Efficient Analysis of Population Protocols and Chemical Reaction Networks

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Motivation
Population protocols and chemical reaction networks model stochastic systems consisting of many interacting entities. Even though every single entity follows simple rules, their interactions lead to complex and hard to understand system behavior. We develop efficient analysis techniques that help us to gain valuable insight into the dynamics of evolving systems.

Population Protocols

Population Protocols Verification

Are there at least 4 sick birds?
- Each bird is in a state of \{0, 1, 2, 3, 4\}
- Initially, sick birds in state 1, healthy birds in state 0
- \((m, n) \rightarrow (m + n, 0)\) if \(m + n < 4\)
- \((m, n) \rightarrow (4, 4)\) if \(m + n \geq 4\)

Tool: Peregrine (https://peregrine.model.in.tum.de)

Chemical Reaction Networks (CRN)

\[
\begin{align*}
2H_2 + O_2 &\rightarrow 2H_2O \\
C + O_2 &\rightarrow CO_2 \\
6CO_2 + 6H_2O &\rightarrow C_6H_{12}O_6 + 6O_2
\end{align*}
\]

Differences to population protocols:
- number of entities does not stay constant
- continuous time (vs. discrete time)
- focus on modeling (vs. programming)

Because numerical analysis is often infeasible, one often has to use simulation to understand CRNs.

Approximate Simulation of CRNs

Simulation-based analysis needs many simulations and each simulation may involve many interactions. We introduce an approximate simulation technique called segmental simulation. The main ideas are:

- Acceleration: Apply multiple reactions at once.
- Memoization: Reuse parts of previous simulations, called segments.
- Abstraction: Split state space into regions to only reuse segments from same region.

Tool: SAQuaiA (https://sequaia.model.in.tum.de)

References

Evolving Systems