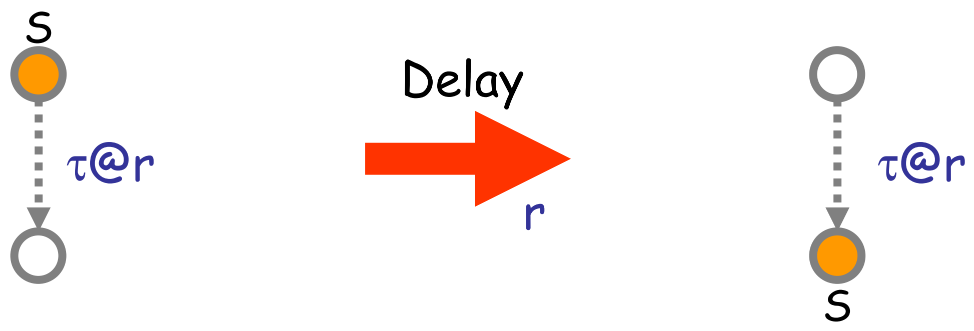
- $?a_i$ input at rate r_i , $i \in 0..\text{arity}(a)-1$
- $!a_i$ output at rate r_i , $i \in 0..\text{arity}(a)-1$
- $\tau@r$ delay at rate r, also written @r

If arity(a)=1, then $?a_0,!a_0$ are written simply ?a,!a (interaction)

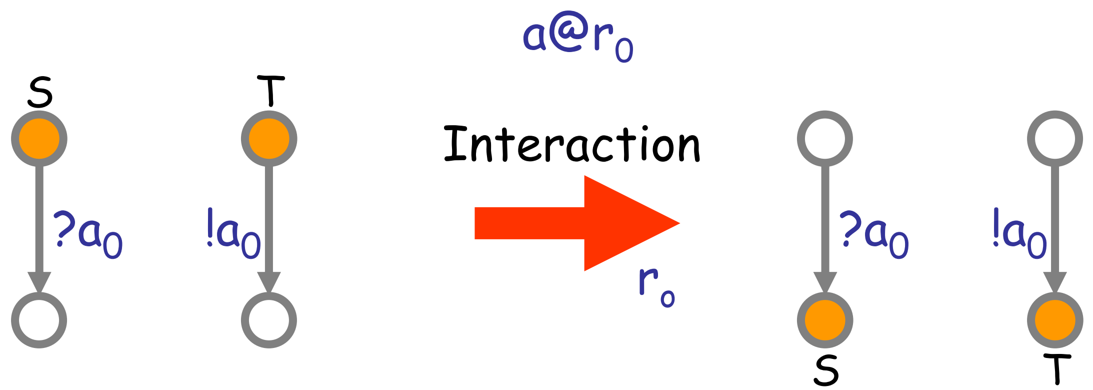
If arity(a)>1 then, for emphasis, $?a_0,!a_0$ may be written &?a,&!a (association), and $?a_i,!a_i$ for i>0 may be written $\%?a_i,\%!a_i$ (dissociation).

If arity(a)=2 then $\%?a_1,\%!a_1$ is written %?a,%!a.

Delay and Interaction Transition Rules



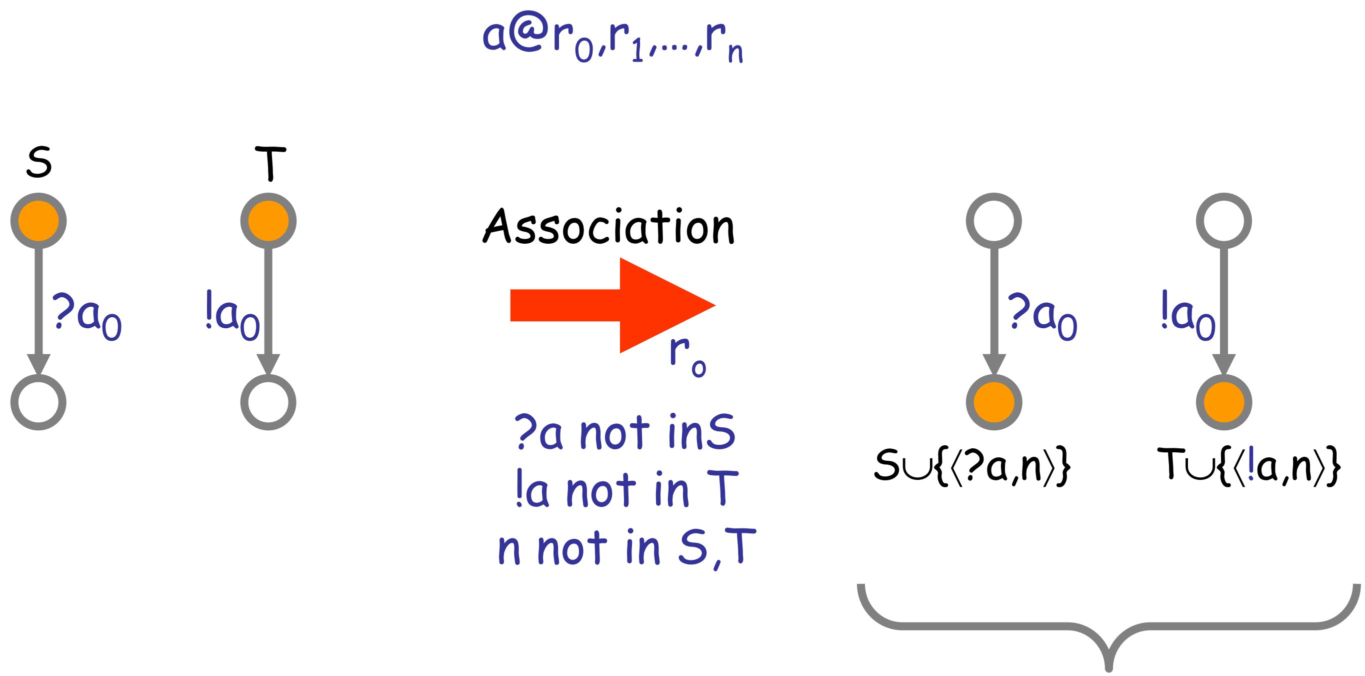
(Label abbreviation: @r)



(Label abbreviation: ?a   !a)

Association Rules

The current state carries a set of association markers S.

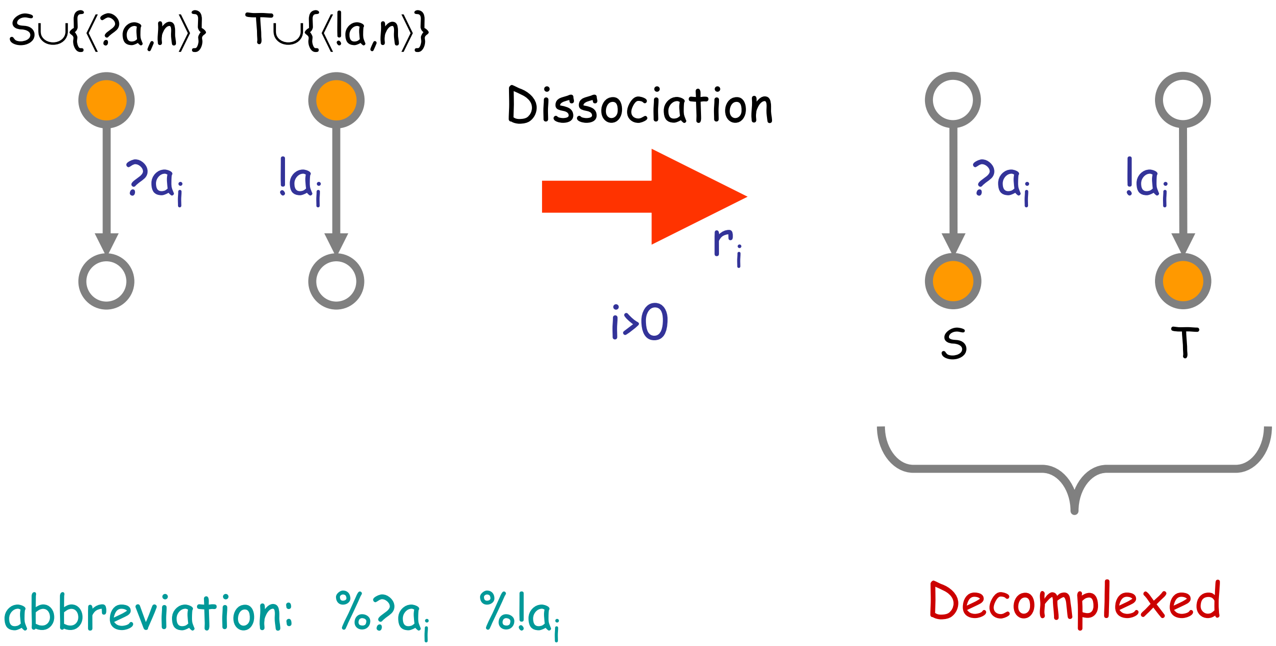


(Label abbreviation: &?a &!a)

Complexed automata, uniquely linked through fresh n, and unable to transition through $?a_0$,$!a_0$ again, but otherwise free to evolve independently.
(They can transition through $!a_0$,$?a_0$ and through $?a_i$,$!a_i$ for i>0 in either order)

Dissociation Rules

$a@r_0,r_1,\ldots,r_n$

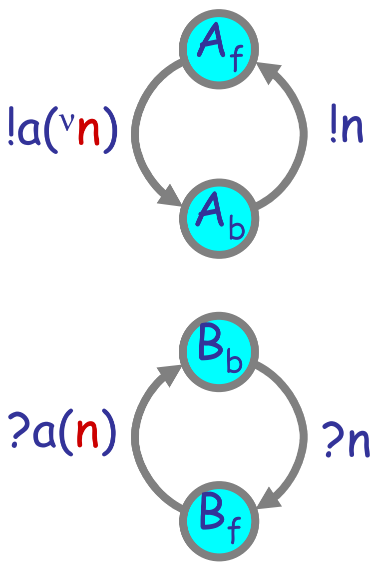


(Label abbreviation: $\%?a_i$ $\%!a_i$
Or, for i=1: $\%?a$ $\%!a$)

Complexation

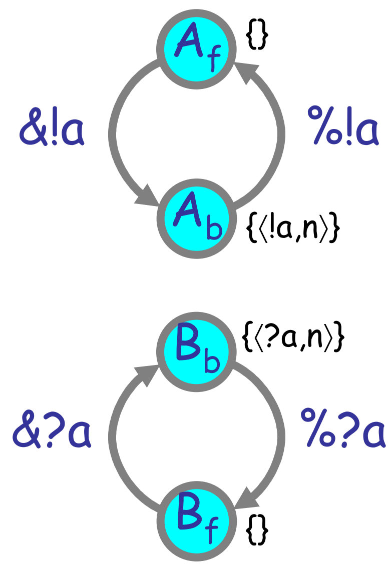
$$A+B \underset{\lambda}{\overset{\mu}{\rightleftharpoons}} AB$$

π-calculus
(informally drawn)



a@μ
n@λ

polyautomata
(formal)

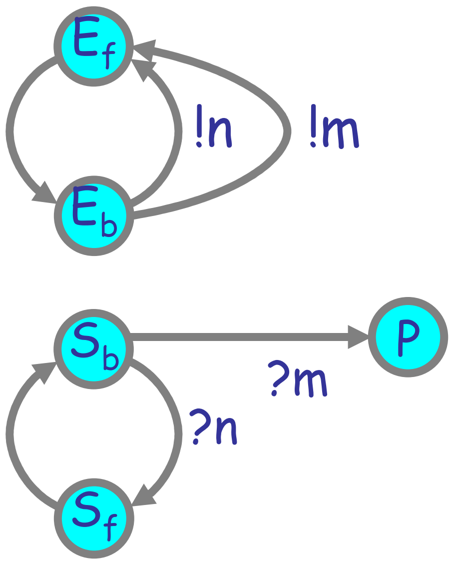


a@μ,λ

Enzymes

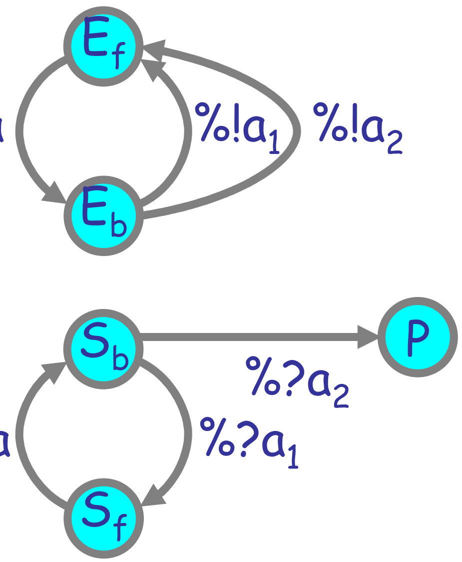
$$E+S \underset{k_1}{\overset{k_0}{\rightleftharpoons}} ES \xrightarrow{k_2} E+P$$

π-calculus (informally drawn)

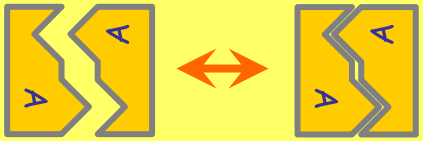


$a@k_0$
$n@k_1$
$m@k_2$

polyautomata (formal)

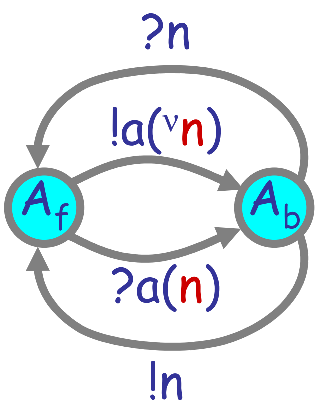


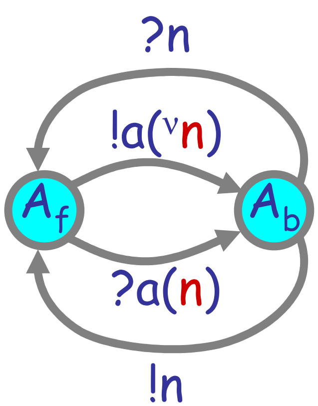
$a@k_0,k_1,k_2$



Homodimerization

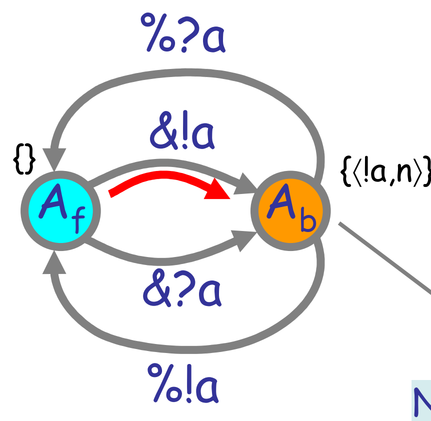
π-calculus
(informally drawn)



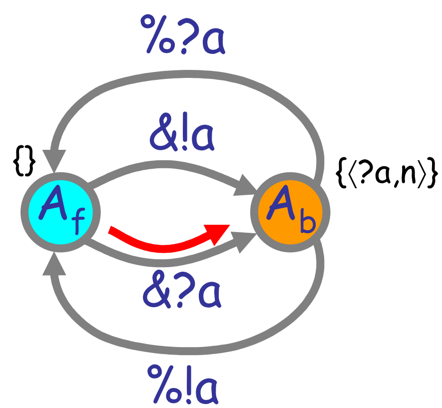


a@k_0, n@k_1

polyautomata
(formal)



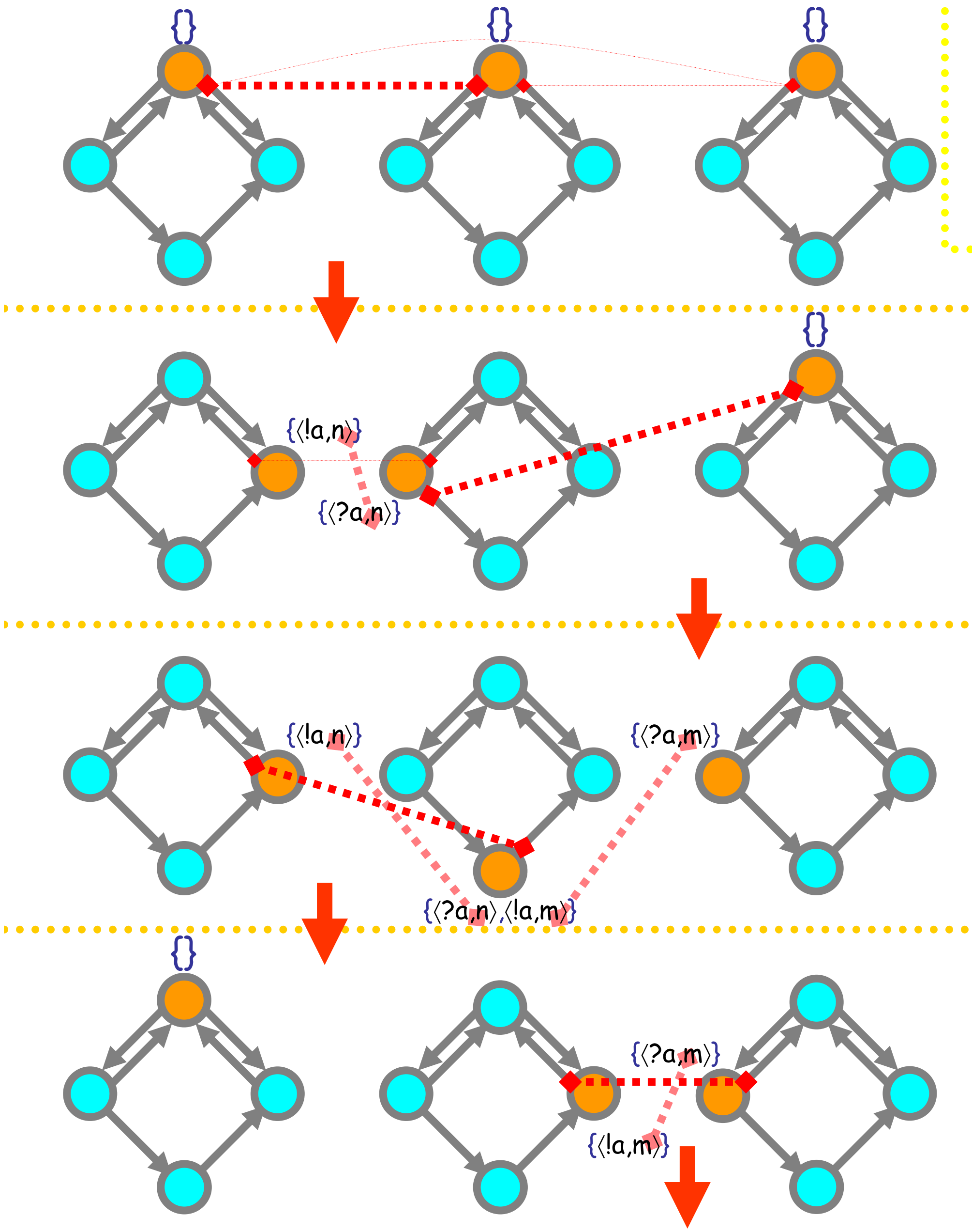
Now this can do only a %!a with the *same copy*

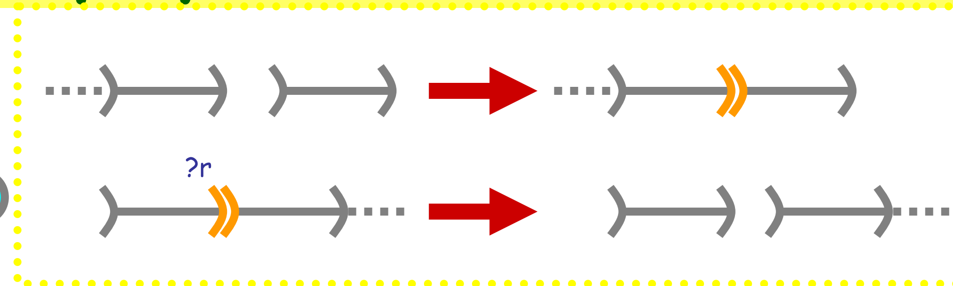


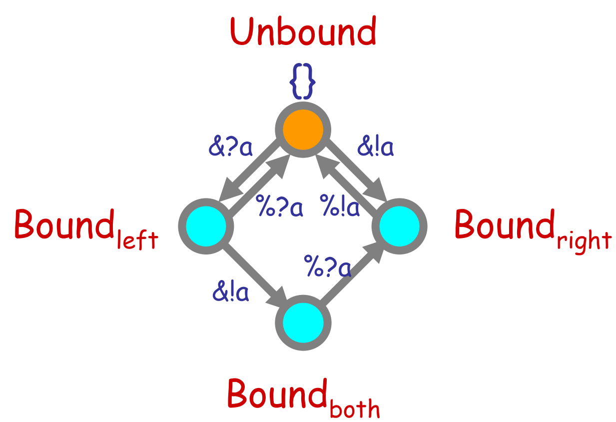
a@k_0,k_1

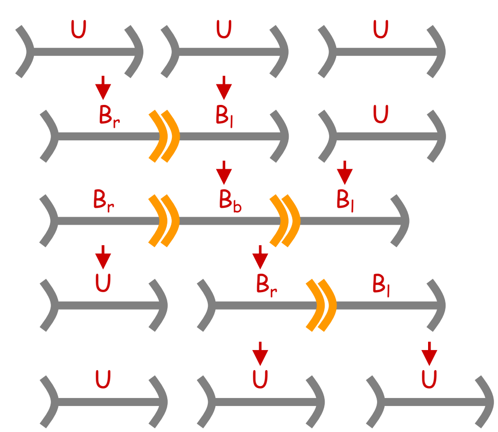
Actin-like

Polymerization/Depolymerization









Summary

- Polyautomata
  - Carry "tokens" in the current state
  - Fresh tokens created on complexation
  - Prevent reusing resources before releasing resources
- Uses
  - As a graphical automata-like notation for complexation
  - As a finite subset of π-calculus, beyond interacting automata
- Applicability
  - Can represent complexation, enzymatic reactions, some polymerization

Q?