Complexity of Model Checking for Reaction Systems

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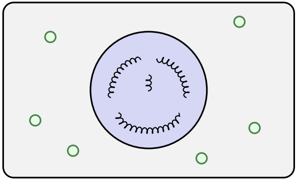
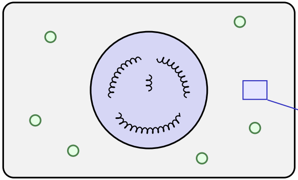
Luca Manzoni, Ion Petre, Antonio E. Porreca

Casys-Mef, March 16

Reaction Systems

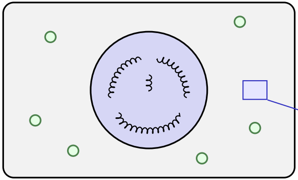


Reaction Systems



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

Reaction Systems



reactants products

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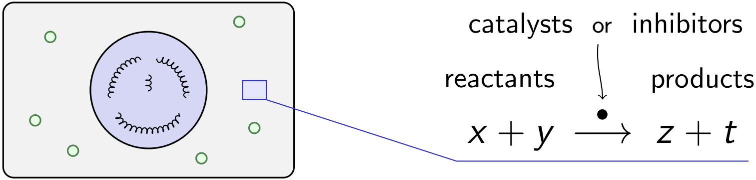

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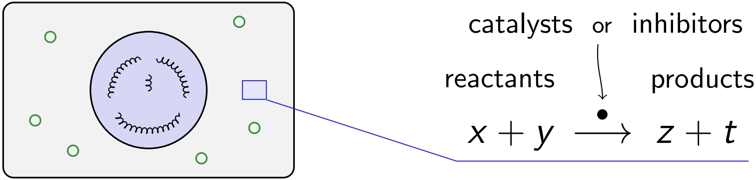

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  $W = \{x, y, u\}$

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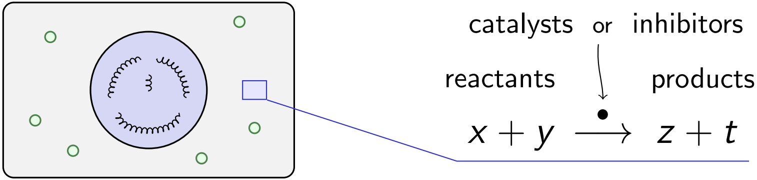

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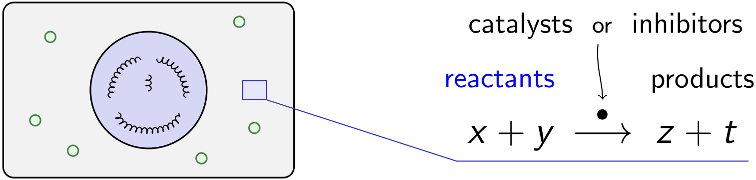

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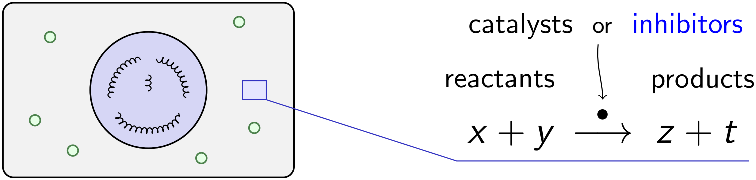

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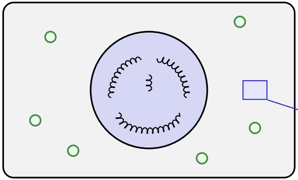

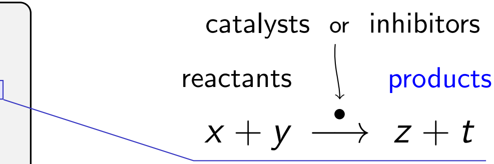

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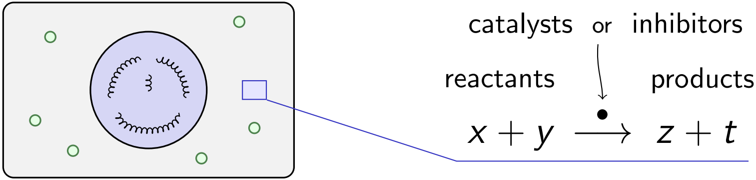

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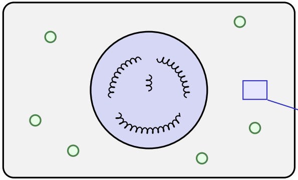

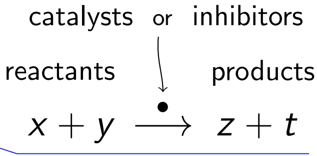

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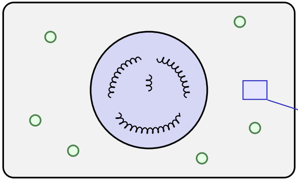

catalysts or inhibitors

reactants products

$$x + y \xrightarrow{\bullet} z + t$$

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- a is not enabled on $\{x\}$ and $\{x, y, f\}$

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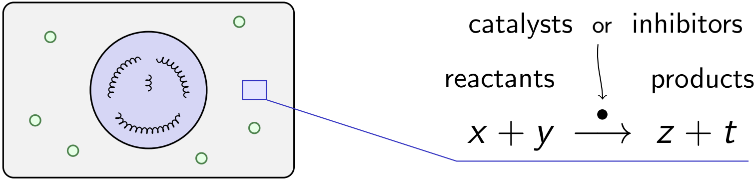

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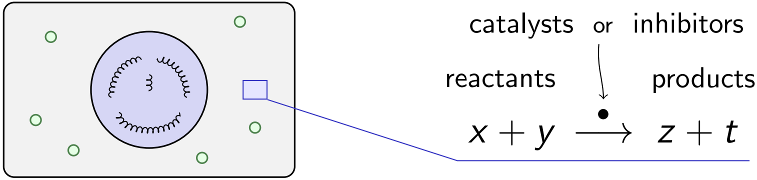

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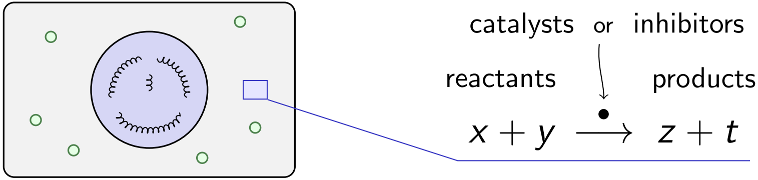

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  - u vanishes
  - threshold assumption

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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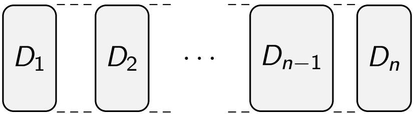

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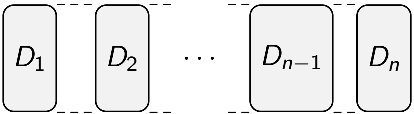

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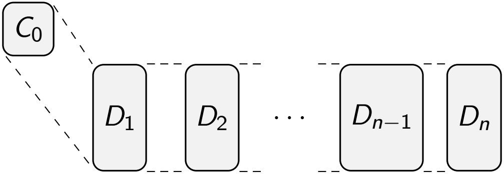

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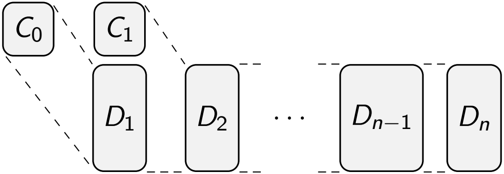

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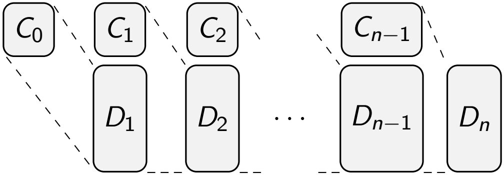

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Use contexts at every step

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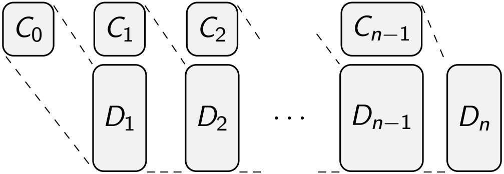

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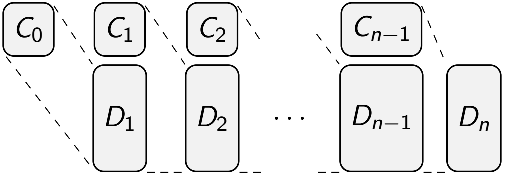

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Presentation Pattern

1. Define property

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3. Show complexity

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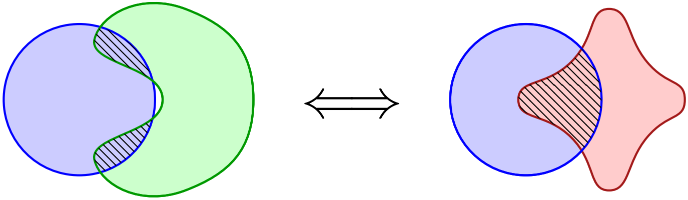

Complexity of Mass Conservation

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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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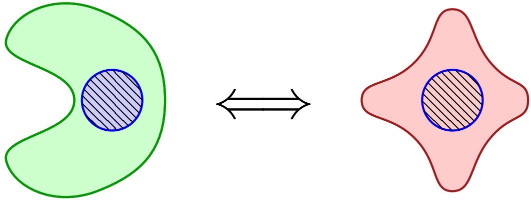

Complexity of Invariance

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- mass conservation is coNP-complete

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

- same as mass conservation

Formula Correspondence

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

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(fixed φ_1 and φ_2)

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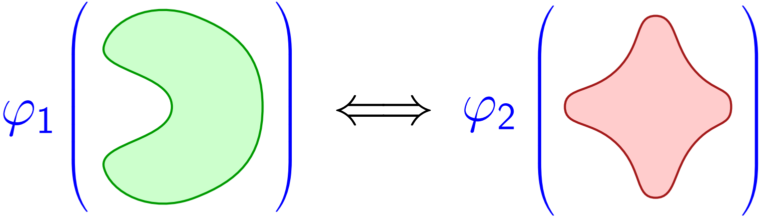

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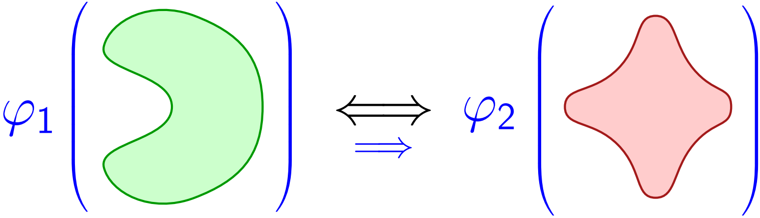

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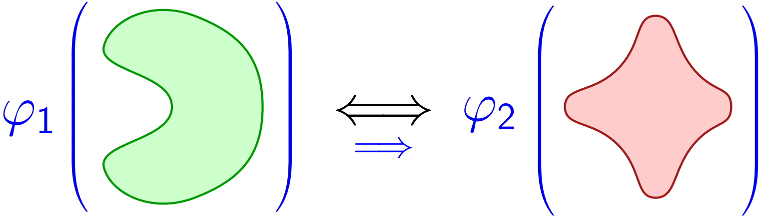

coNP-complete problem

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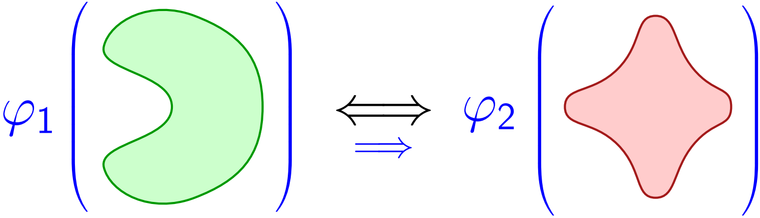

coNP-complete problem

- because mass conservation and invariance are

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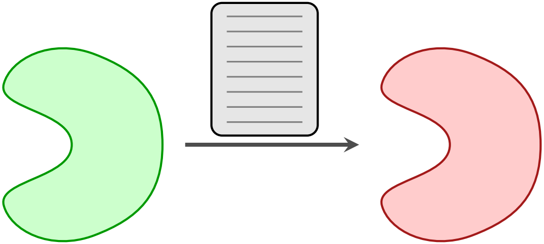

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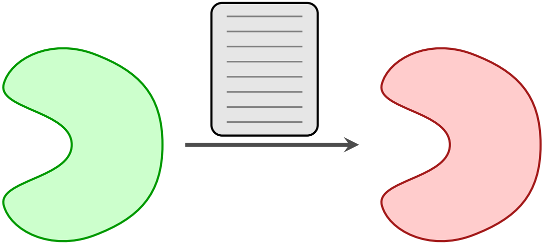

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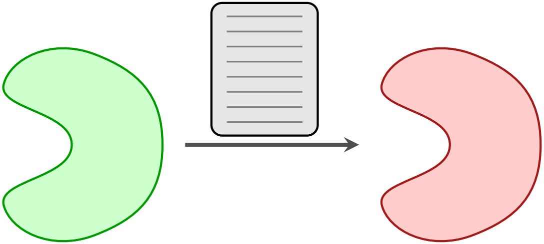

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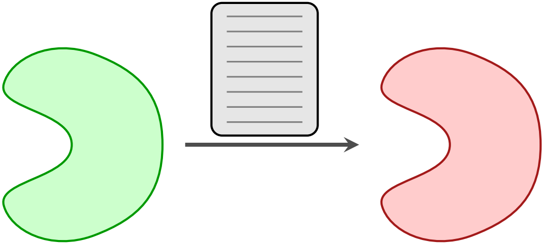

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Steady States

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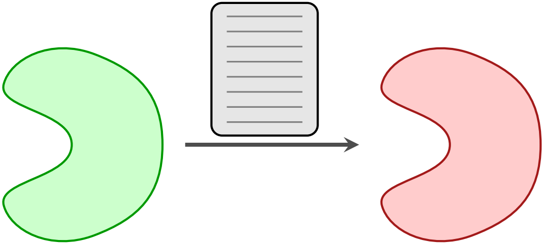

"Is given W a steady state?" – trivial

"$\exists$ steady state W?" – NP-complete

- Take $\varphi = \ldots \wedge (x_1 \vee \ldots \vee x_n \vee \bar{y}_1 \vee \ldots \vee \bar{y}_m) \wedge \ldots$
- Consider reactions $(\{y_1, \ldots, y_n\}, \{x_1, \ldots, x_n, \spadesuit\}, \{\spadesuit\})$ and $(\{x\}, \{\spadesuit\}, \{x\})$, for all variables x

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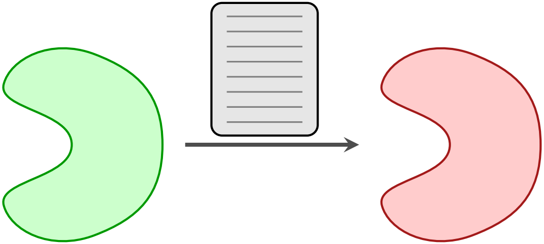

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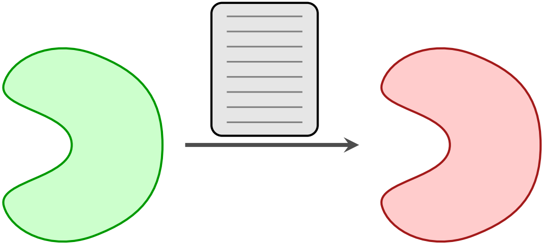
- Consider reactions $\left(\{y_1, \ldots, y_n\}, \{x_1, \ldots, x_n, \spadesuit\}, \{\spadesuit\}\right)$ and $\left(\{x\}, \{\spadesuit\}, \{x\}\right)$, for all variables x
- $res_{\mathcal{A}}(T) = T$ iff T satisfies all disjunctions in φ

Elementary Fluxes

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



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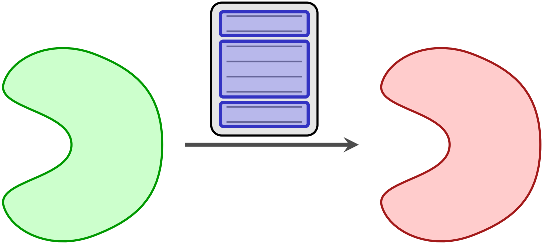

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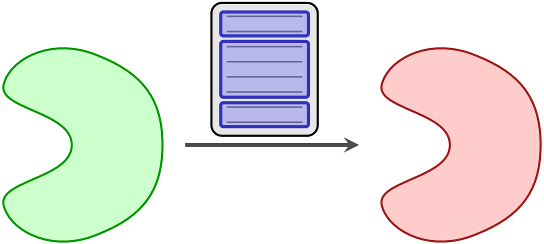
$A_E \subseteq A$ – elementary flux if $W = res_{A_E}(W)$



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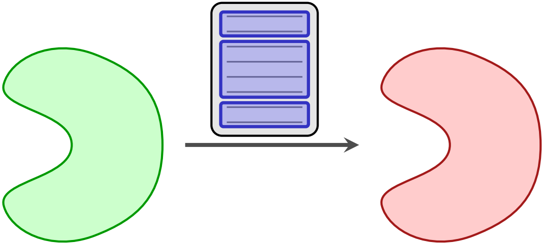

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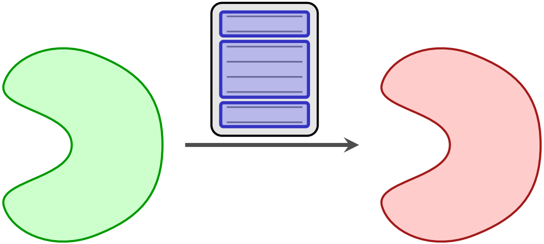

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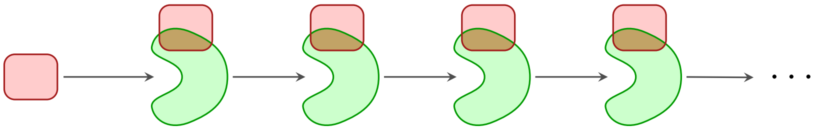
- (equivalent to the set covering problem)

Periodic Processes

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



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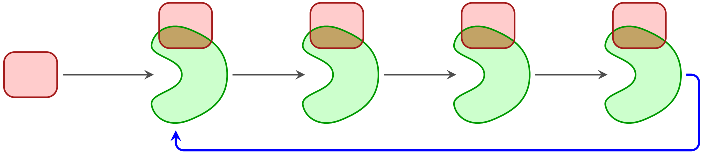

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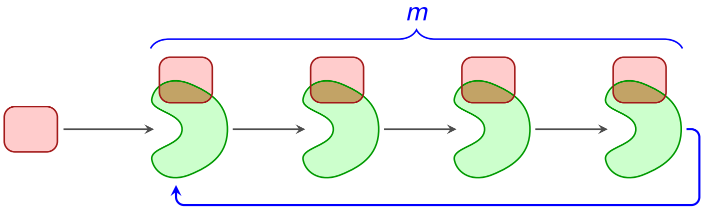
Consider $\pi = \big((C_n)_{n \geq 0}, (D_n)_{n > 0}\big)$

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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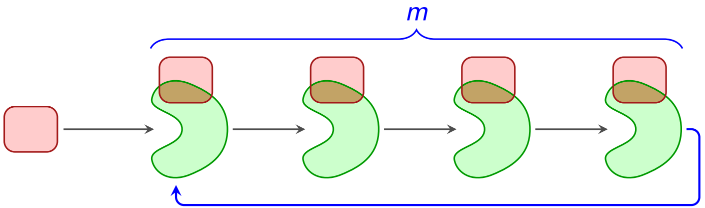

PSPACE-complete for periodic contexts

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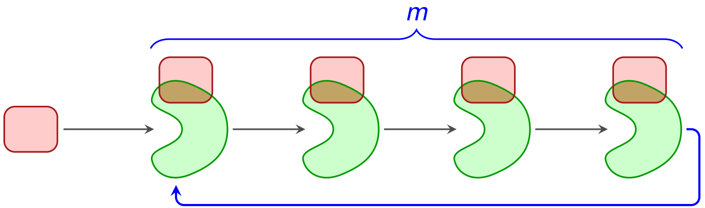

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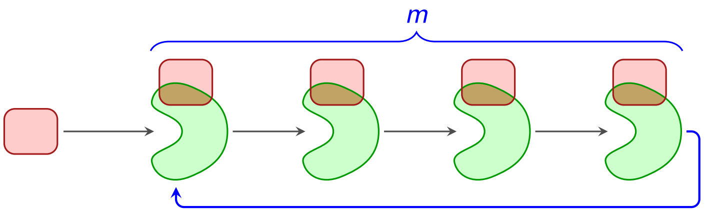

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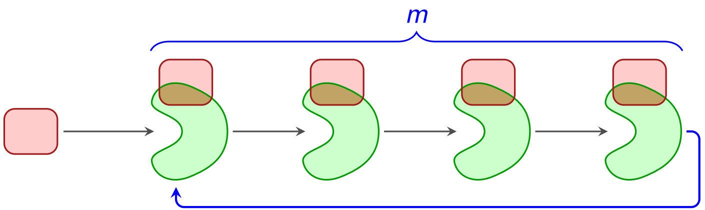

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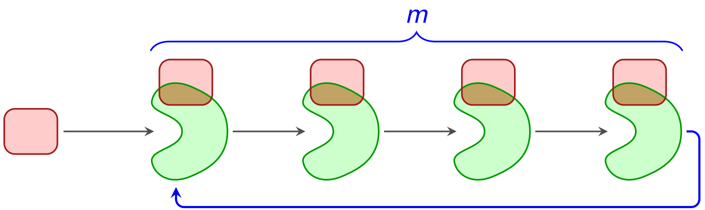

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Undecidable for more complex contexts

- cannot be solved by a Turing machine

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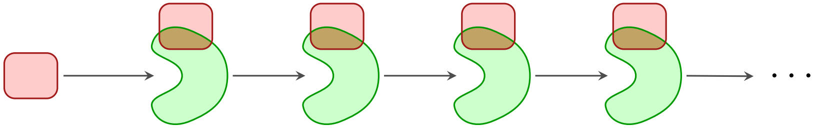

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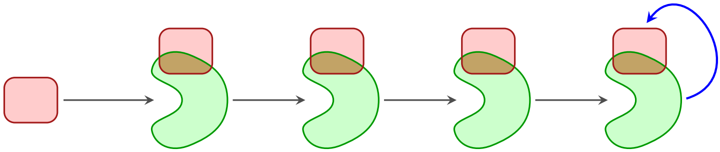

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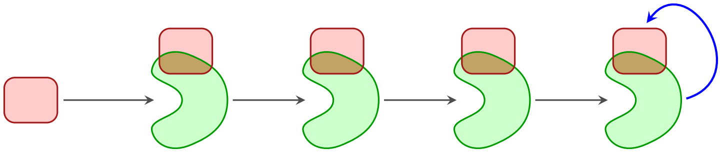

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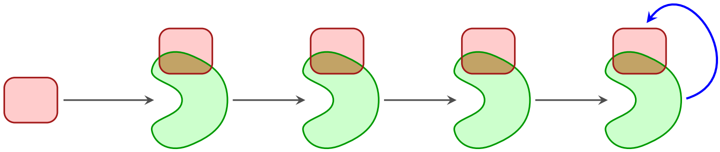

Check first p states

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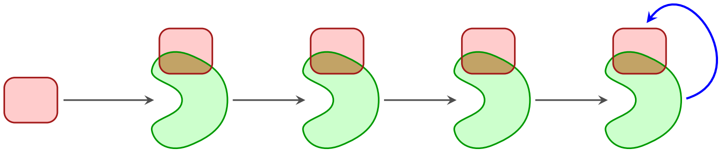

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Relatively easy answer

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