Biological Systems as Concurrent Processes

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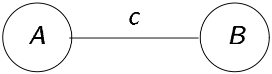
Modeling Systems

- Software/hardware systems consisting of multiple components:
  - Concurrency: Components execute simultaneously.
  - Interaction: Components may communicate with their neighbors.
  - Mobility: Components may move to another neighborhood.
- May be formally modelled in some calculus.
  - E.g. π-calculus (Milner, 1992).
- Example: components A and B sharing a communication channel c.

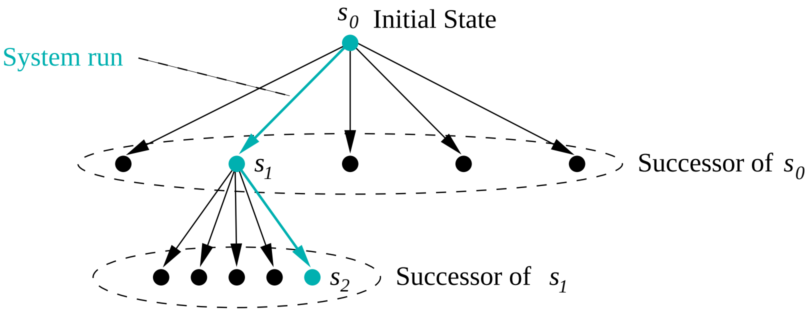


  - System: new c $(A \mid B)$.
  - Components: $A := \overline{c}\langle a \rangle.A', B := c(x).B'$.
  - Interaction: new c $(A \mid B) \rightarrow$ new c $(A' \mid B'[a/x])$.

The semantics of a concurrent system is defined by its formal model.

Behaviors of Systems

The possible system runs are paths in the graph of system states.

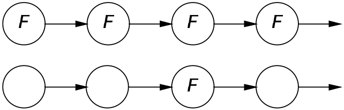


From an initial state, multiple runs may emerge (non-determinism).

Properties of Systems

We need to specify properties required from every possible system run.

- Temporal logic:
  - $\Box F$: "F will always hold".
  - $\Diamond F$: "eventually F will hold".



- Specification: $\Box(x > 0 \Rightarrow \Diamond x = 0)$.

  Every time x becomes greater than 0, it will become 0 again.
- Verification: prove that every run of a system (e.g. modelled in π-calculus) satisfies a specification (e.g. described in temporal logic).
- Model checking: check that above holds in a system that has only a finite number of states.

Hardware and software verification is a very active research area today.

Biological Systems

From the BioSPI project (http://www.wisdom.weizmann.ac.il/~biospi):

We employ 5 major principles in modeling biochemical processes as concurrent systems:

- *Pathways, molecules and molecular domains as computational processes.*
- *Complementary molecular determinants as communication channels.*
- *Molecular interaction and modification as communication and change of channel names.*
- *The integrity of molecules, complexes and compartment as channels with restricted scope.*
- *The formation of complexes and translocation of molecule as extrusion of restricted channels.*

Based on this strong correspondence between the calculus and biochemical networks, we can incrementally represent detailed information on biochemical systems in a structured, biologically faithful fashion. The resulting representations can be used in simulation, analysis and verification.

Example: A Chemical Reaction

- A reaction equation: $\mathrm{Na} + \mathrm{Cl} \leftrightarrow \mathrm{Na}^{+} + \mathrm{Cl}^{-}$

  A salt (NaCL) molecule consists of a Na atom and a Cl atom shared by a "ionic bond": the Na atom gives an electron to the Cl atom such that the resulting ions are coupled by electrostatic attraction; to separate the atoms, the process has to be reversed.

- A corresponding *pi*-calculus model with four atoms:

  $System := \mathrm{new}\ e_1, e_2\ (Na \mid Na \mid Cl \mid Cl).$
  $Na := \overline{e_1}\langle\rangle.NaPlus.$
  $NaPlus := e_2().Na.$
  $Cl := e_1().ClMinus.$
  $ClMinus := \overline{e_2}\langle\rangle.Cl.$

Molecules can be modelled as concurrent systems of atoms that emit and absorb electrons.