Molecules as Automata
(Refresh)

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Chemical Systems

- Finite Stochastic Reaction Networks

$A \rightarrow^{r} B_1 + \ldots + B_n$	$(n \geq 0)$	Unary Reaction	$d[A]/dt = -r[A]$	Exponential Decay
$A_1 + A_2 \rightarrow^{r} B_1 + \ldots + B_n$	$(n \geq 0)$	Hetero Reaction	$d[A_i]/dt = -r[A_1][A_2]$	Mass Action Law
$A + A \rightarrow^{r} B_1 + \ldots + B_n$	$(n \geq 0)$	Homeo Reaction	$d[A]/dt = -2r[A]^2$	Mass Action Law

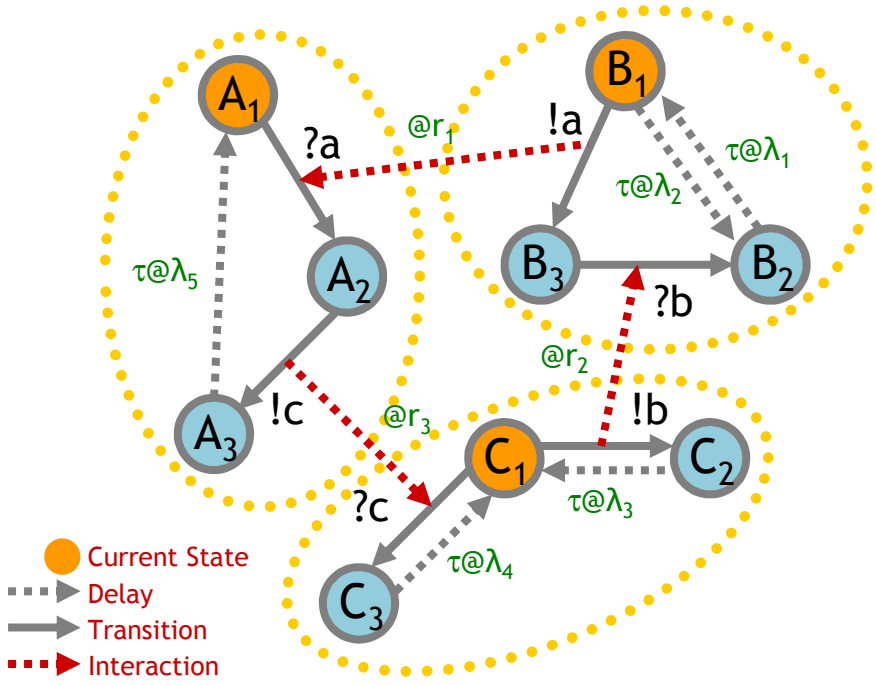
(assuming $A \neq B_i \neq A_j$ for all i,j)

Process Algebra

[Hoare, Milner, Pnueli, etc.]

- Reactive systems (living organisms, computer networks, operating systems, …)
  - Math is based on *entities that react/interact with their environment ("processes")*, not on functions from domains to codomains.
- Concurrent
  - Events (reactions/interactions) happen concurrently and asynchronously, not sequentially like in function composition.
- Stochastic
  - Or probabilistic, or nondeterministic, but is never about deterministic system evolution.
- Stateful
  - Each concurrent activity ("process") maintains its own local state, as opposed to stateless functions from inputs to outputs.
- Discrete
  - Evolution through discrete transitions between discrete states, not incremental changes of continuous quantities.
- Kinetics of interaction
  - An "interaction" is anything that moves a system from one state to another.

Interacting Automata



Interactions have rates. Actions DO NOT have rates.

The equivalent process algebra model

new $a@r_1$
new $b@r_2$
new $c@r_3$

Communication channels

$A_1 = ?a; A_2$
$A_2 = !c; A_3$
$A_3 = \tau@\lambda_5; A_1$

$B_1 = \tau@\lambda_2; B_2 + !a; B_3$
$B_2 = \tau@\lambda_1; B_1$
$B_3 = ?b; B_2$

$C_1 = !b; C_2 + ?c; C_3$
$C_2 = \tau@\lambda_3; C_1$
$C_3 = \tau@\lambda_4; C_2$

Automata

$A_1 \mid B_1 \mid C_1$

The system and initial state

Chemical Ground Form (CGF)

$E ::= 0 \;:\; X=M,\, E$ — Reagents

$M ::= 0 \;:\; \pi;P \oplus M$ — Molecules

$P ::= 0 \;:\; X \mid P$ — Solutions

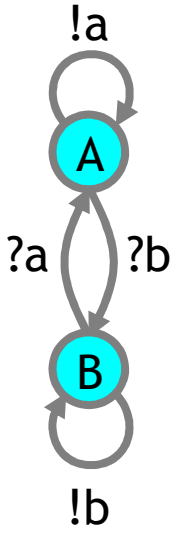
$\pi ::= \tau_{(r)} \;:\; ?a_{(r)} \;:\; !a_{(r)}$ — Actions (delay, input, output)

$CGF ::= E,P$ — Reagents plus Initial Conditions

A stochastic subset of CCS
(no values, no restriction)

(To translate chemistry to processes we need a bit more than interacting automata: we may have "+" on the right of $\rightarrow$, that is we may need "|" after π.)

$\oplus$ is stochastic choice (vs. + for chemical reactions)
0 is the null solution ($P|0 = 0|P = P$)
and null molecule ($M \oplus 0 = 0 \oplus M = M$)
Each X in E is a distinct *species*
Each name a is assigned a fixed rate r: $a_{(r)}$



Ex: Interacting Automata
(= finite-control CGFs: they use "|" only in initial conditions):

$A = !a;A \oplus ?b;B$ — Automaton in state A

$B = !b;B \oplus ?a;A$ — Automaton in state B

$A|A|B|B$ — Initial conditions: 2A and 2B

Quantitative Process Semantics