Using semantic equivalences to model biological behaviour

Vashti Galpin*, Federica Ciocchetta†, Jane Hillston‡

*Laboratory for Foundations of Computer Science, School of Informatics, University of Edinburgh; †COSBI, Trento, Italy; ‡CSBE, University of Edinburgh

Process algebra modelling of biological systems

Biochemical reactions

\[ S \in E \xrightarrow{\text{SE}} P + E \]

- Bio-PEPA model
  - \[ S = \{s_1, s_2, \ldots, s_n\} \]
  - \[ E = \{e_1, e_2, \ldots, e_m\} \]
  - \[ SE = \{s_i \cdot e_j : s_i \in S, e_j \in E\} \]
  - \[ P = \{p_1, p_2, \ldots, p_k\} \]
- \[ \text{discretisation} \]
- Semantic equivalences
  - \[ \text{ODE analysis} \]
  - \[ \text{stochastic simulation} \]

Biological reactions

\[ S \in E \xrightarrow{\text{SE}} P + E \]

- Bio-PEPA model with levels
  - \[ S = \{s_1, s_2, \ldots, s_n\} \]
  - \[ E = \{e_1, e_2, \ldots, e_m\} \]
  - \[ SE = \{s_i \cdot e_j : s_i \in S, e_j \in E\} \]
  - \[ P = \{p_1, p_2, \ldots, p_k\} \]
- \[ \text{Labelled transition system (LTS) with levels} \]
  - \[ \text{transition} \]
  - \[ \text{for a species} \]
  - \[ \text{for each state in} \]
  - \[ \text{for reaction} \]

Equivalent behaviour based on two discretisations of same model: compression bisimulation

\[ S \in E \xrightarrow{\text{SE}} P + E \]

- \[ \text{transition system over sets of states} \]
  - \[ \text{maximum level for all species is 7} \]
- \[ \text{transition system over sets of states with the same reactions} \]
  - \[ \text{maximum level for all species is 7} \]

Equivalent behaviour based on different abstractions of reactions: parameterised bisimulation

\[ S \in E \xrightarrow{\text{SE}} P + E \]

- \[ \text{parameterised bisimulation uses functions on transition labels to determine which transitions match} \]
- \[ \text{for this example, reaction names need to be matched using the functions} \]
- \[ \text{for this example, rate information can be extracted by summing over transitions with the same reaction name (after applying function)} \]
- \[ \text{state (5, 2, 1, 2) has two transitions} \]
- \[ \text{applying name function and rate extraction} \]
- \[ \text{if } r = \alpha + \beta \text{ and target states match then state (5, 2, 2) has a matching transition} \]

References and acknowledgments

- V. Galpin, Equivalences for a biological process algebra, submitted for publication.

Vashti Galpin is supported by EPSRC Grant EP-E014139/1.
Jane Hillston is supported by EPSRC ARP EF/C55396/01.
The Centre for Systems Biology at Edinburgh is a Centre for Integrative Systems Biology (CSB) funded by the BBSRC and EPSRC in 2006.