Feasibility of Organizations - A Refinement of Chemical Organization Theory with Application to P Systems

Stephan Peter, Tomas Veloz, Peter Dittrich
University Jena

Bio Systems Analysis

JCB
Jena Centre for Bioinformatics

Contents

- Chemical Reaction Networks
- Chemical Organizations
- Fixed Points
- Feasibility
- P Systems
- Conclusions & Future Work

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P. Dittrich

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1) Set of species $S = \{s_{1,} \ldots, s_m\}$ s_1, s_2, s_3, s_4

Statics

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1) Set of species $S=\{s_1,\ldots,s_m\}$ s_1, s_2, s_3, s_4

2) Set of reaction rules $R=\{r_1,\ldots,r_n\}$

$$r_1:\ s_1+s_3 \rightarrow 2s_3$$
$$r_2:\ s_2+s_3 \rightarrow s_1+s_2,$$
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1) Set of species $S=\{s_1,\ldots,s_m\}$ s_1, s_2, s_3, s_4

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$$
\begin{aligned}
r_1&: s_1 + s_3 \rightarrow 2s_3\\
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r_4&: s_1 + s_4 \rightarrow s_1 + s_2
\end{aligned}
$$

Stoichiometric matrix

$$
N=\begin{pmatrix} -1 & +1 & 0 & 0\\ 0 & 0 & -1 & +1\\ +1 & -1 & 0 & 0\\ 0 & 0 & +1 & -1 \end{pmatrix} \in \mathbb{Z}^{m\,x\,n}
$$

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Dynamics

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1) IVP

$$\dot{x} = N \cdot v(x;k),\ x(0) \equiv x_0$$

Dynamics

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$$\dot{x} = N \cdot v(x;k),\ x(0) \equiv x_0$$

2) Mass action kinetics

$$(v(x;k))_r = k_r \cdot \prod_{s=1}^{m} x^{a_{rs}}$$

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Definition

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A **chemical organization** is a subset of species $O \subseteq S$, which is:

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A **chemical organization** is a subset of species $O \subseteq S$, which is:

1) **closed**: The products of all reactions possible on O are elements of O.

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Definition

A **chemical organization** is a subset of species $O \subseteq S$, which is:

1) **closed**: The products of all reactions possible on O are elements of O.

2) **self-maintaining**: There is a flux vector $v \in \mathbb{R}^n_+$ with

$$N \cdot v \geq 0$$

and

$v_r > 0$ iff the reaction r is possible with the species of O.

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Organizational structure

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Lattice of organizations:

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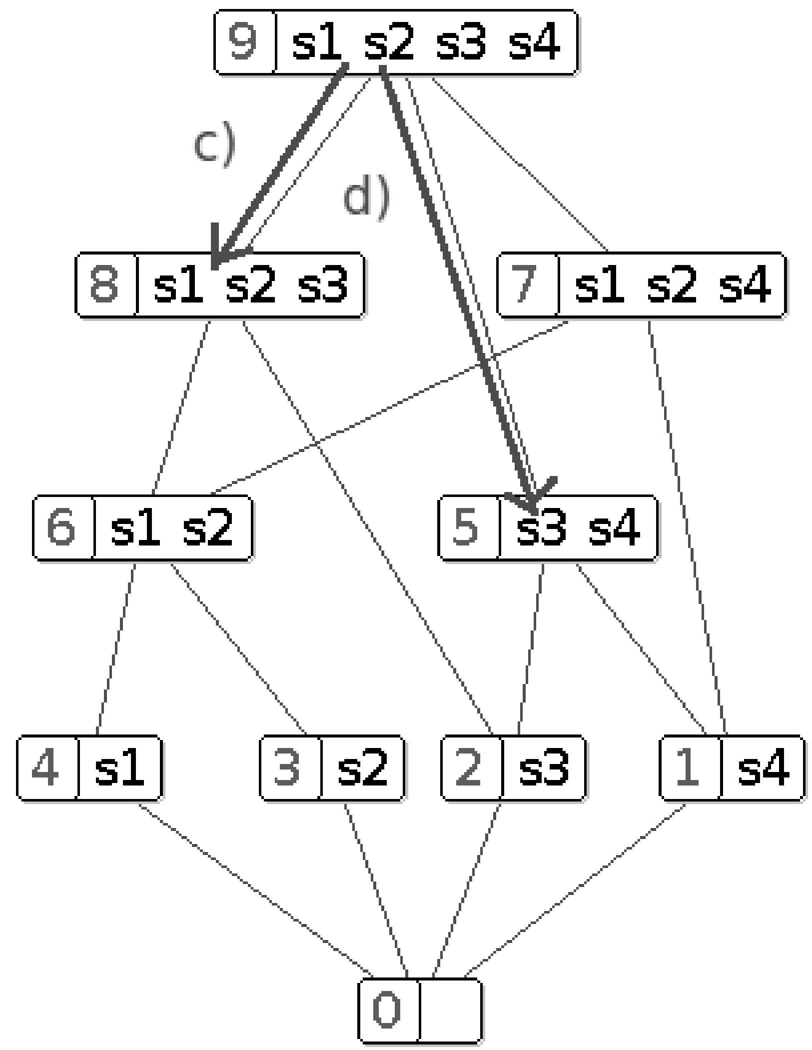
Lattice of organizations:



Organizational structure

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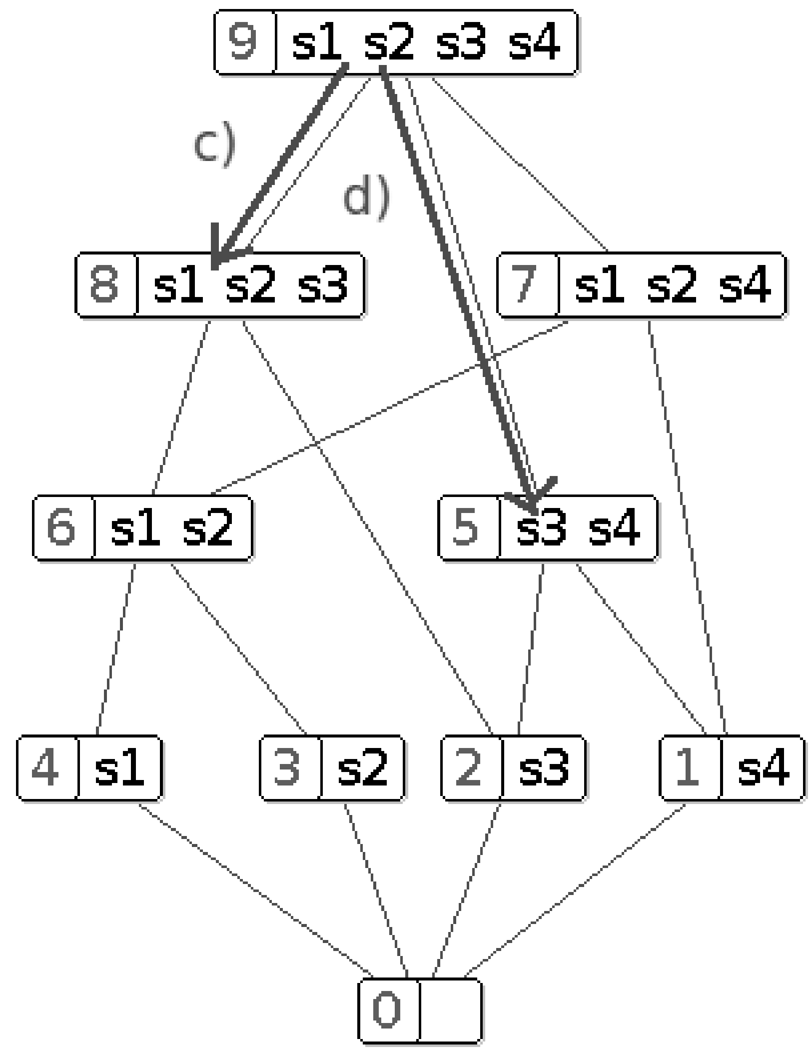
Lattice of organizations:



high level of abstraction

Theory

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Definition: A **fixed point** $\hat{x}$ is a state with $0 = N \cdot v(\hat{x}; k)$.

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Theorem: The species present in a fixed point form an organization.

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Definition: A **fixed point** $\hat{x}$ is a state with $0 = N \cdot v(\hat{x}; k)$.

Theorem: The species present in a fixed point form an organization.

→ **converse** does not hold in general!

→ **Feasibility**

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Example

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ODE System

$$\dot{x}_1 = -k_1 x_1 x_3 + k_2 x_2 x_3 \qquad \dot{x}_2 = -k_3 x_2 x_4 + k_4 x_1 x_4$$

$$\dot{x}_3 = +k_1 x_1 x_3 - k_2 x_2 x_3 \qquad \dot{x}_4 = +k_3 x_2 x_4 - k_4 x_1 x_4$$

Example

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Fixed points

Subsets of species

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Fixed points

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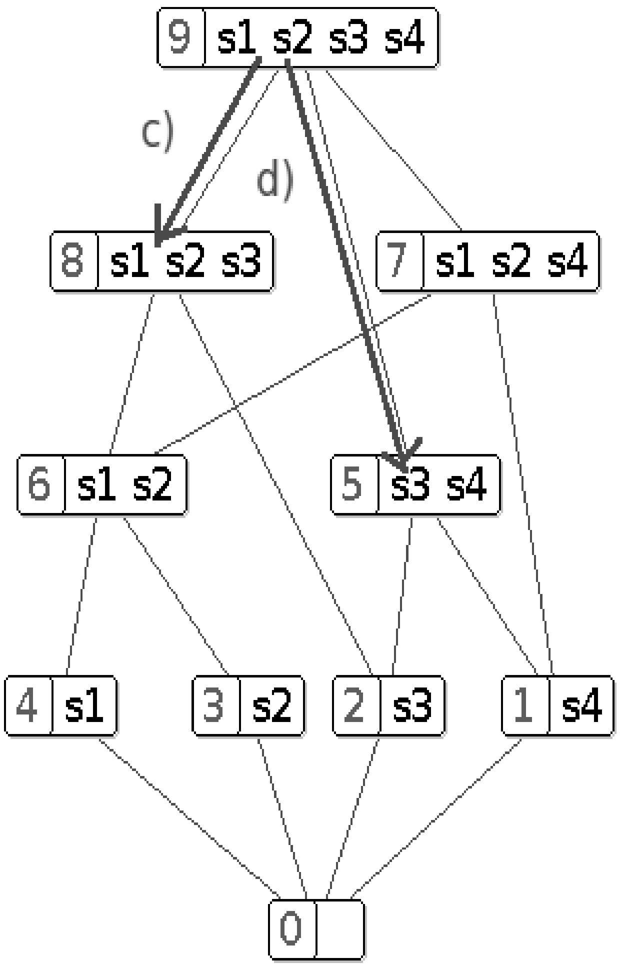

Example

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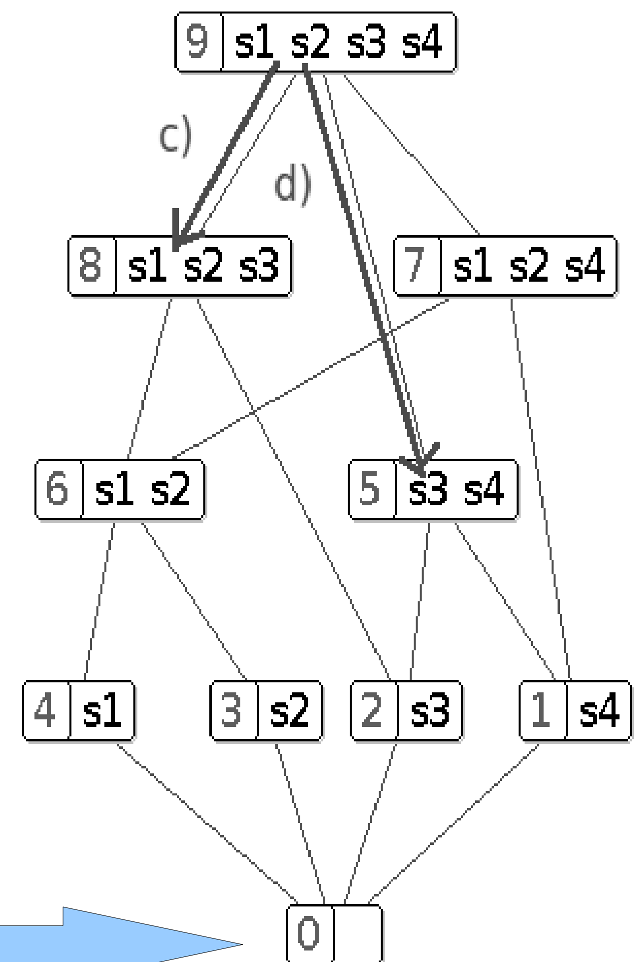
Fixed points

$$(0,0,0,0)$$

Subsets of species



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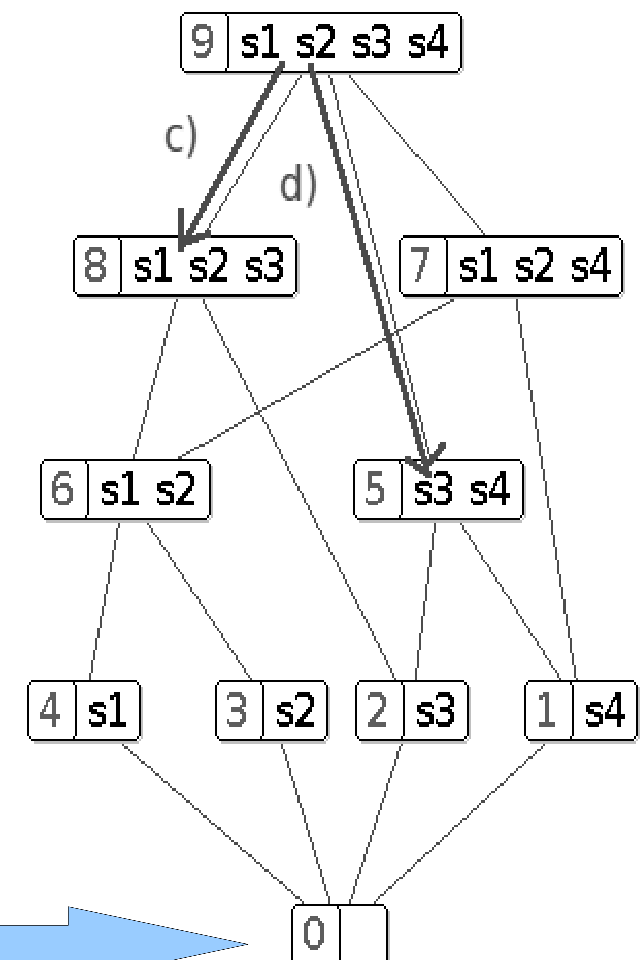
Fixed points

$$(*, 0, 0, 0), (0, *, 0, 0),$$
$$(0, 0, *, 0), (0, 0, 0, *)$$

$$(0, 0, 0, 0)$$

Subsets of species



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Fixed points

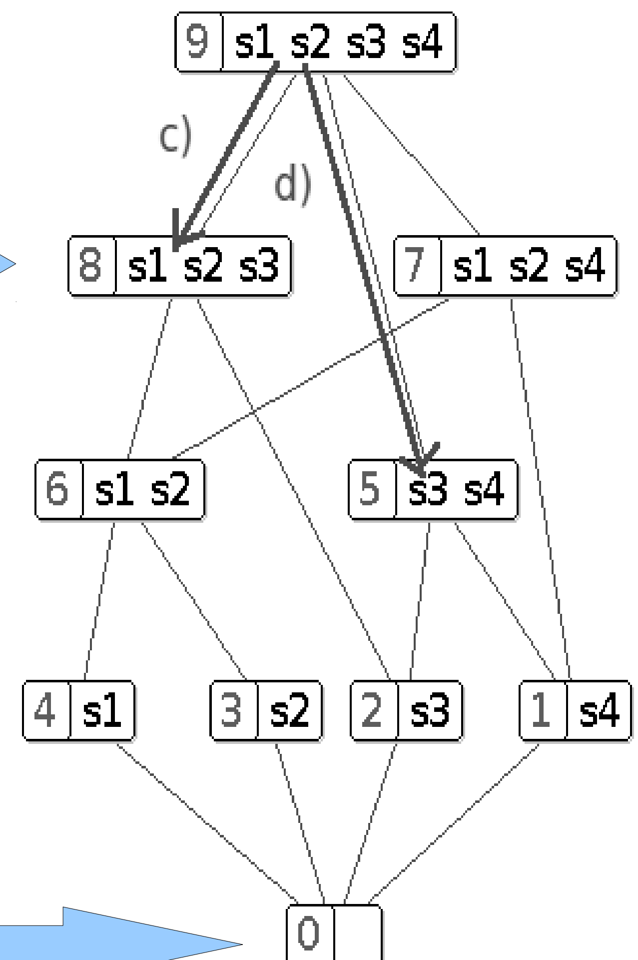
$$(\frac{k_2}{k_1} x_2, x_2, *, 0), \ (\frac{k_3}{k_4} x_2, x_2, *, 0)$$

$$(*, *, 0, 0), (0, 0, *, *)$$

$$(*, 0, 0, 0), (0, *, 0, 0),$$
$$(0, 0, *, 0), (0, 0, 0, *)$$

$$(0, 0, 0, 0)$$

Subsets of species



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Fixed points

$$\left(\frac{k_2}{k_1}x_2, x_2, *, *\right), \quad \frac{k_2}{k_1} = \frac{k_3}{k_4}$$

$$\left(\frac{k_2}{k_1}x_2, x_2, *, 0\right), \left(\frac{k_3}{k_4}x_2, x_2, *, 0\right)$$

$$(*, *, 0, 0), (0, 0, *, *)$$

$$(*, 0, 0, 0), (0, *, 0, 0),$$
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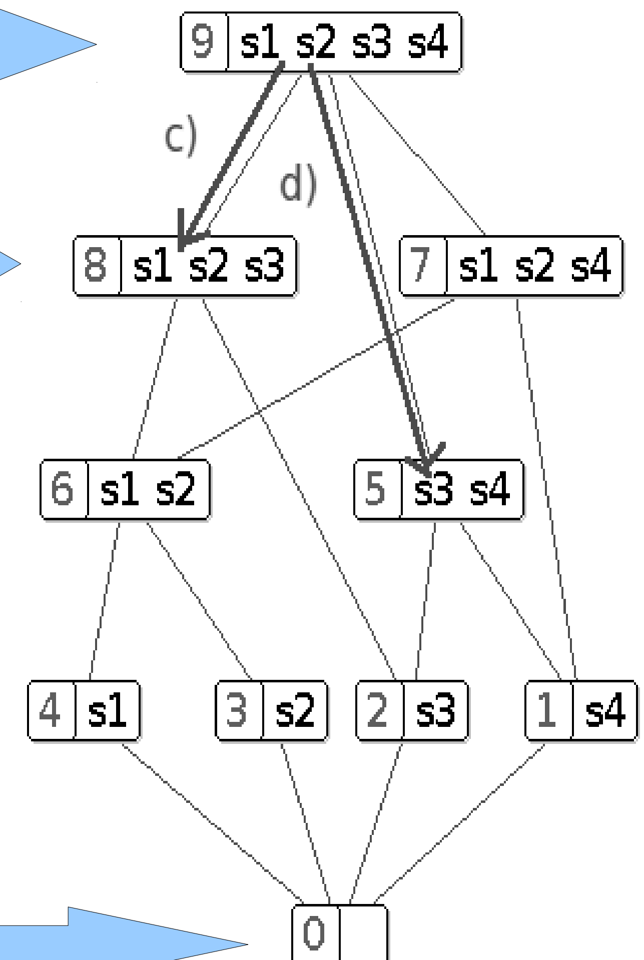
$$(0, 0, 0, 0)$$

Subsets of species



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Fixed points

$$\left(\frac{k_2}{k_1} x_2, x_2, *, *\right), \quad \frac{k_2}{k_1} = \frac{k_3}{k_4}$$

Unfeasible organization

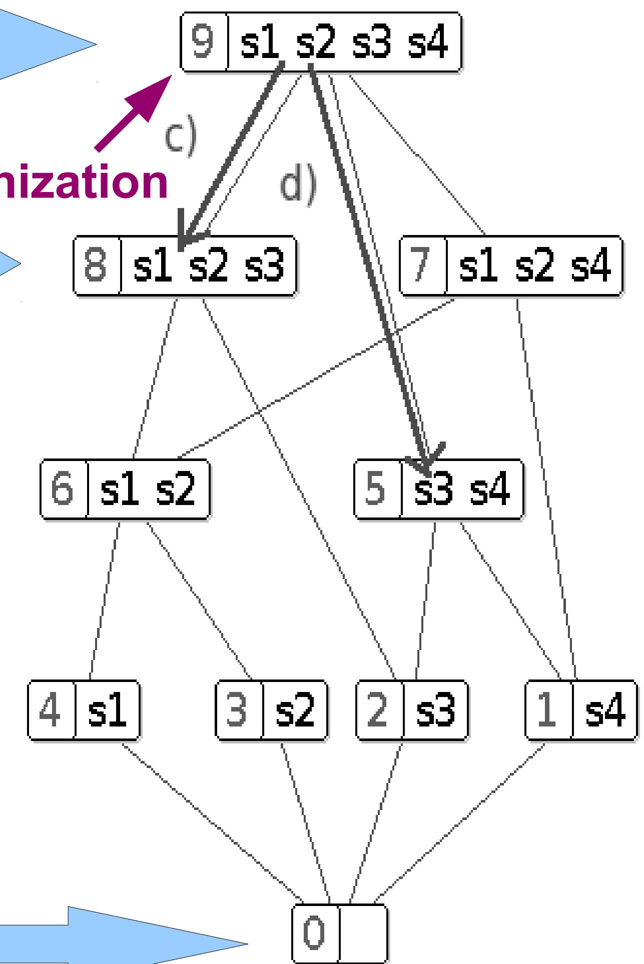
$$\left(\frac{k_2}{k_1} x_2, x_2, *, 0\right), \left(\frac{k_3}{k_4} x_2, x_2, *, 0\right)$$

$$(*, *, 0, 0), (0, 0, *, *)$$

$$(*, 0, 0, 0), (0, *, 0, 0),$$
$$(0, 0, *, 0), (0, 0, 0, *)$$

$$(0, 0, 0, 0)$$

Subsets of species



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Definition & Criterion

Definition & **Criterion** for feasibility of an organization

➡ See paper! 🙂

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Definition & Criterion

Definition & **Criterion** for feasibility of an organization

→ See paper!

→ feasible ← **Organization** → unfeasible

feasible ↓ probable to be observed

unfeasible ↓ not probable to be observed

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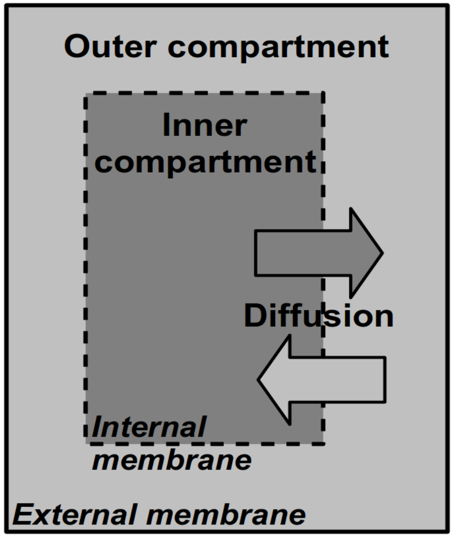
Organizations and Membranes



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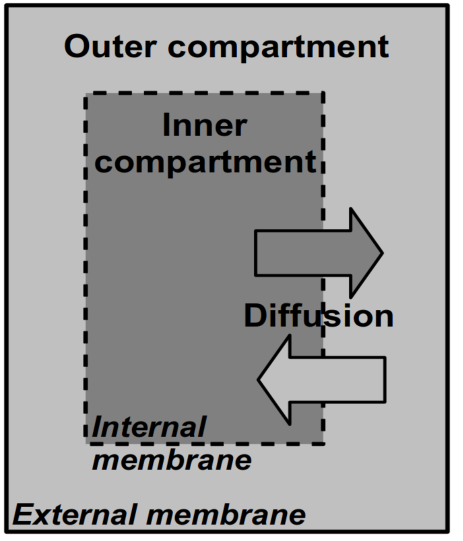

Reactions

$$r_1^i : s_1^i + s_3^i \rightarrow 2s_3^i$$
$$r_2^i : s_2^i + s_3^i \rightarrow s_1^i + s_2^i,$$
$$r_3^i : s_2^i + s_4^i \rightarrow 2s_4^i$$
$$r_4^i : s_1^i + s_4^i \rightarrow s_1^i + s_2^i$$

Inner reactions

$$r_1^o : s_1^o + s_3^o \rightarrow 2s_3^o$$
$$r_2^o : s_2^o + s_3^o \rightarrow s_1^o + s_2^o,$$
$$r_3^o : s_2^o + s_4^o \rightarrow 2s_4^o$$
$$r_4^o : s_1^o + s_4^o \rightarrow s_1^o + s_2^o$$

Outer reactions

s_j^i and s_j^o, $j = 1,2,3,4$, represent the same species in each compartment.

Organizations and Membranes

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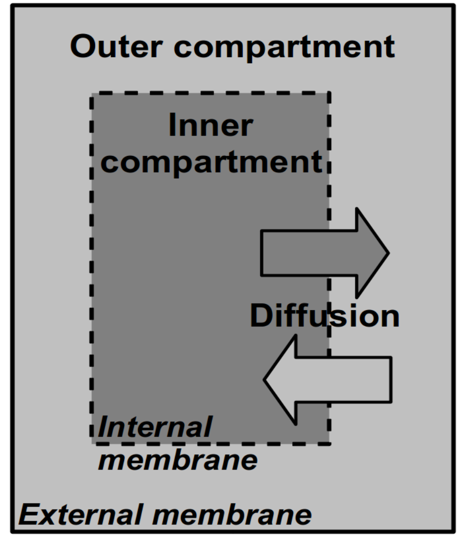


Reactions

Inner reactions

$$r^i_1 : s^i_1 + s^i_3 \to 2s^i_3$$
$$r^i_2 : s^i_2 + s^i_3 \to s^i_1 + s^i_{2,}$$
$$r^i_3 : s^i_2 + s^i_4 \to 2s^i_4$$
$$r^i_4 : s^i_1 + s^i_4 \to s^i_1 + s^i_2$$

Diffusion reactions

$$r^d_1 : s^o_1 \leftrightarrow s^i_1$$
$$r^d_2 : s^o_2 \leftrightarrow s^i_2$$
$$r^d_3 : s^o_3 \leftrightarrow s^i_3$$
$$r^d_4 : s^o_2 \leftrightarrow s^i_2$$

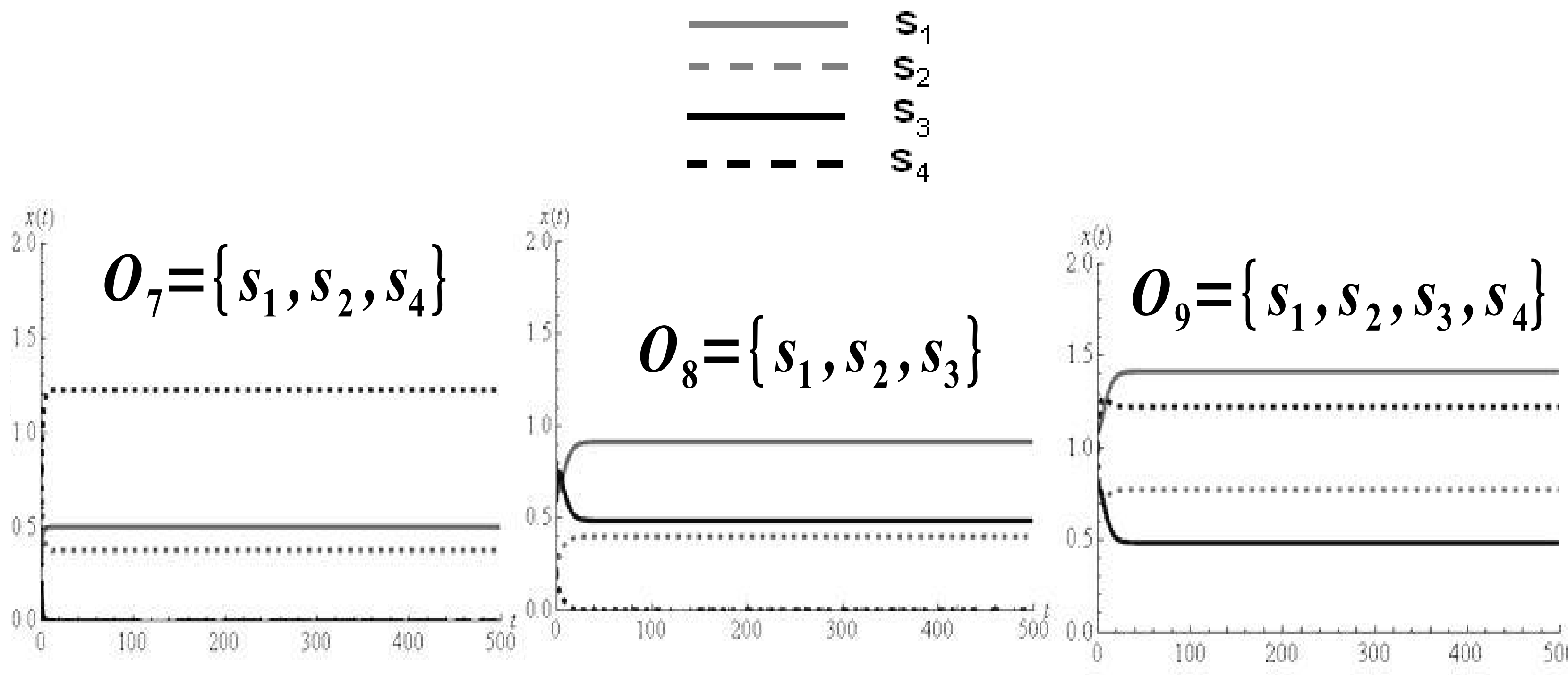
Outer reactions

$$r^o_1 : s^o_1 + s^o_3 \to 2s^o_3$$
$$r^o_2 : s^o_2 + s^o_3 \to s^o_1 + s^o_{2,}$$
$$r^o_3 : s^o_2 + s^o_4 \to 2s^o_4$$
$$r^o_4 : s^o_1 + s^o_4 \to s^o_1 + s^o_2$$

s^i_j and s^o_j, $j = 1,2,3,4$, represent the same species in each compartment.

Simulations

without diffusion



inner | outer | inner + outer

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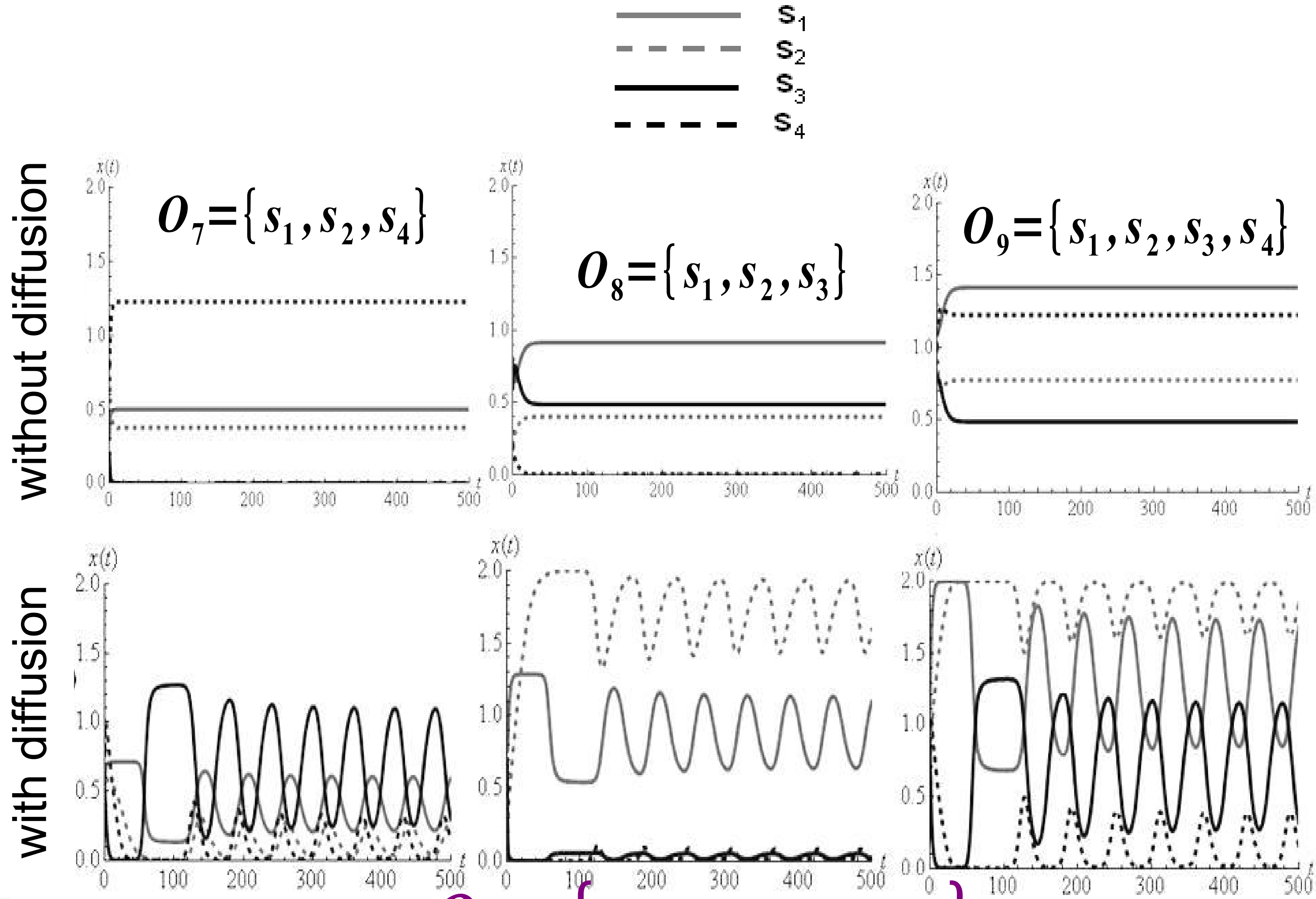
Simulations



$$O_9=\{s_1, s_2, s_3, s_4\}$$

inner | outer | inner + outer

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Conclusions

- **Feasibility** = refinement of organization theory

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Conclusions

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- **Feasibility** = refinement of organization theory

- **P-system**: organization theory applicable (to each compartment)

  membranes and feasibility are complementary principles

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Future Work

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- formalization of various ecological-like phenomena in nature, e.g., competition, depredation, symbiosis, etc.

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Future Work

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- organization theory for P systems (dynamics)

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Future Work

- formalization of various ecological-like phenomena in nature, e.g., competition, depredation, symbiosis, etc.

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- relation between different kinetic laws and feasibility of organizations

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Future Work

- formalization of various ecological-like phenomena in nature, e.g., competition, depredation, symbiosis, etc.

- organization theory for P systems (dynamics)

- relation between different kinetic laws and feasibility of organizations

- computational aspects of feasibility

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