Biology Inspired Modelling of Distributed Computing

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What is distributed computing?

- Separated components communicate and coordinate their actions by passing messages.
- They have local memory.
- Additional properties (like independent failure, ad-hoc network structure) are sometimes assumed.
- Components may work on a common goal or try to achieve their own goals.

What has that to do with Biology?

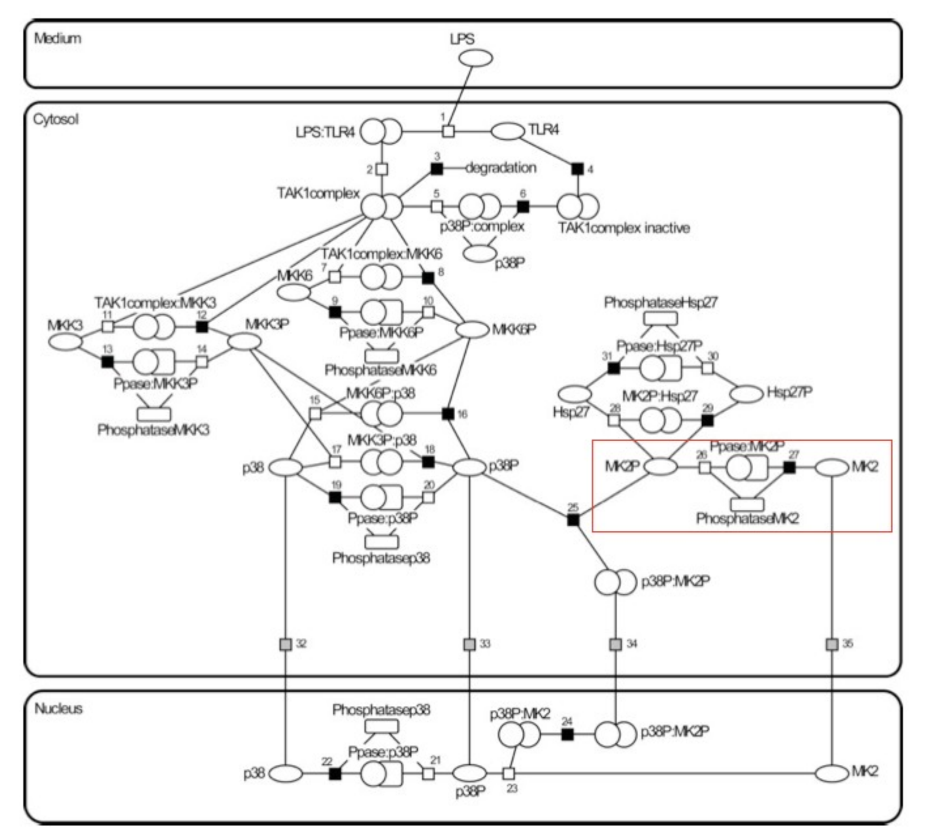
- Independent entities exist in many forms.
- Organisms, cells, proteins, small molecules, atoms …
- They do not share a global memory, but interact by sending “messages”.
- Systems are compositional, their behaviour is emergent.

How do they come together?

- Similar techniques are used for modelling.
- Methods used include Petri nets, cellular automata, state machines...
- Process calculi are used in both fields.
- “Process calculi provide a tool for the high-level description of interactions, communications, and synchronizations between a collection of independent agents or processes” (wikipedia)

Existing applications

- Stochastic process algebras, e. g. BioPEPA.
- Network is fully specified, with all possible reactions.
- Kinetic rates enable prediction of concentrations
- Allows testing of inhibitors and their effects on the overall network
- The structure of the network is not considered



Baroukh et al. 2010 IEEE International Conference on Bioinformatics and Biomedicine Workshops

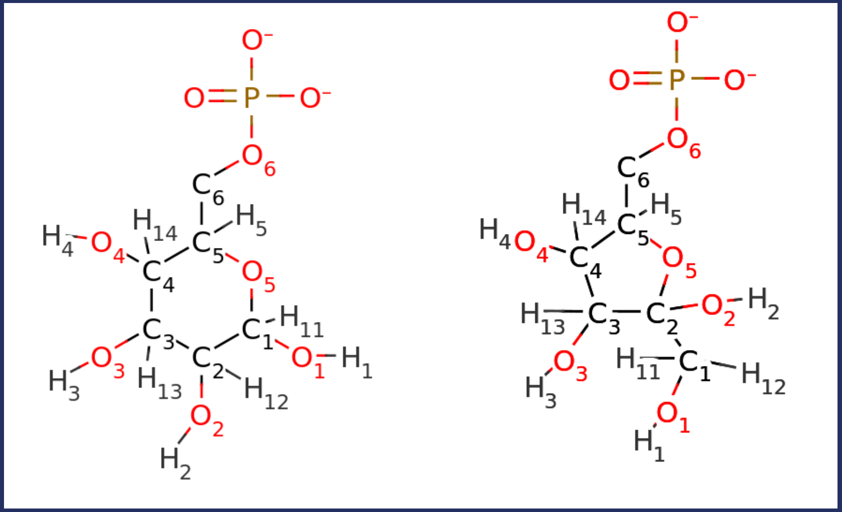
Existing applications

- What is a process here?
- How far do processes change?
- Which role plays state?
- Anything about causality and reversibility?

What do we want to do?

- Give a more structural view of the components
- The network is then an emergent property of the components
- For this, causality and reversibility should play a major role
- Reversibility can get us to states which are unreachable otherwise

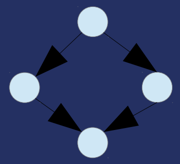
Example



- Small molecule-protein interaction
- Overall change in molecule is small
- Change is done in three phases: ring opening, movement of charge, ring closure
- The third phase is a reversal of the first phase in a different place
- 12 atoms participating

Example

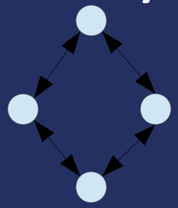
- How would a calculus work?
- We have four atoms, which can interact in pairs. The order is arbitrarily
- $a.P \mid \overline{a}.Q \mid b.R \mid \overline{b}.S$
- This leaves the options to do a and b in any order, giving us a state diagram like this:



- We build the system behaviour from components

Reversibility

- Can we model reversibility?
- Traditional CCS does not remember where we came from
- “Communication keys” can do this:
- a.P | $\overline{a}$.Q | b.R | $\overline{b}$.S becomes
  a[1].P | $\overline{a[1]}$.Q | b[2].R | $\overline{b[2]}$.S
- By breaking bonds we can go back in any order, giving us a state diagram like this:



Causality

- Can we model causality?
- a.b.P | a.b.Q would imply “a causing b”
- Reversing only possible in causal order
- Is there out-of-causal-order reversibility?
- How can we model this?
- If events of the same process are independent, how do we model that?
- CCS has “choice”: a.b.P + b.a.P

Things to do

- Search for more examples
- How far can we model them with existing calculi?
- What do we need to include?
- How do reversibility and causality influence each other?

Questions?