Complexity of Model Checking for Reaction Systems

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Luca Manzoni, Ion Petre, Antonio E. Porreca

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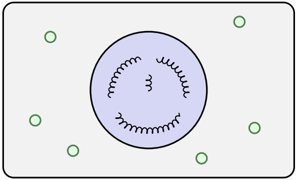
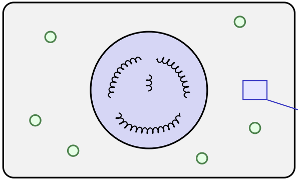
Reaction Systems

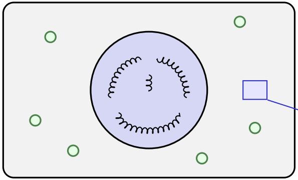


Reaction Systems



$$x + y \longrightarrow z + t$$

Reaction Systems



reactants products

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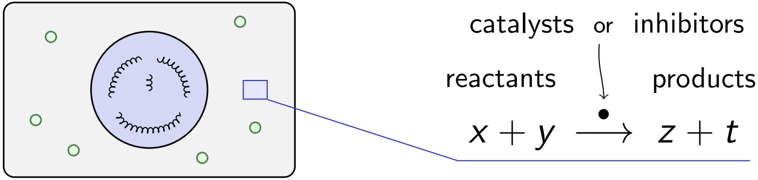

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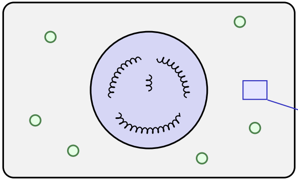

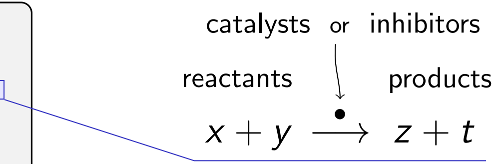

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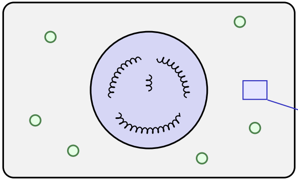
  $W = \{x, y, u\}$

Reaction Systems



catalysts or inhibitors

reactants → products

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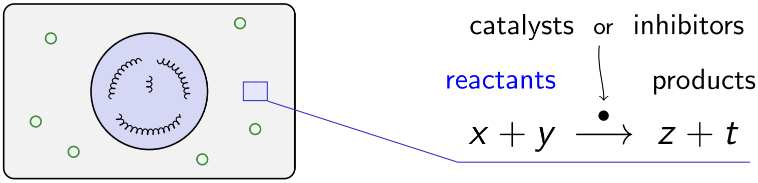

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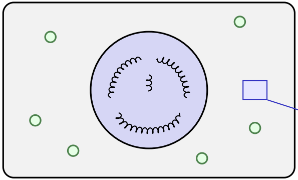

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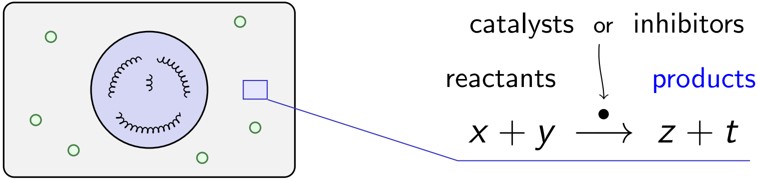

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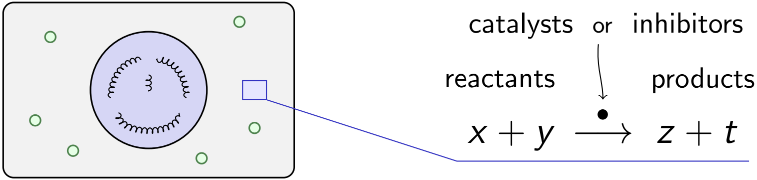

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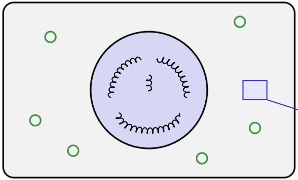

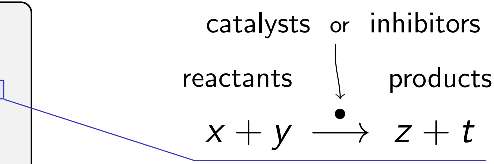

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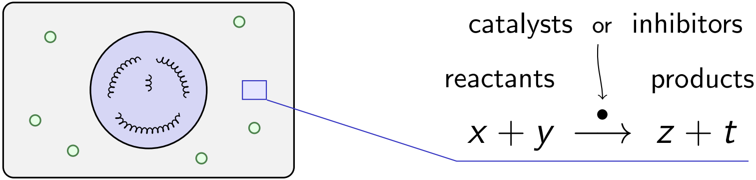

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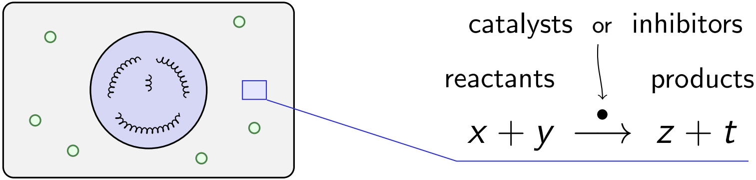

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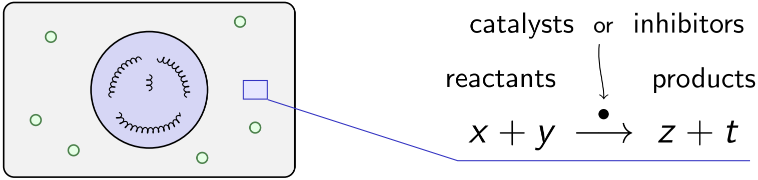

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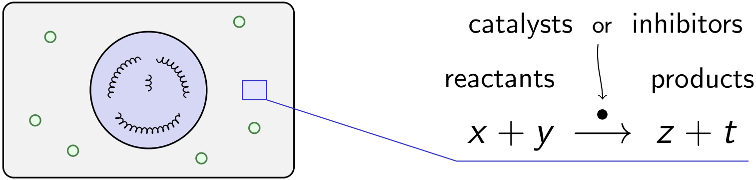

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  - u vanishes
  - threshold assumption

Dynamics of Reaction Systems

$$\text{State at } t_i \quad \mapsto \quad \text{Set of species } W_i$$

Dynamics of Reaction Systems

State at t_i $\mapsto$ Set of species W_i

State transition $\mapsto$ Running of reactions

- $W_{i+1} = res_{\mathcal{A}}(W_i)$

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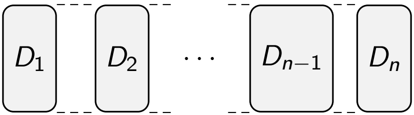

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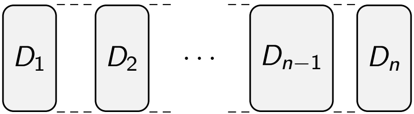

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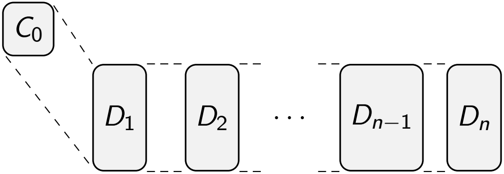

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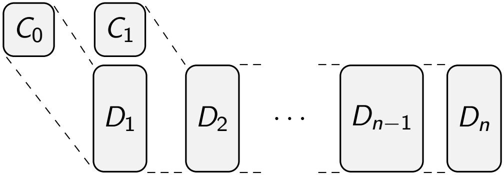

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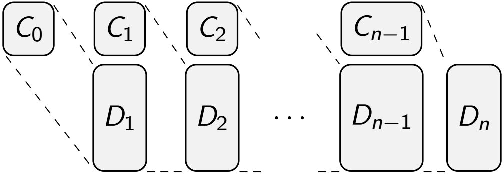

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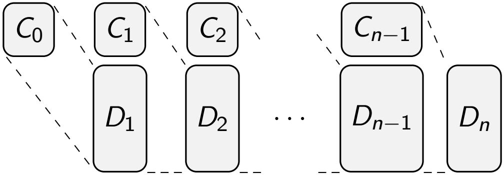

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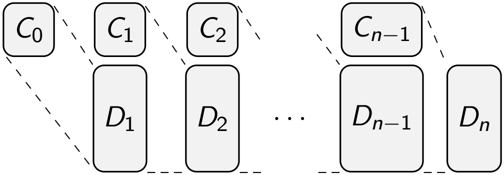

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Presentation Pattern

1. Define property

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3. Show complexity

Mass Conservation

Reactions systems are qualitative

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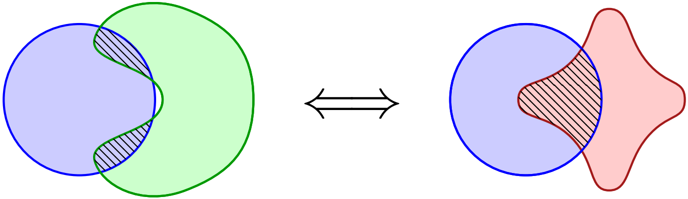

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- can be non-deterministically answered in polynomial time, given an oracle for coNP-complete problems

Invariant Sets

Stronger conservation

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M – invariant if $\forall W \,.\, M \subseteq W \iff M \subseteq res_{\mathcal{A}}(W) \neq \varnothing$

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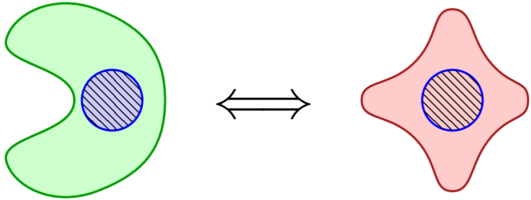

Complexity of Invariance

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- mass conservation is coNP-complete

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"Is given M invariant?" – coNP-complete

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"$\exists$ invariant M?" – coNP-hard, in Σ_2^P

- same as mass conservation

Formula Correspondence

Conserved set $\quad \forall W\,. \quad M \cap W \neq \varnothing \quad \Longleftrightarrow \quad M \cap res_{\mathcal{A}}(W) \neq \varnothing$

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Generalisation	$\forall W\,.$	$\varphi_1(W)$	$\iff$	$\varphi_2(res_{\mathcal{A}}(W))$

(fixed φ_1 and φ_2)

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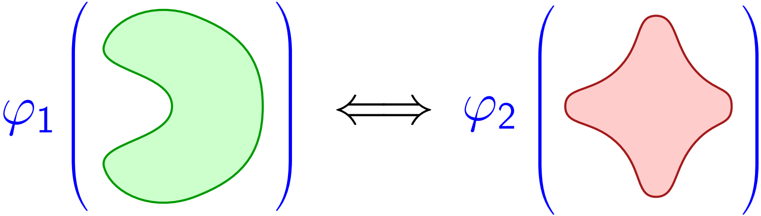

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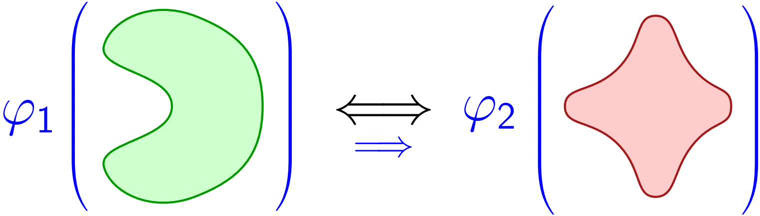

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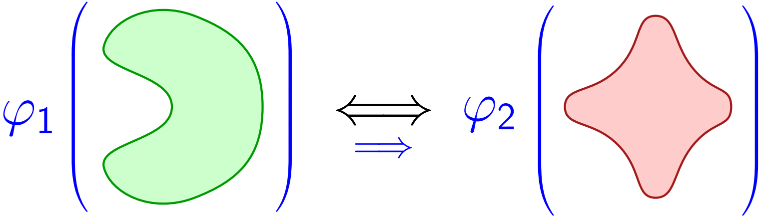

coNP-complete problem

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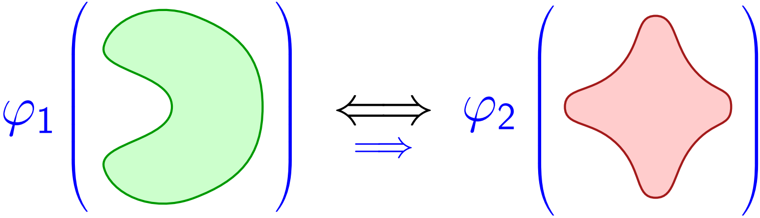

coNP-complete problem

- because mass conservation and invariance are

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$$W \text{ – steady state if } W = res_{\mathcal{A}}(W)$$

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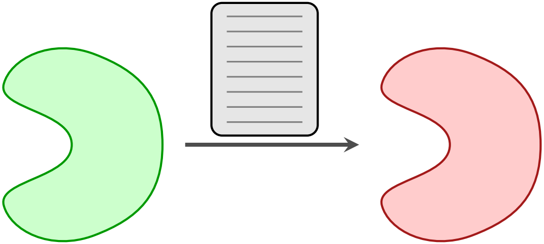

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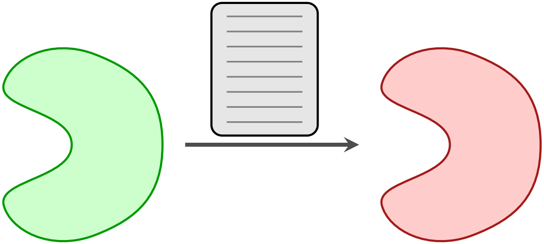

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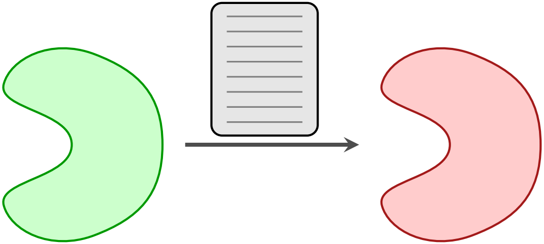

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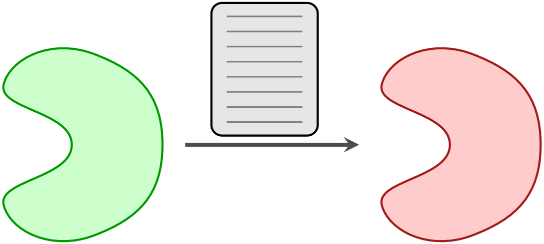

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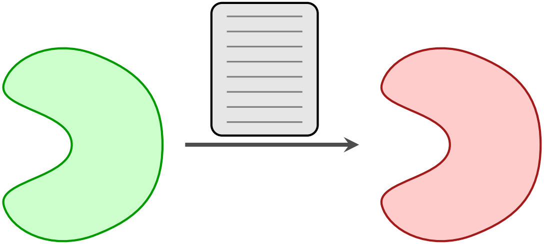
- Take $\varphi = \ldots \wedge \left(x_1 \vee \ldots \vee x_n \vee \bar{y}_1 \vee \ldots \vee \bar{y}_m\right) \wedge \ldots$

Steady States

W – steady state if $W = res_{\mathcal{A}}(W)$



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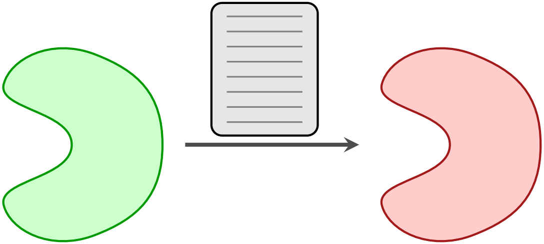

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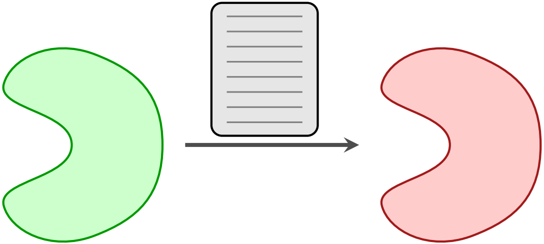
- $res_{\mathcal{A}}(T) = T$ iff T satisfies all disjunctions in φ

Elementary Fluxes

Take a steady state W, $W = res_{\mathcal{A}}(W)$



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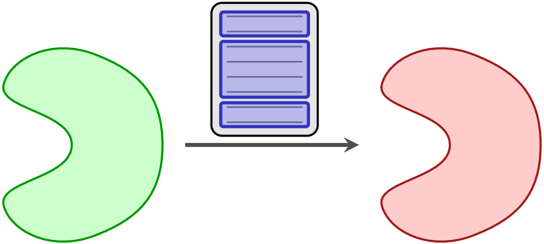

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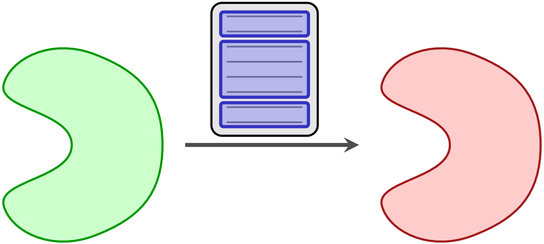
$A_E \subseteq A$ – elementary flux if $W = res_{A_E}(W)$



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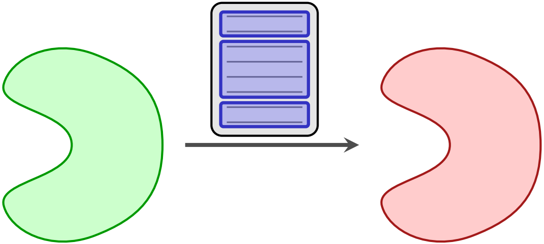

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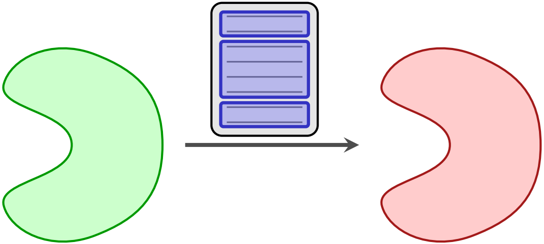

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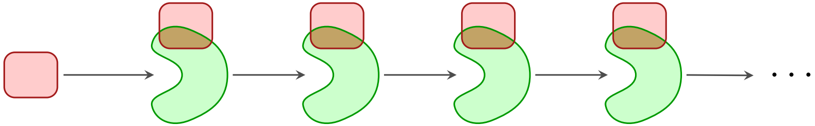
- (equivalent to the set covering problem)

Periodic Processes

Consider $\pi = \left((C_n)_{n\geq 0}, (D_n)_{n>0}\right)$



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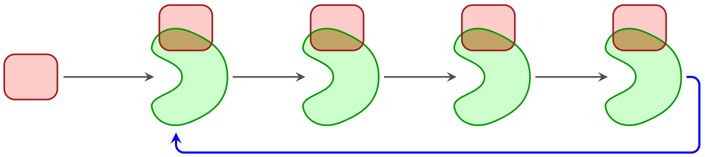

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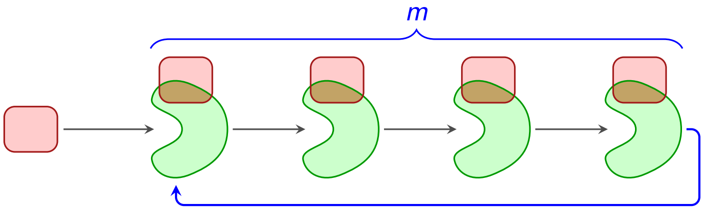
Consider $\pi = \big((C_n)_{n \geq 0}, (D_n)_{n > 0}\big)$

π is periodic if $\exists m > 1 .\ C_k \cup D_k = C_{k+m} \cup D_{k+m}$, for all $k > k_0$



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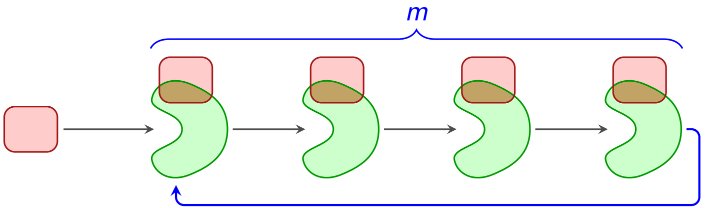

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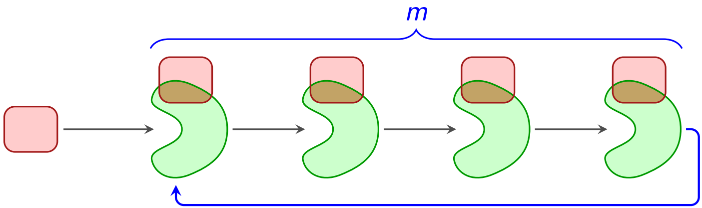

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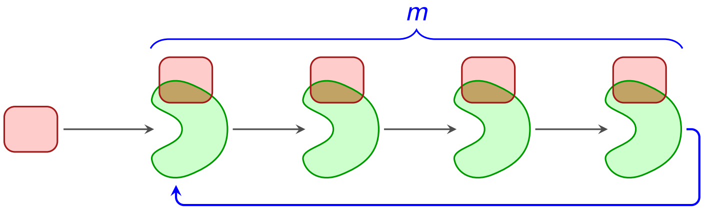

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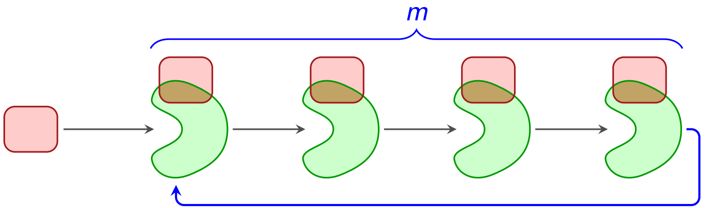

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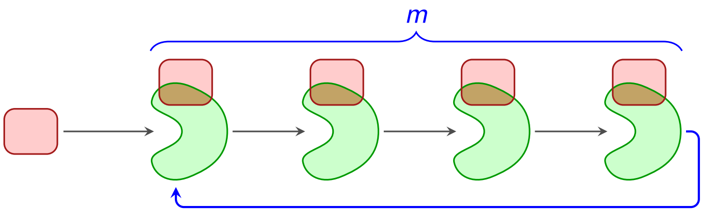

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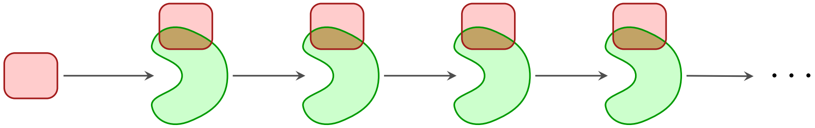

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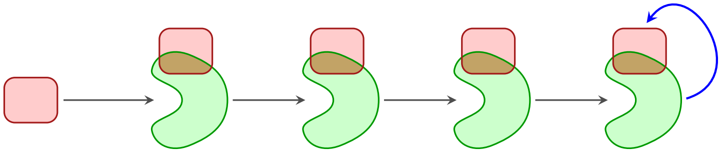

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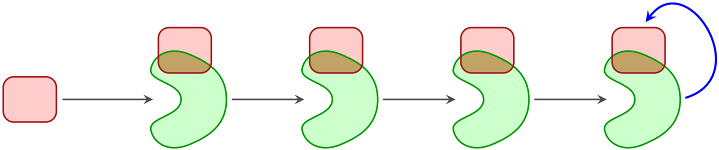

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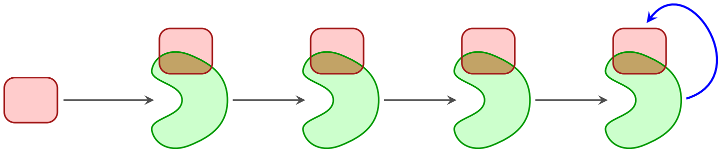

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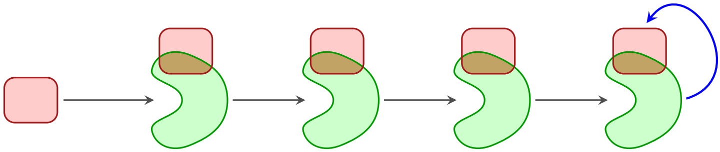

Check first p states

- p = length of context period

Relatively easy answer

Conclusion

Mass conservation and invariant sets

- deciding – coNP-complete
- existence – coNP-hard, in Σ_2^P

Steady states and elementary fluxes

- existence – NP-complete

Periodic processes (periodic contexts)

- deciding – PSPACE-complete

Stationary processes (periodic contexts)

- deciding – polynomial