



Chemical Pure Reaction Automata in Maximally Parallel manner

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DEGLI STUDI
DI TRIESTE**

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CPRA in *mp*

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Definition

Given a finite set S , a *chemical reaction* over S is a couple (R, P) of multisets of S :

- R is the multiset of *reactants*,
- P is the multiset of *products*.

(R, P) is *enabled* in a state $T \in S^\#$ when $R \leq T$.

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The reaction $(\{a\}, \{b\})$ is enabled by $\{a, a, b\}$ since

$$\{a\} \leq \{a, a, b\}$$

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- R is the multiset of *reactants*,
- P is the multiset of *products*.

(R, P) is *enabled* in a state $T \in S^\#$ when $R \leq T$.

The reaction $(\{a\}, \{b\})$ is enabled by $\{a, a, b\}$ since

$$\{a\} \leq \{a, a, b\}$$

but $(\{a, a, a\}, \{b, b, b\})$ is not enabled by $\{a, a, b\}$ since

$$\{a, a, a\} \not\leq \{a, a, b\}.$$

Maximally parallel criterion



$$\mathbf{A} = \{\mathbf{r}_1 = (\{a, a\}, \{b\}),$$
$$\mathbf{r}_2 = (\{a, a, b\}, \{a\})\}$$

$$T = \{a, a, b\}$$

The reaction \mathbf{r}_1 is enabled by T in *maximally parallel* manner since both

$$\mathbf{r}_1 + \mathbf{r}_2 = (\{a, a, a, a, b\}, \{b, a\})$$

and

$$\mathbf{r}_1 + \mathbf{r}_1 = 2\mathbf{r}_1 = (\{a, a, a, a\}, \{b, b\})$$

are not enabled by T .

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and

$$\mathbf{r}_1 + \mathbf{r}_1 = 2\mathbf{r}_1 = (\{a, a, a, a\}, \{b, b\})$$

are not enabled by T .

$$\Rightarrow \text{En}_{\mathbf{A}}^{mp}(T) = \{\mathbf{r}_1, \mathbf{r}_2\}$$

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Maximally parallel criterion



$$\mathbf{A}' = \{\mathbf{r}'_1 = (\{a\}, \{b\}), \\ \mathbf{r}'_2 = (\{a, a, b\}, \{a\})\}$$

$$T = \{a, a, b\}$$

The reaction \mathbf{r}'_1 is not enabled by T in *maximally parallel* manner since

$$\mathbf{r}'_1 + \mathbf{r}'_1 = (\{a, a\}, \{b, b\})$$

is enabled by T .

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Result¹

$$\mathbf{A} = \{\mathbf{r}_1 = (\{a, a\}, \{b\}),$$
$$\mathbf{r}_2 = (\{a, a, b\}, \{a\})\}$$
$$T = \{a, a, b\}$$
$$\text{En}_{\mathbf{A}}^{mp}(T) = \{\mathbf{r}_1, \mathbf{r}_2\}$$



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¹Okubo, Kobayashi, and Yokomori 2012.

Result¹

$$\mathbf{A} = \{\mathbf{r}_1 = (\{a, a\}, \{b\}),$$
$$\mathbf{r}_2 = (\{a, a, b\}, \{a\})\}$$
$$T = \{a, a, b\}$$
$$\text{En}_{\mathbf{A}}^{mp}(T) = \{\mathbf{r}_1, \mathbf{r}_2\}$$

$$\left. \begin{array}{l} T = \{a, a, b\} \xrightarrow{\mathbf{r}_1} P_{\mathbf{r}_1} + \underbrace{T - R_{\mathbf{r}_1}}_{\{b\}} = \{b, b\} \\ T = \{a, a, b\} \xrightarrow{\mathbf{r}_2} P_{\mathbf{r}_2} + \underbrace{T - R_{\mathbf{r}_2}}_{\emptyset} = \{a\} \end{array} \right\} = \text{Res}_{\mathbf{A}}^{mp}(T)$$

¹Okubo, Kobayashi, and Yokomori 2012.



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$$\mathbf{A} = \{\mathbf{r}_1 = (\{a, a\}, \{b\}), \\ \mathbf{r}_2 = (\{a, a, b\}, \{a\})\}$$
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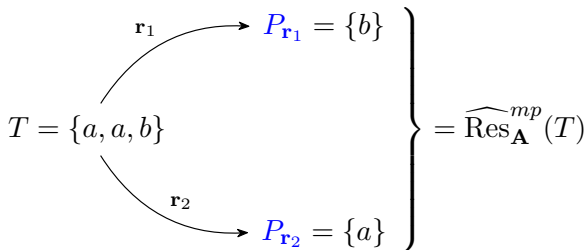
References

²Ascone et al. 2024.

$$\mathbf{A} = \{ \mathbf{r}_1 = (\{a, a\}, \{b\}), \\ \mathbf{r}_2 = (\{a, a, b\}, \{a\}) \}$$

$$T = \{a, a, b\}$$

$$\text{En}_{\mathbf{A}}^{mp}(T) = \{ \mathbf{r}_1, \mathbf{r}_2 \}$$



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Example with *mp* manner

$$\Sigma = \{a, b\}, D_0 = \{s_0, f\}, F = \{f\}.$$

$$\mathbf{A} = \{\mathbf{r}_1 = (\{s_0, a\}, \{s_1\}),$$

$$\mathbf{r}_2 = (\{s_1, b\}, \{s_0\}),$$

$$\mathbf{r}_3 = (\{s_1, a\}, \{\clubsuit\}),$$

$$\mathbf{r}_4 = (\{\clubsuit\}, \{\clubsuit\}),$$

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$$w = ab \in \Sigma^* :$$

$$D_0 = \{s_0, f\}$$

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Example with *mp* manner

$$\Sigma = \{a, b\}, D_0 = \{s_0, f\}, F = \{f\}.$$

$$\mathbf{A} = \{\mathbf{r}_1 = (\{s_0, a\}, \{s_1\}), \leftarrow$$

$$\mathbf{r}_2 = (\{s_1, b\}, \{s_0\}),$$

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$$\mathbf{r}_5 = (\{f\}, \{f\}) \leftarrow\}$$

$$w = ab \in \Sigma^* :$$

$$D_0 = \{s_0, f\} \xrightarrow[a]{\mathbf{r}_1 + \mathbf{r}_5}$$



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Example with *mp* manner



$$\Sigma = \{a, b\}, D_0 = \{s_0, f\}, F = \{f\}.$$

$$\mathbf{A} = \{\mathbf{r}_1 = (\{s_0, a\}, \{s_1\}), \leftarrow$$

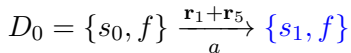
$$\mathbf{r}_2 = (\{s_1, b\}, \{s_0\}),$$

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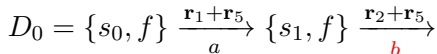
Example with *mp* manner



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$$w = ab \in \Sigma^* :$$

$$D_0 = \{s_0, f\} \xrightarrow[a]{\mathbf{r}_1 + \mathbf{r}_5} \{s_1, f\} \xrightarrow[b]{\mathbf{r}_2 + \mathbf{r}_5} \{s_0, f\}$$

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$\Rightarrow ab$ is accepted by the CPRA working in *mp*

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$$\mathbf{r}_5 = (\{f\}, \{f\}) \quad \}$$

$$w = aa \in \Sigma^*:$$

$$D_0 = \{s_0, f\} \xrightarrow[a]{\mathbf{r}_1 + \mathbf{r}_5} \{s_1, f\}$$

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$$w = a\mathbf{a} \in \Sigma^*:$$

$$D_0 = \{s_0, f\} \xrightarrow[a]{\mathbf{r}_1 + \mathbf{r}_5} \{s_1, f\} \xrightarrow[a]{\mathbf{r}_3 + \mathbf{r}_5}$$

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$$w = aa \in \Sigma^*:$$

$$D_0 = \{s_0, f\} \xrightarrow[a]{\mathbf{r}_1 + \mathbf{r}_5} \{s_1, f\} \xrightarrow[a]{\mathbf{r}_3 + \mathbf{r}_5} \{\clubsuit, f\} \xrightarrow{\mathbf{r}_4 + \mathbf{r}_5} \underbrace{\{\clubsuit, f\}}_{\neq F} \cup$$

$\Rightarrow aa$ is not accepted by the CPRA working in *mp*

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Non deterministic CPRA in mp are Turing complete



Theorem

Given any chemical reaction automaton $\mathcal{A} = (S, \Sigma, \mathbf{A}, D_0, S_f)$ working in mp manner, there exists a chemical pure reaction automaton \mathcal{M} working in mp manner such that they accepts the same language in λ input mode.

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Theorem (Okubo and Yokomori 2016)

$$CRA_{mp}^{\lambda} = RE.$$

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Theorem (Okubo and Yokomori 2016)

$$CRA_{mp}^{\lambda} = \mathcal{RE}.$$

Corollary

$$CPRA_{mp}^{\lambda} = \mathcal{RE}.$$

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Definition

If the pure result $\widehat{\text{Res}}_{\mathbf{A}}^{mp}(T)$ consists of one element only, for any reachable state T , we say that the CPRA is *deterministic*.

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Definition

If the pure result $\widehat{\text{Res}}_{\mathbf{A}}^{mp}(T)$ consists of one element only, for any reachable state T , we say that the CPRA is *deterministic*.

Given a deterministic CPRA, the following map is well defined on reachable states:

$$R : S^\# \longrightarrow S^\#$$
$$T \longmapsto R(T) \in \widehat{\text{Res}}_{\mathbf{A}}^{mp}(T).$$

Deterministic CPRA

Example

$$\Sigma = \{a, b\}, D_0 = \{s_0, f\}, F = \{f\}.$$

$$\mathbf{A} = \{\mathbf{r}_1 = (\{s_0, a\}, \{s_1\}),$$

$$\mathbf{r}_2 = (\{s_1, b\}, \{s_0\}),$$

$$\mathbf{r}_3 = (\{s_1, a\}, \{\clubsuit\}),$$

$$\mathbf{r}_4 = (\{\clubsuit\}, \{\clubsuit\}),$$

$$\mathbf{r}_5 = (\{f\}, \{f\})\}$$

$$w = ab \in \Sigma^*:$$

$$D_0 = \{s_0, f\} \xrightarrow{a} \{s_1, f\} \xrightarrow{b} \{s_0, f\} \rightarrow \{f\} = F.$$



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Deterministic CPRA

Example

$$\Sigma = \{a, b\}, D_0 = \{s_0, f\}, F = \{f\}.$$

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$$\mathbf{r}_4 = (\{\clubsuit\}, \{\clubsuit\}),$$

$$\mathbf{r}_5 = (\{f\}, \{f\})\}$$

$$w = ab \in \Sigma^*:$$

$$D_0 = \{s_0, f\} \xrightarrow{a} \{s_1, f\} \xrightarrow{b} \{s_0, f\} \rightarrow \{f\} = F.$$

$$\Rightarrow R(\{s_0, f, a\}) = \{s_1, f\}$$

$$R(\{s_1, f, b\}) = \{s_0, f\}$$

$$R(\{s_0, f\}) = \{f\}$$



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Topology on $S^\#$

Example

$$V = \{a, a, b, b, b, b\} \mapsto (2, 4) \in \mathbb{N}^2$$



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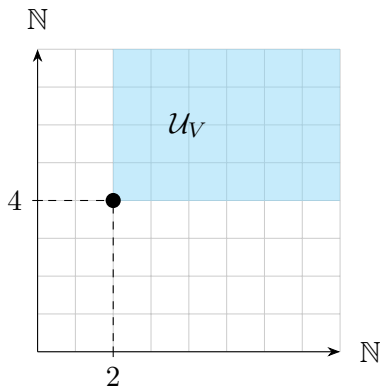
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Example

$$V = \{a, a, b, b, b, b\} \mapsto (2, 4) \in \mathbb{N}^2$$



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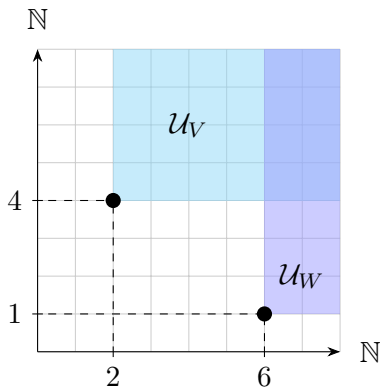
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Example

$$V = \{a, a, b, b, b, b\} \mapsto (2, 4) \in \mathbb{N}^2$$

$$W = \{a, a, a, a, a, a, b\} \mapsto (6, 1) \in \mathbb{N}^2$$



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As a corollary of Dickson's Lemma, we prove the following result.

Corollary

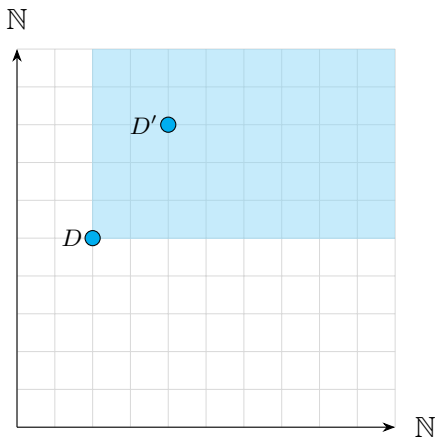
Given a sequence of multisets $\{D_n\}_{n \in \mathbb{N}} \subseteq S^\#$, there exist $M, k \in \mathbb{N}$, such that $D_{M+k} \geq D_M$.

Deterministic CPRA in mp are monotone



Lemma

Let $D, D' \in S^\#$ such that $D \leq D'$, then $R(D) \leq R(D')$.



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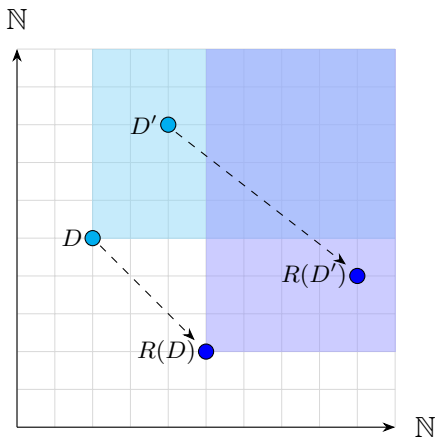
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Deterministic CPRA in mp are monotone



Lemma

Let $D, D' \in S^\#$ such that $D \leq D'$, then $R(D) \leq R(D')$.



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Deterministic CPRA in mp are not Turing complete



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References

Given an input word $w = w_1 \cdots w_n \in \Sigma^*$, consider the process reading w :

$$D_0 \xrightarrow{w_1} D_1 \xrightarrow{w_2} D_2 \cdots D_{n-1} \xrightarrow{w_n} D_n \rightarrow D_{n+1} \rightarrow \cdots$$

Deterministic CPRA in mp are not Turing complete

Proof



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Deterministic CPRA in mp are not Turing complete

Proof



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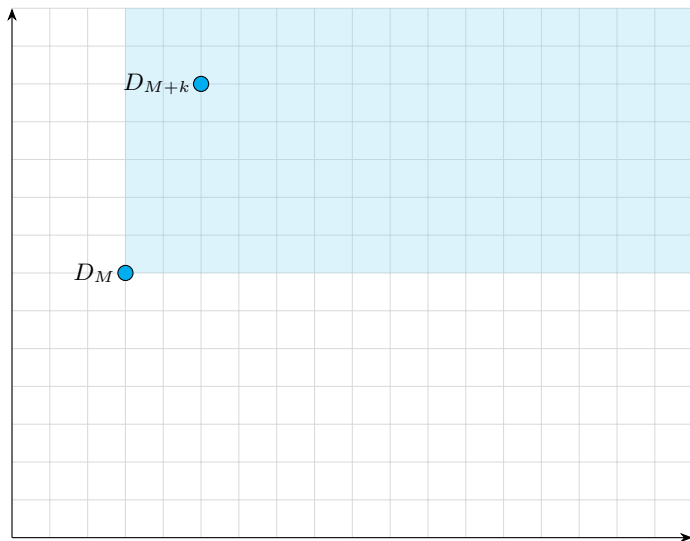
References

Given an input word $w = w_1 \cdots w_n \in \Sigma^*$, consider the process reading w :

$$D_0 \xrightarrow{w_1} D_1 \xrightarrow{w_2} D_2 \cdots D_{n-1} \xrightarrow{w_n} \underbrace{D_n \rightarrow D_{n+1} \rightarrow \cdots}$$

Dickson's Lemma $\Rightarrow \exists M \geq n$ and $k \in \mathbb{N}$ s.t. $D_{M+k} \geq D_M$

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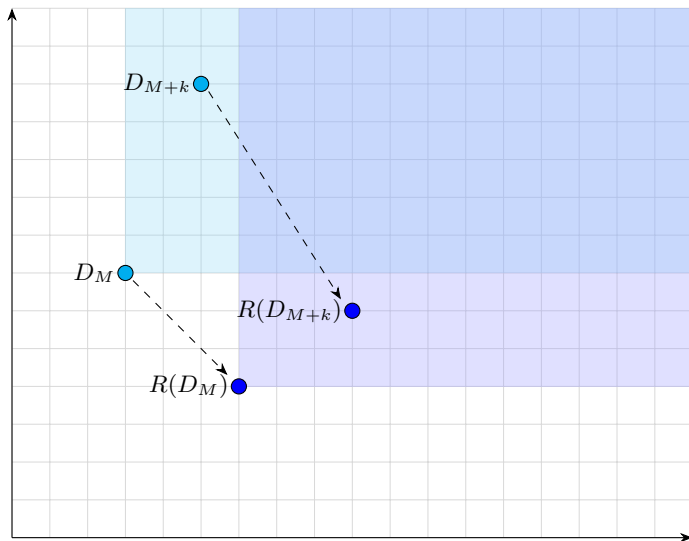
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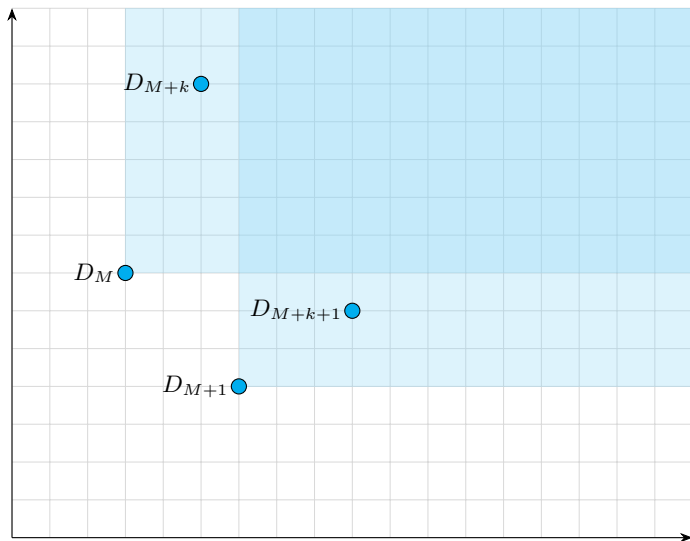
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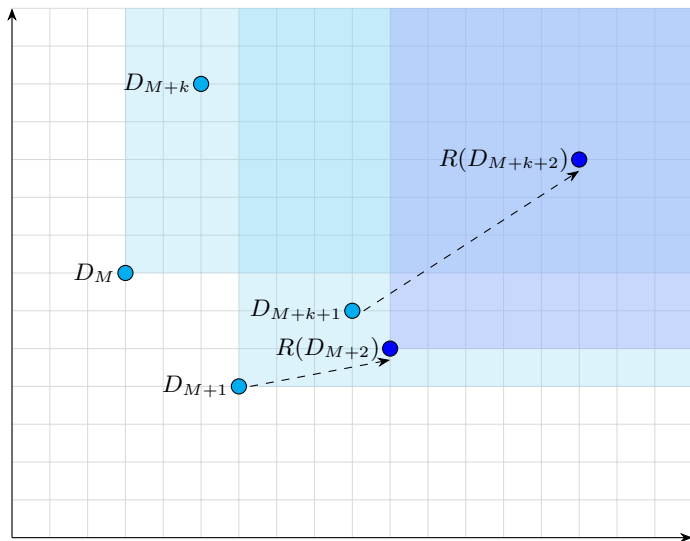
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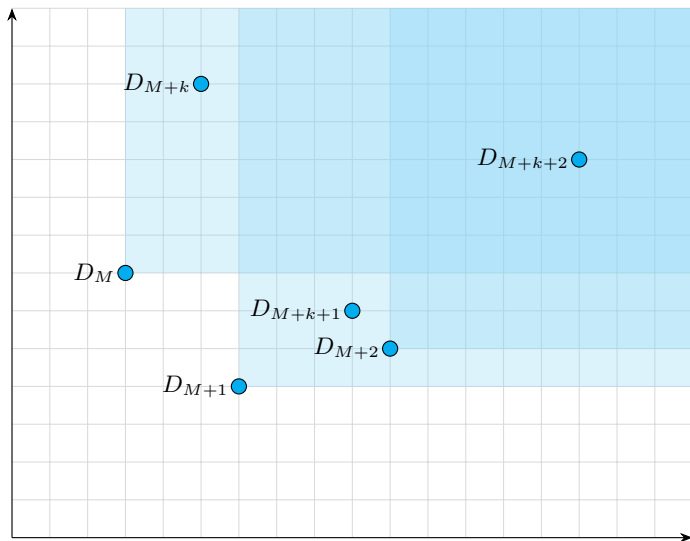
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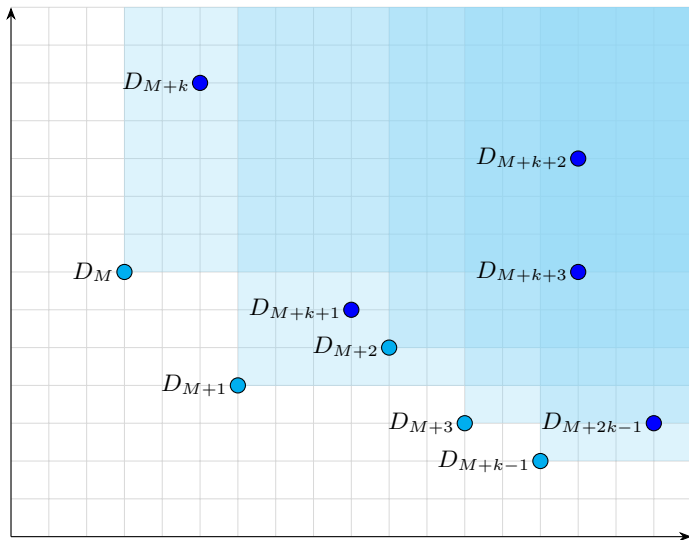
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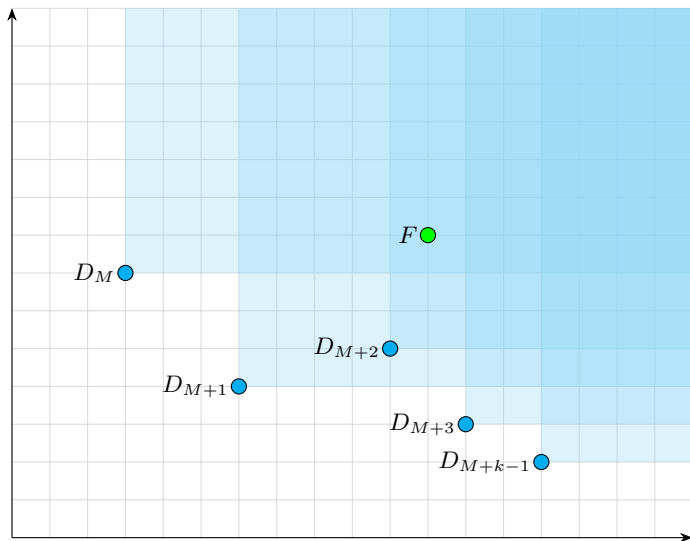
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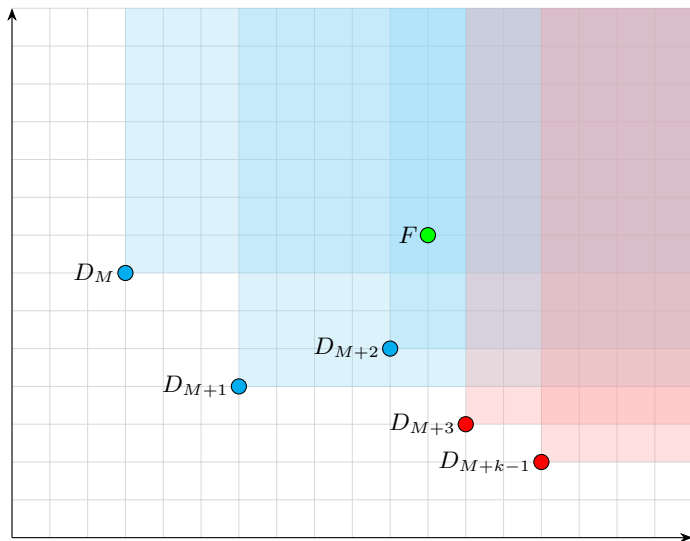
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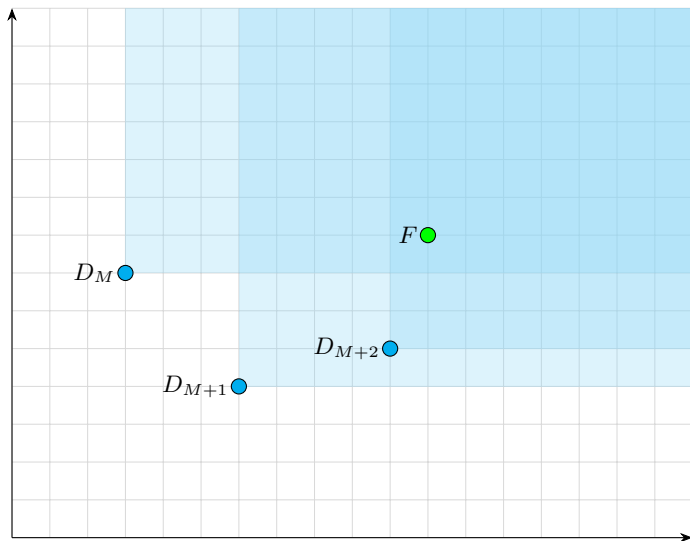
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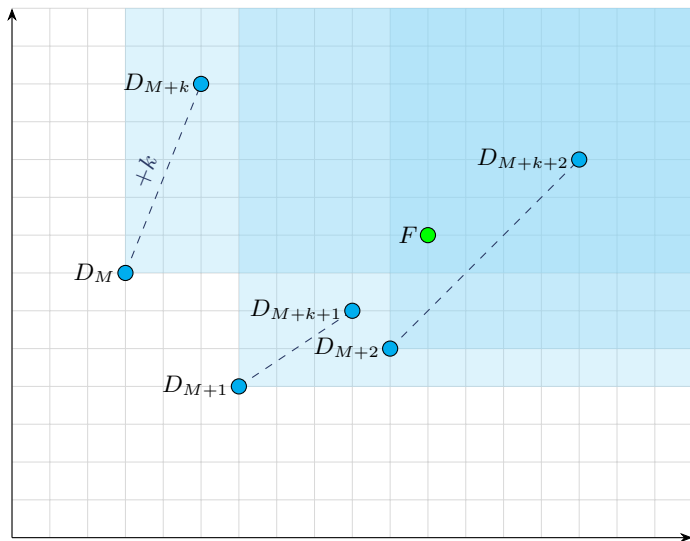
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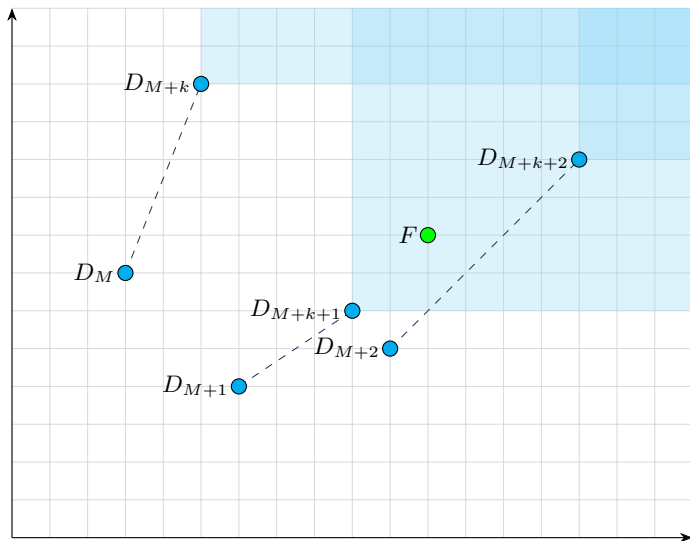
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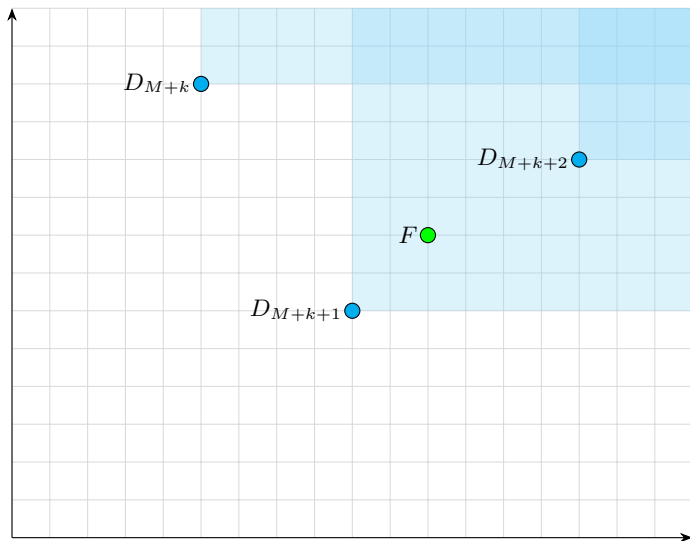
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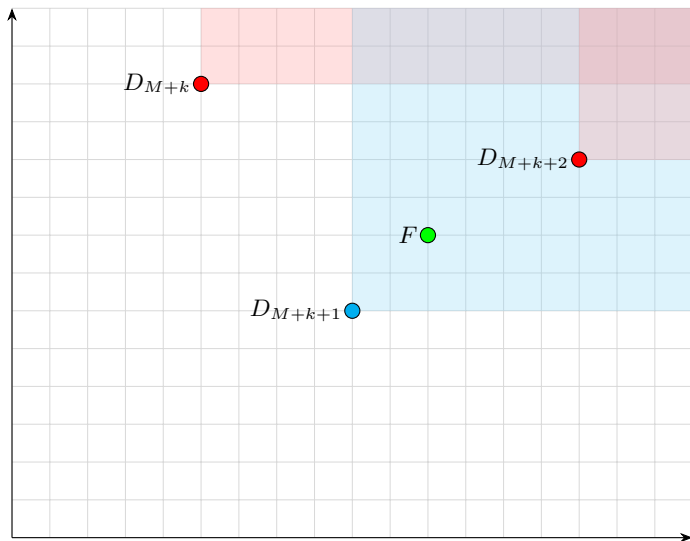
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- Determine DCPRA's exact computation power. (Petri Nets?)

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- Determine DCPRA's exact computation power. (Petri Nets?)
- DCRA in mp : still open.

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- Determine DCPRA's exact computation power. (Petri Nets?)
- DCRA in mp : still open.
- Investigate the computation power given by *maximally reactive* criterion of execution for CPRA and DCPRA.

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References



- Determine DCPRA's exact computation power. (Petri Nets?)
- DCRA in mp : still open.
- Investigate the computation power given by *maximally reactive* criterion of execution for CPRA and DCPRA.
- Build a solid connection with the existing derivation modes for P systems.

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References



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