Efficient Analysis of Population Protocols and Chemical Reaction Networks

Martin Helfrich

helfrich@in.tum.de

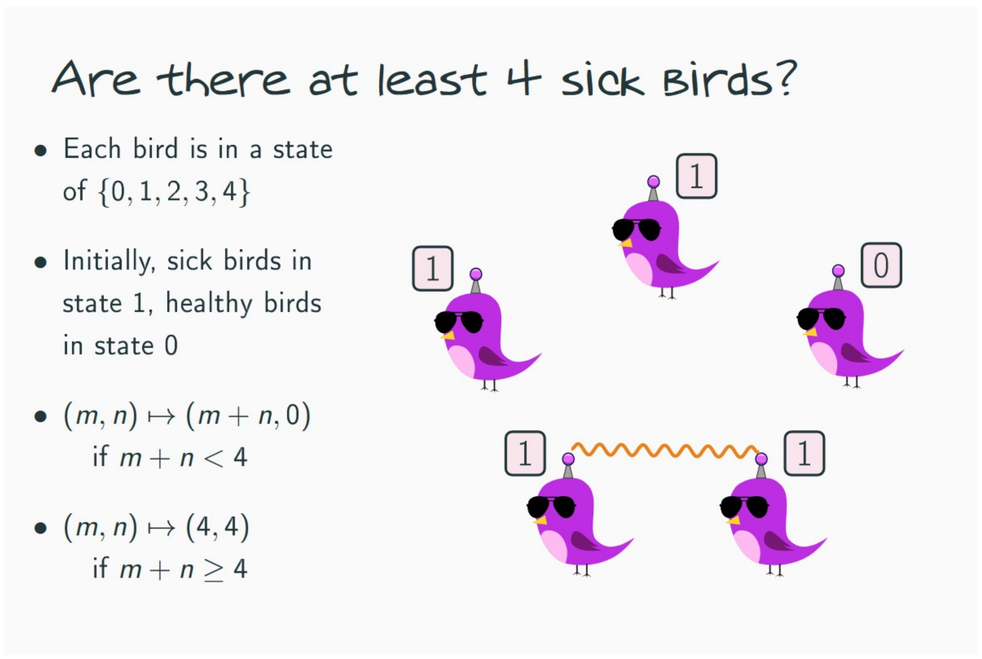
Supervisors: Javier Esparza & Jan Křetínský

Collaborators: Philipp Czerner (ConVeY) & Javier Esparza (ConVeY)

Motivation

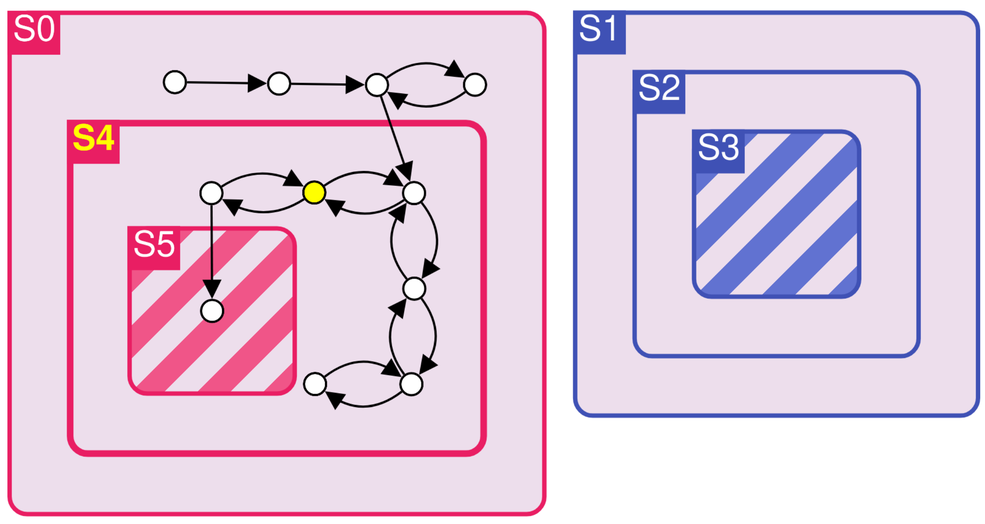
Population protocols and *chemical reaction networks* model stochastic systems consisting of many interacting entities. Even through every single entity follows simple rules, their interactions lead to complex and hard to understand system behavior. We develop efficient analysis techniques that help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

Population Protocols



Population Protocols Verification

Stage graphs are formal objects that can efficiently verify population protocols.



They help us understand:

- How does the protocol work?
- Why is it correct / incorrect?
- How fast does it compute?

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

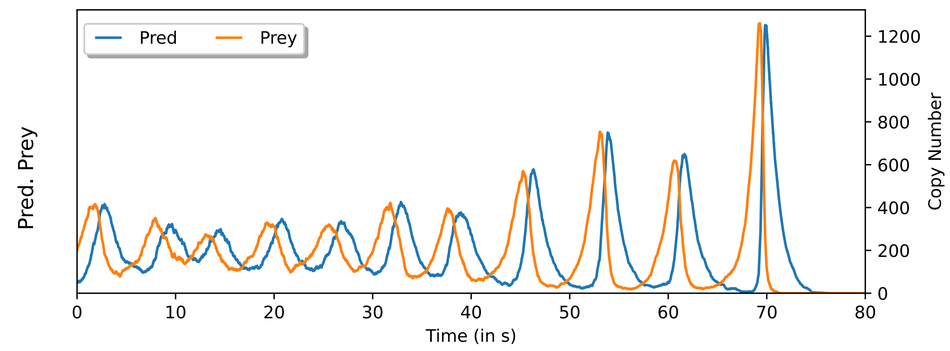
Chemical Reaction Networks (CRN)

$$2H_2 + O_2 \to 2H_2O$$
$$C + O_2 \to CO_2$$
$$6CO_2 + 6H_2O \to C_6H_{12}O_6 + 6O_2$$

Differences to population protocols:

- number of entities does not stay constant
- continuous time (vs. discrete time)
- focus on modeling (vs. programming)

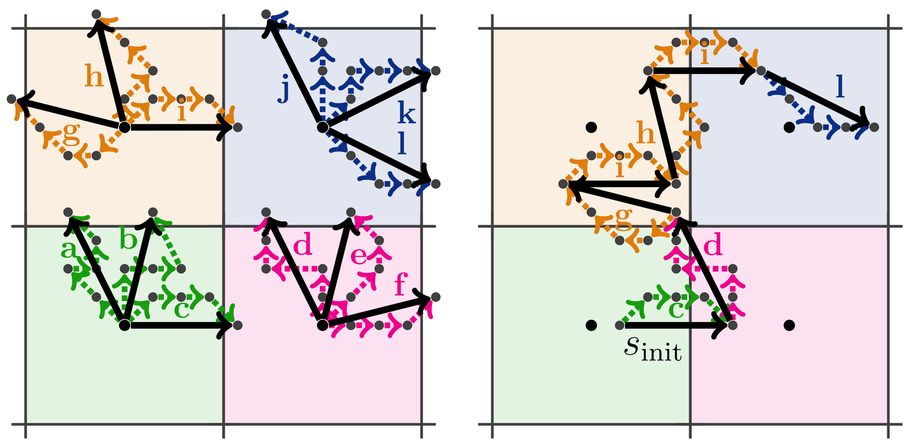
Because numerical analysis is often infeasible, one often has to use simulation to understand CRNs.



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

[1] M. Blondin et al. "Checking Qualitative Liveness Properties of Replicated Systems with Stochastic Scheduling". In: *Computer Aided Verification*. Ed. by S. K. Lahiri et al. Cham: Springer International Publishing, 2020, pp. 372–397.

[2] M. Helfrich et al. "Abstraction-Based Segmental Simulation of Chemical Reaction Networks". In: *Computational Methods in Systems Biology*. Ed. by I. Petre et al. Cham: Springer International Publishing, 2022, pp. 41–60.