Quantitative Analysis of Time Petri Nets Used for Modelling Biochemical Networks

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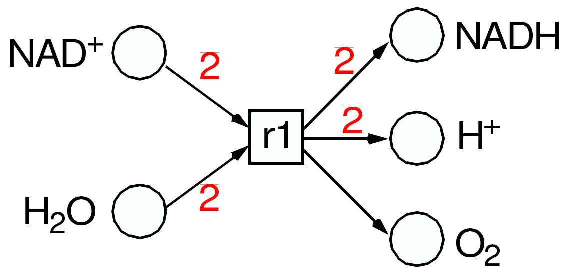
Outline

- **chemical reactions -> atomic actions -> Petri net transitions**

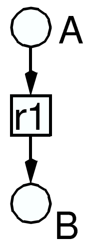
$$2\ NAD^+ + 2\ H_2O \rightarrow 2\ NADH + 2\ H^+ + O_2$$

input compounds



output compounds

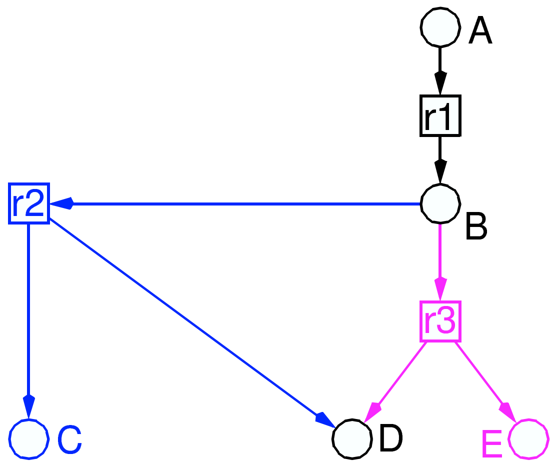
r1: A -> B



r1: A -> B

r2: B -> C + D

r3: B -> D + E



-> alternative reactions

r1: A -> B

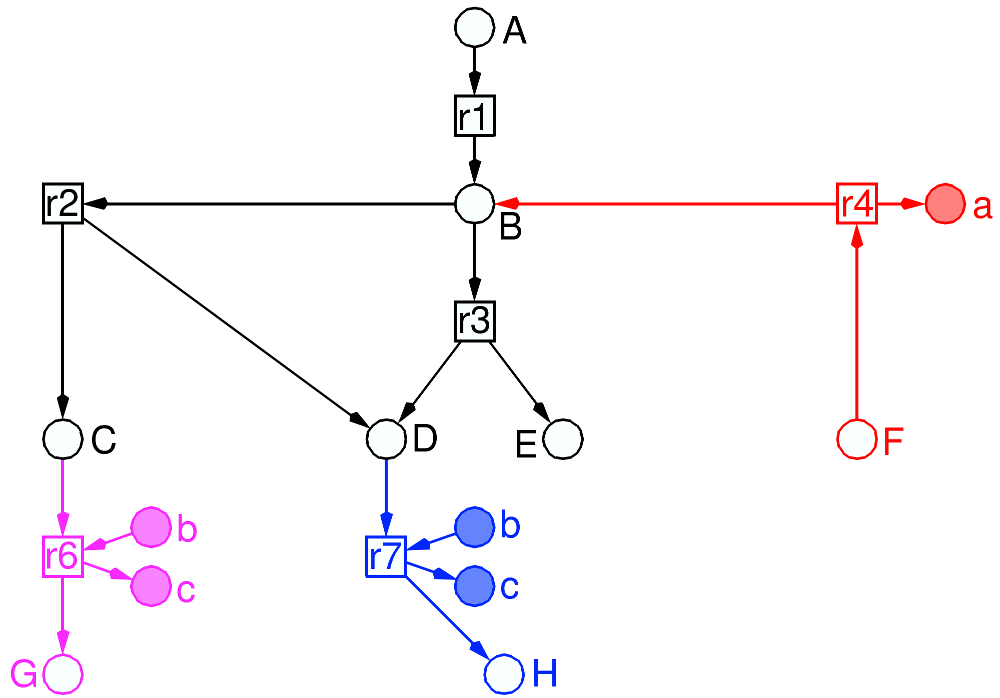
r2: B -> C + D

r3: B -> D + E

r4: F -> B + a

r6: C + b -> G + c

r7: D + b -> H + c



-> concurrent reactions

r1: A -> B

r2: B -> C + D

r3: B -> D + E

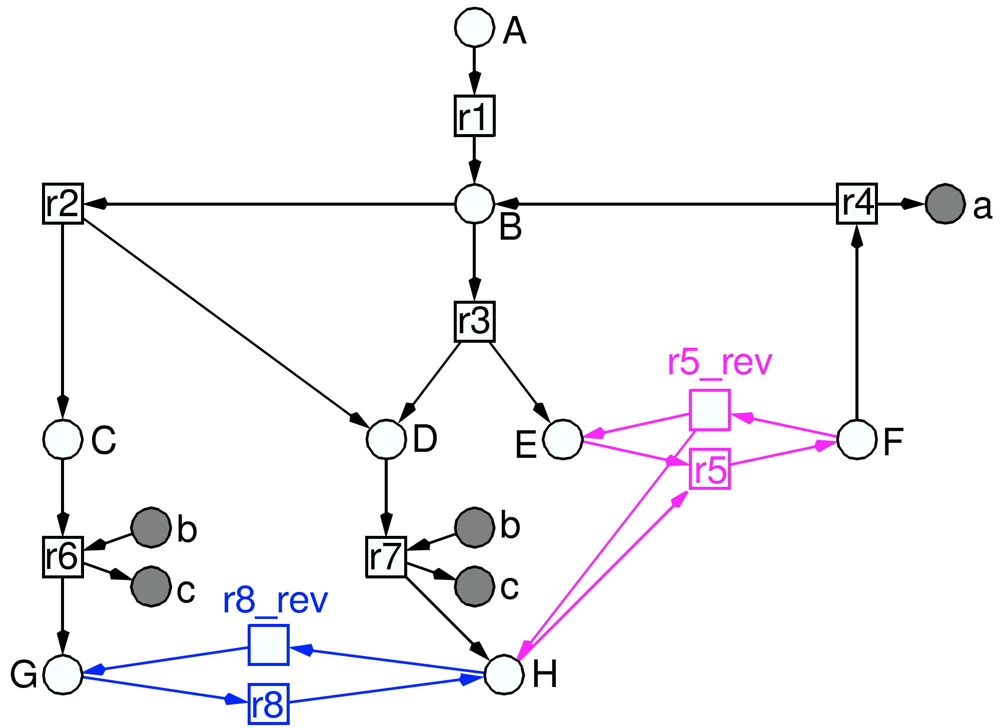
r4: F -> B + a

r5: E + H <-> F

r6: C + b -> G + c

r7: D + b -> H + c

r8: H <-> G



-> reversible reactions

r1: A -> B

r2: B -> C + D

r3: B -> D + E

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r5: E + H <-> F

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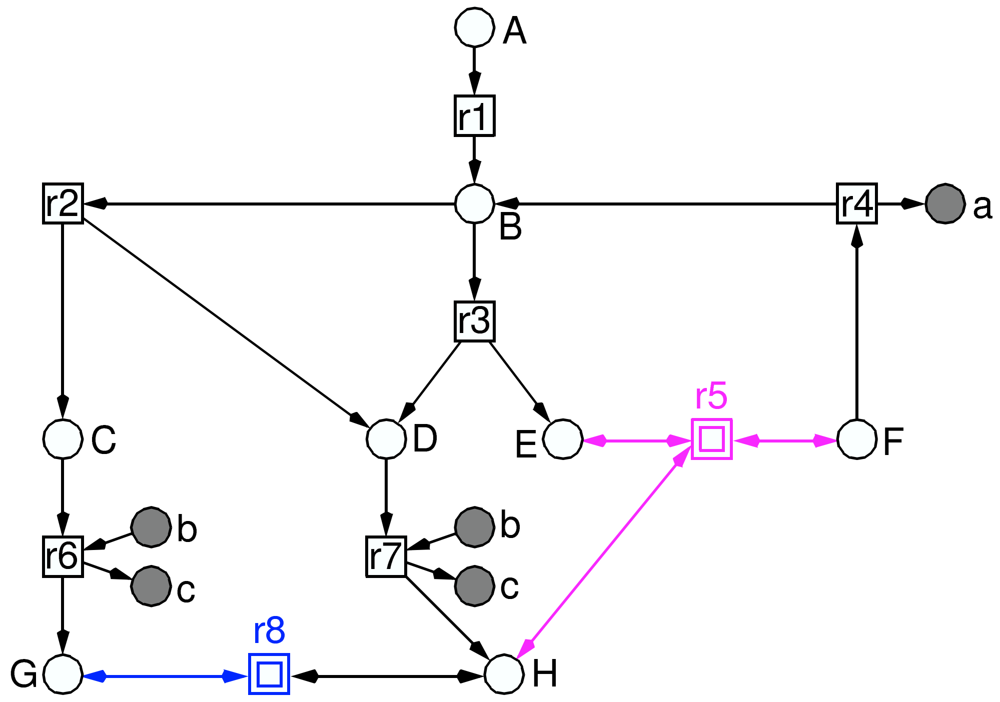


-> reversible reactions
- hierarchical nodes

r1: A -> B

r2: B -> C + D

r3: B -> D + E

r4: F -> B + a

r5: E + H <-> F

r6: C + b -> G + c

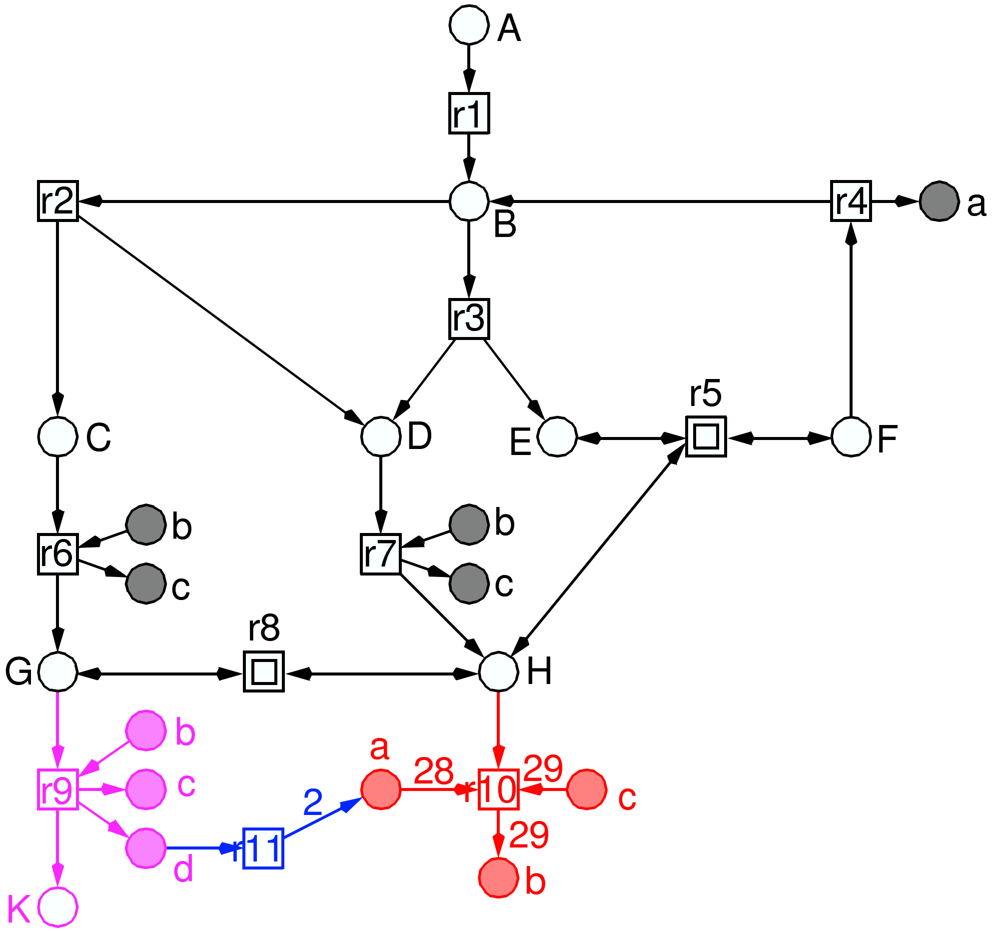
r7: D + b -> H + c

r8: H <-> G

r9: G + b -> K + c + d

r10: H + 28a + 29c -> 29b

r11: d -> 2a



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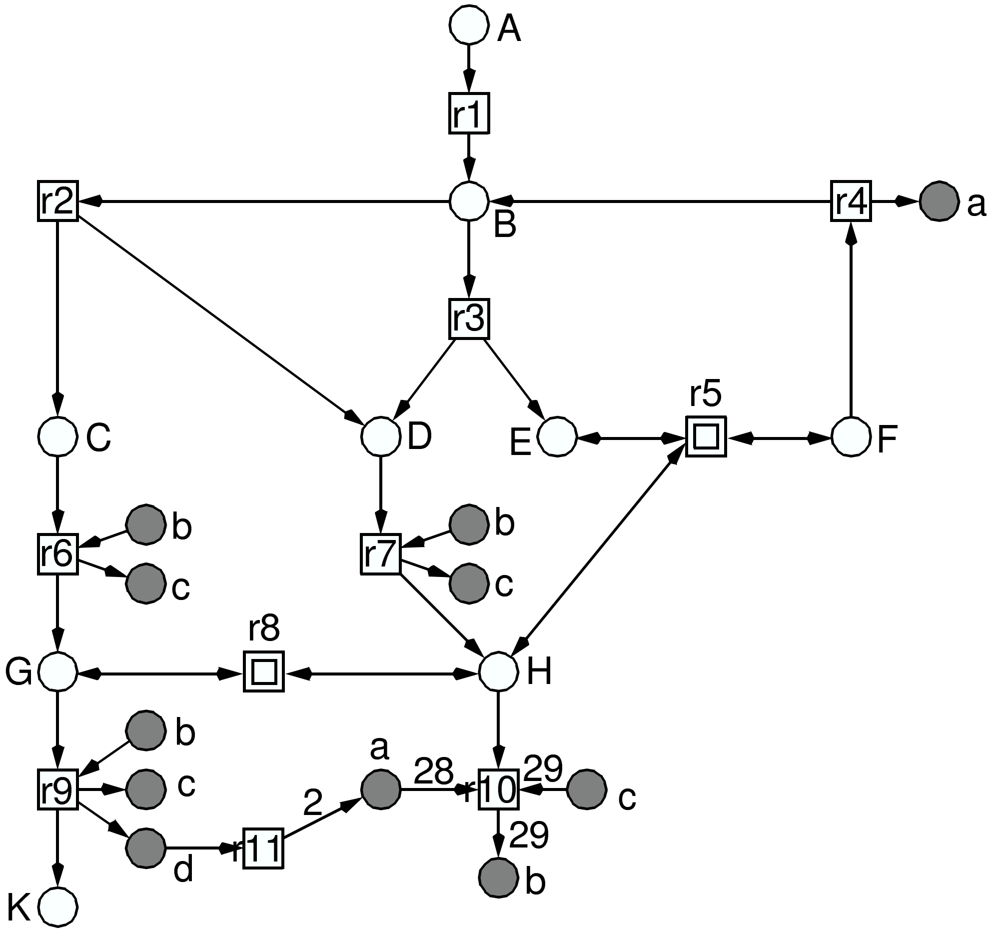

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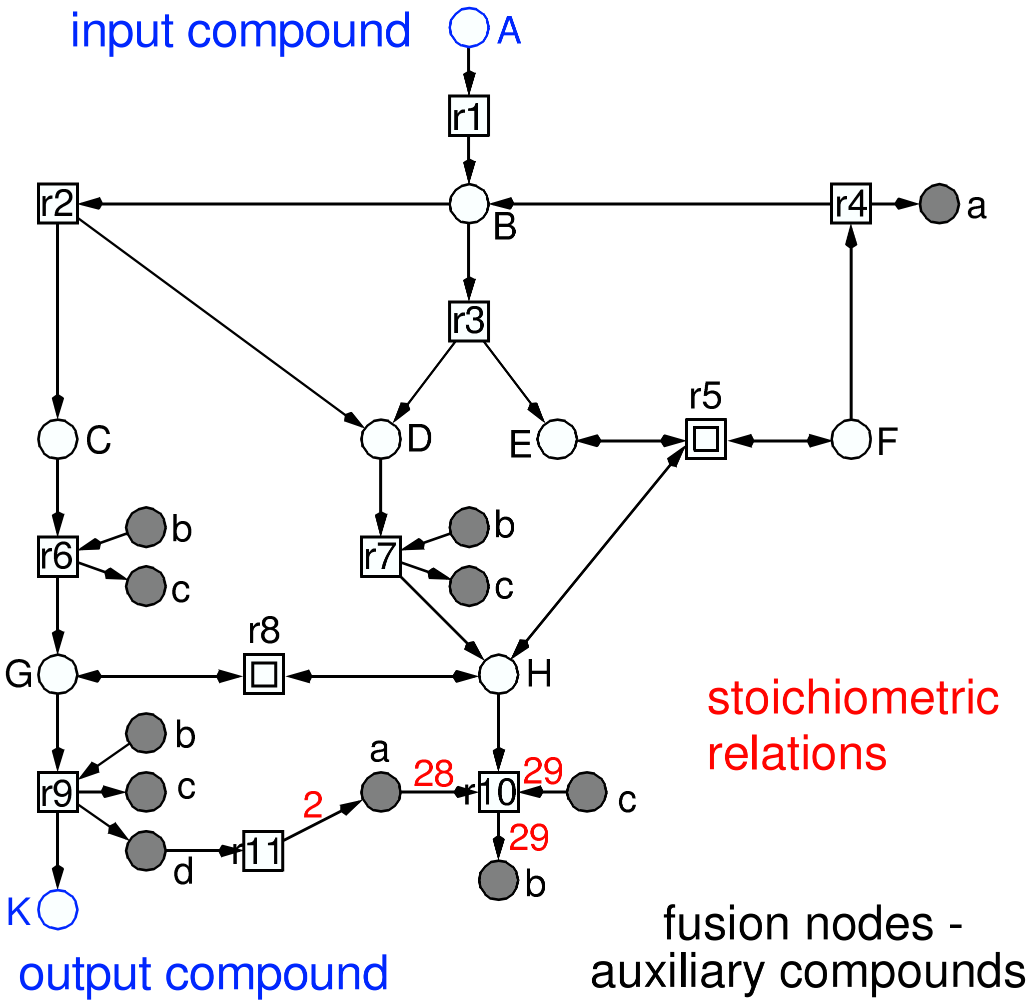
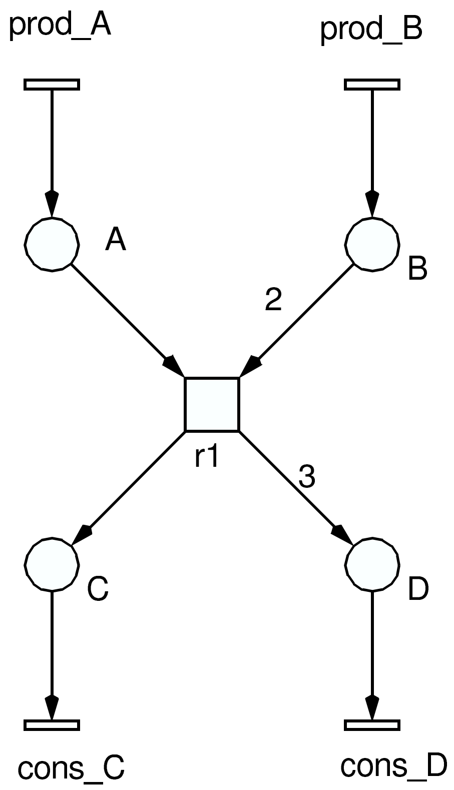


TRANSFORMATION, EX1



-> properties as time-less net

INA

ORD	HOM	NBM	PUR	CSV	SCF	CON	SC	Ft0	tF0	Fp0	pF0	MG	SM	FC	EFC	ES
N	Y	N	Y	N	Y	Y	N	Y	Y	N	N	Y	N	Y	Y	Y

CPI	CTI	B	SB	REV	DSt	BSt	DTr	DCF	L	LV	L&S
N	Y	N	N	Y	N	?	N	Y	Y	Y	N

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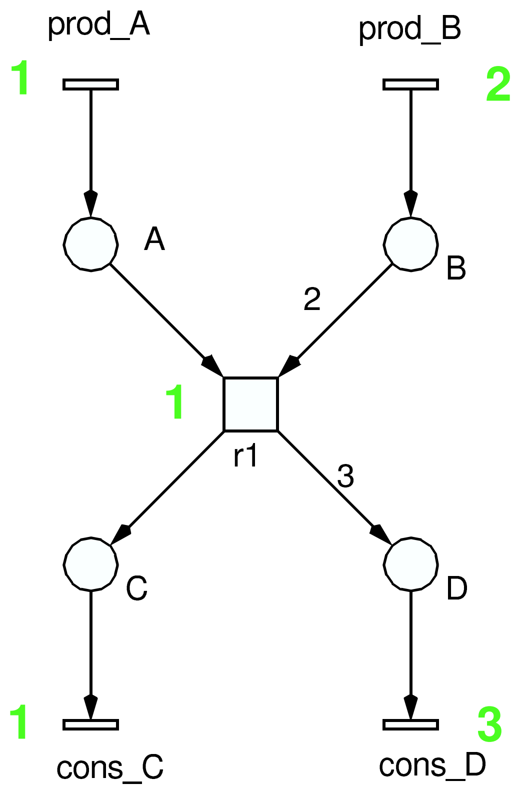

T-INVARIANTE

-> properties as time-less net

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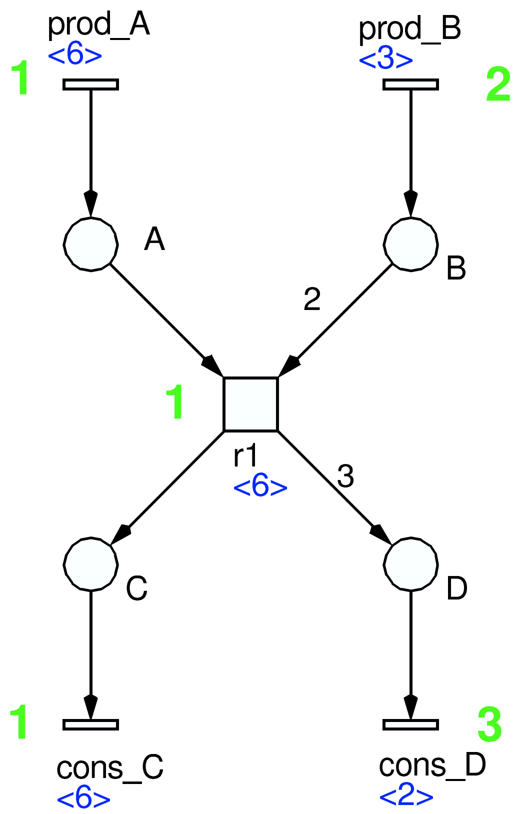
N	Y	N	N	Y	N	?	N	Y	Y	Y	N



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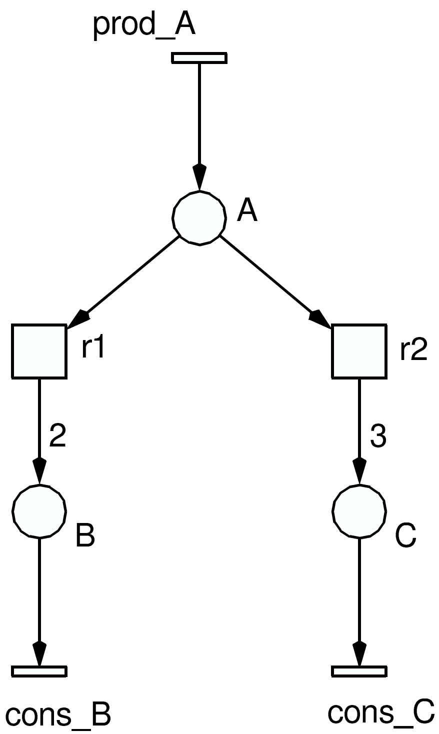

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N	Y	N	Y	N	Y	Y	N	Y	Y	N	N	Y	N	Y	Y	Y

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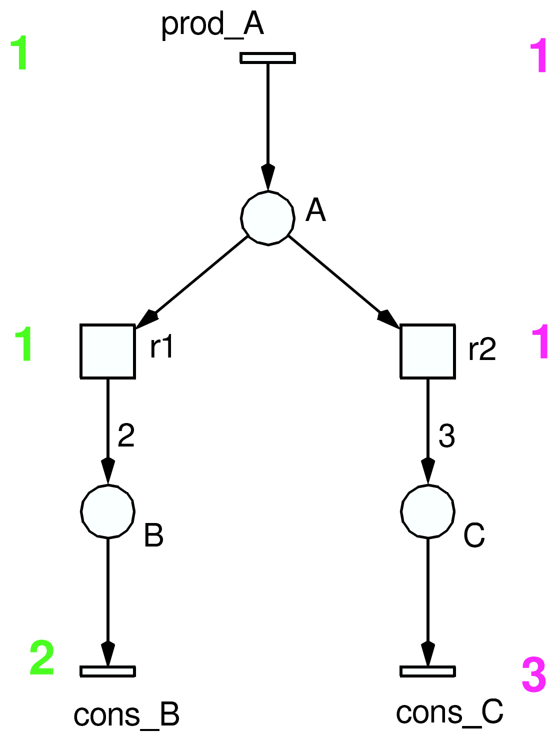

T-INVARIANTE1

T-INVARIANTE2

-> properties as time-less net

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N	Y	N	Y	N	Y	Y	N	Y	Y	N	N	Y	N	Y	Y	Y

CPI	CTI	B	SB	REV	DSt	BSt	DTr	DCF	L	LV	L&S
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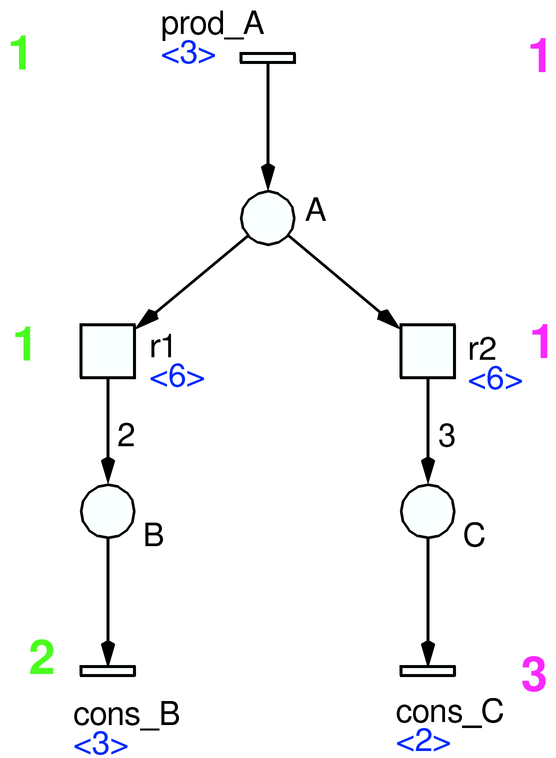

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The structure $N = (P, T, F, V, m_0)$ is a **Petri Net (PN)**, iff

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- $V : F \longrightarrow \mathbb{N}^+$ (weights of edges)

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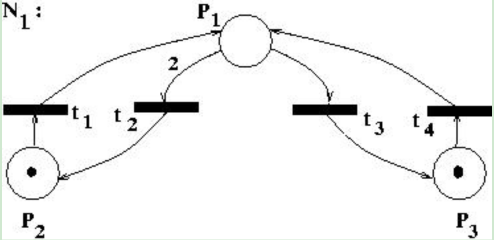
- $V : F \longrightarrow \mathbb{N}^+$ (weights of edges)
- $m_0 : P \longrightarrow \mathbb{N}$ (initial marking)

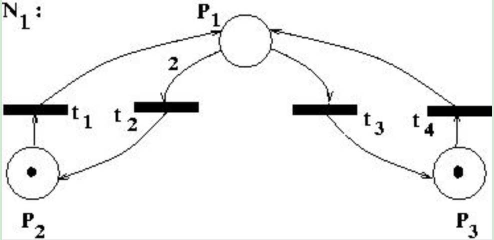
Petri Net

Example



Petri Net

Example



- $m_0 = (0, 1, 1)$

Petri Net

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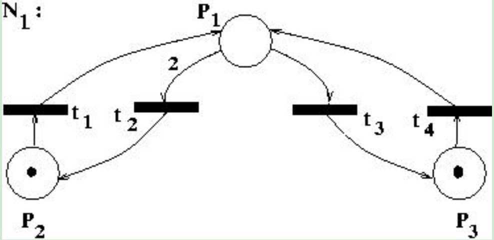
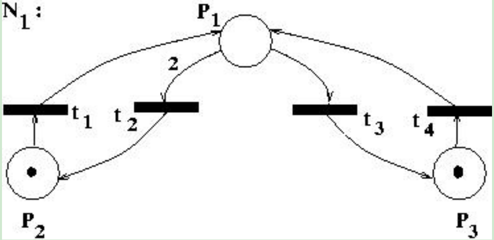


- $m_0 = (0, 1, 1)$
- $t_1^- = (0, 1, 0)$

Petri Net

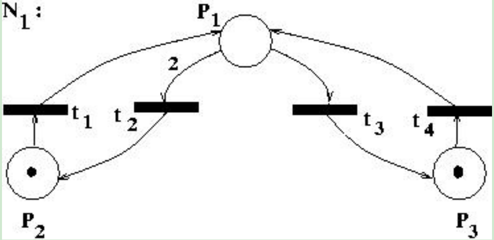
Example



- $m_0 = (0,1,1)$
- $t_1^- = (0,1,0)$ $t_1^+ = (1,0,0)$

Petri Net

Example



- $m_0 = (0, 1, 1)$
- $t_1^- = (0, 1, 0)$ $\quad$ $t_1^+ = (1, 0, 0)$
- $\Delta(t_1) = -t_1^- + t_1^+ = (1, -1, 0)$

Firing transition

Definition

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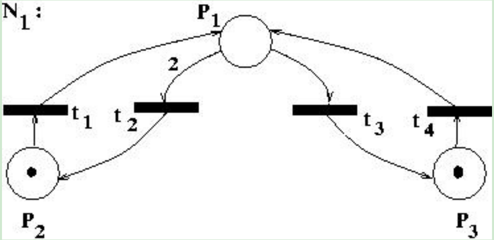
  denoted by $m \xrightarrow{t} m'$.

firing transition

Example



firing transition

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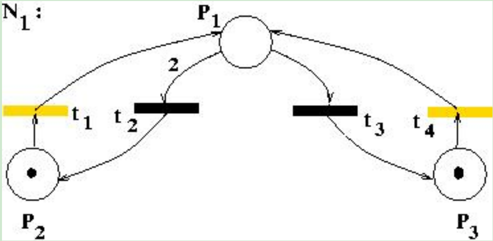

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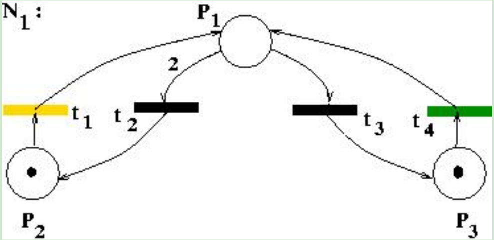

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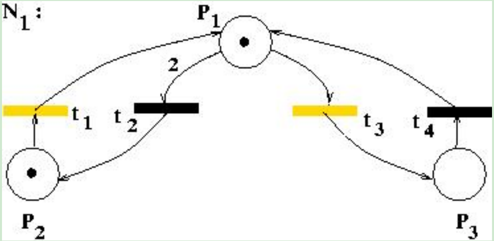

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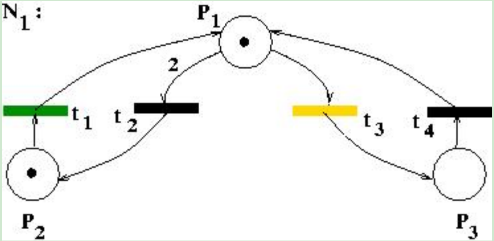

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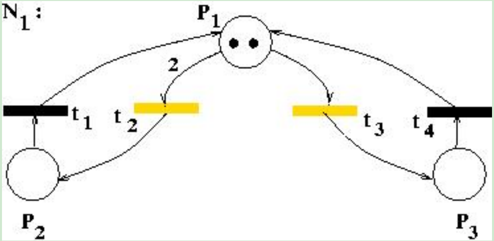

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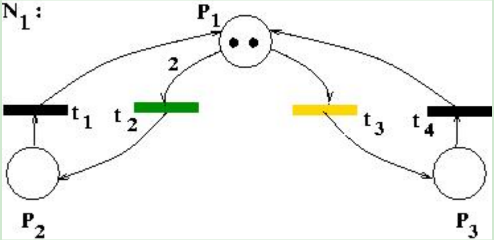
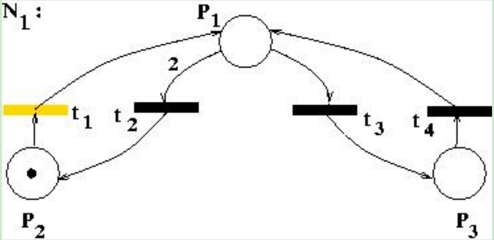


firing transition

Example



Time Petri Net

Definition (Time Petri net)

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- $I : T \longrightarrow \mathbb{Q}_0^+ \times (\mathbb{Q}_0^+ \cup \{\infty\})$ and $I_1(t) \leq I_2(t)$ for each $t \in T$, where $I(t) = (I_1(t), I_2(t))$.

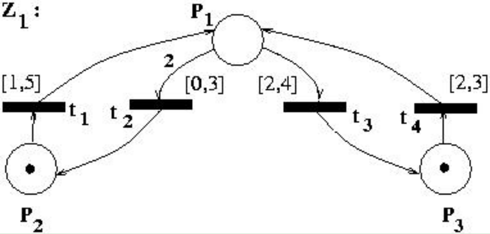
Time Petri Net

Definition (FTPN)

A TPN is called finite Time Petri net (FTPN) iff
$I : T \longrightarrow \mathbb{Q}_0^+ \times \mathbb{Q}_0^+$.

Time Petri Net

Example



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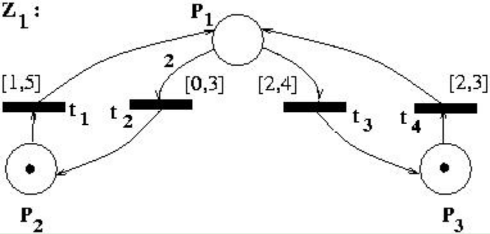
Example



- $m_0 = (0, 1, 1)$ p-marking

Time Petri Net

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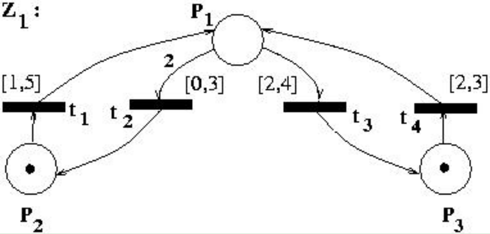

- $m_0 = (0, 1, 1)$ p-marking
- $h_0 = (0, \sharp, \sharp, 0)$ t-marking

state

Definition (state)

Let $Z = (P, T, F, V, m_o, I)$ be a TPN and $h : T \longrightarrow \mathbb{R}_0^+ \cup \{\#\}$.
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  and
  $\forall t \; (\; (t \in T \wedge t^- \not\leq m) \; \longrightarrow \; h(t) = \#).$

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$z = (m, h)$, $z' = (m', h')$ be two states.

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state changing

Definition (state changing)

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(iii) $\forall t\ (\ t \in T \longrightarrow$

$$h'(t) =: \begin{cases} \# & \text{iff} \quad t^- \not\leq m' \\ h(t) & \text{iff} \quad t^- \leq m \wedge t^- \leq m' \wedge Ft \cap F\hat{t} = \emptyset \\ 0 & \text{otherwise} \end{cases} \quad).$$

state changing

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(c) the state $z = (m, h)$ is **changed** into the state $z' = (m', h')$ **by the time elapsing** $\tau \in \mathbb{R}_0^+$, denoted by $z \xrightarrow{\tau} z'$, iff

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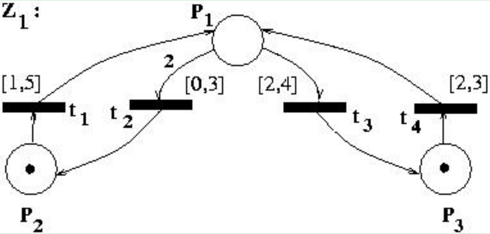
Time Petri Net

Example



$$(m_0, \begin{pmatrix} 0 \\ \sharp \\ \sharp \\ 0 \end{pmatrix})$$

Time Petri Net

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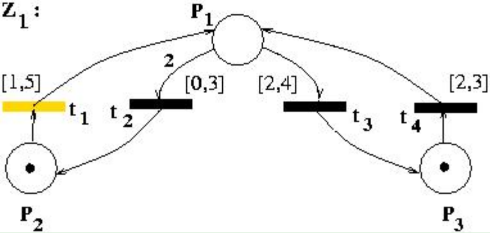

$$(m_0, \begin{pmatrix} 0 \\ \sharp \\ \sharp \\ 0 \end{pmatrix}) \xrightarrow{1.3} (m_1, \begin{pmatrix} 1.3 \\ \sharp \\ \sharp \\ 1.3 \end{pmatrix})$$

Time Petri Net

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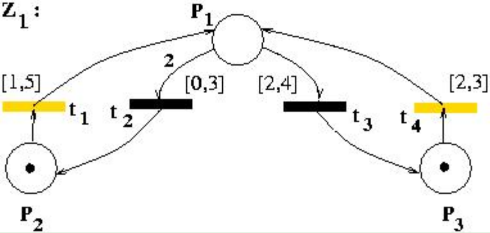

$$z_0 \xrightarrow{1.3} (m_1, \begin{pmatrix} 1.3 \\ \sharp \\ \sharp \\ 1.3 \end{pmatrix}) \xrightarrow{1.0} (m_2, \begin{pmatrix} 2.3 \\ \sharp \\ \sharp \\ 2.3 \end{pmatrix})$$

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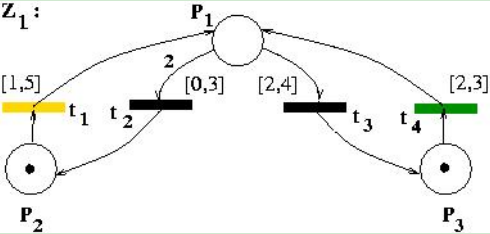

$$z_0 \xrightarrow{1.3} \xrightarrow{1.0} \left(m_2, \begin{pmatrix} 2.3 \\ \sharp \\ \sharp \\ 2.3 \end{pmatrix}\right) \xrightarrow{t_4}$$

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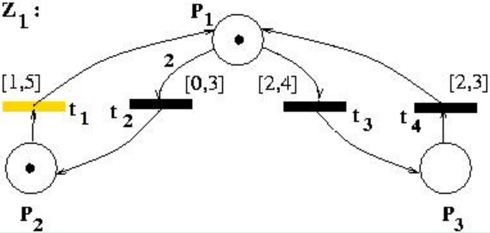

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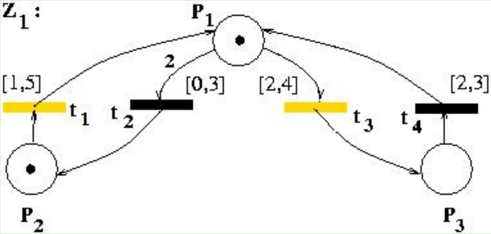
Time Petri Net

Example



$$z_0 \xrightarrow{1.3} \xrightarrow{1.0} \xrightarrow{t_4} (m_3, \begin{pmatrix} 2.3 \\ \sharp \\ 0.0 \\ \sharp \end{pmatrix}) \xrightarrow{2.0} (m_4, \begin{pmatrix} 4.3 \\ \sharp \\ 2.0 \\ \sharp \end{pmatrix})$$

Time Petri Net

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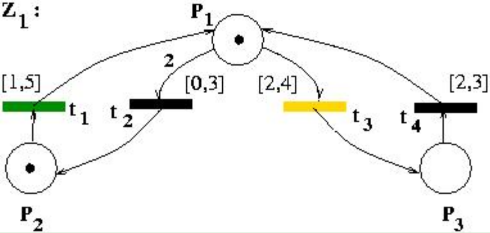

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Time Petri Net

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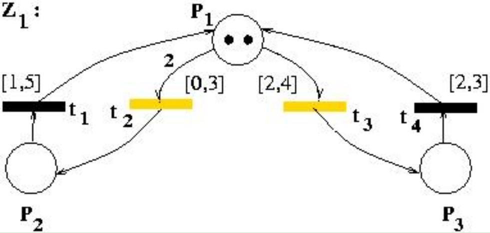

$$z_0 \xrightarrow{1.3} \xrightarrow{1.0} \xrightarrow{t_4} \xrightarrow{2.0} \left(m_4, \begin{pmatrix} 4.3 \\ \sharp \\ 2.0 \\ \sharp \end{pmatrix}\right) \xrightarrow{t_1} \left(m_5, \begin{pmatrix} \sharp \\ 0.0 \\ 2.0 \\ \sharp \end{pmatrix}\right)$$

Time Petri Net

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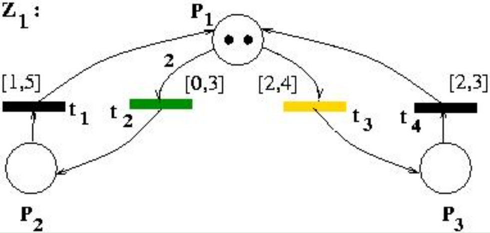

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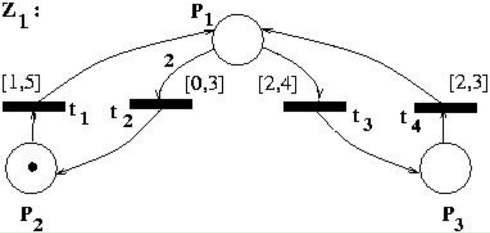

$$z_0 \xrightarrow{1.3} \xrightarrow{1.0} \xrightarrow{t_4} \xrightarrow{2.0} \xrightarrow{t_1} \left(m_5, \begin{pmatrix} \sharp \\ 0.0 \\ 2.0 \\ \sharp \end{pmatrix}\right) \xrightarrow{t_2} \left(m_6, \begin{pmatrix} 0.0 \\ \sharp \\ \sharp \\ \sharp \end{pmatrix}\right)$$

Transition sequences, Runs

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- **feasable transition sequence :** σ is feasable if there ex. a feasable run $\sigma(\tau)$

Reachable state, Reachable marking, State space

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- The set of all reachable states in Z is the **state space** of Z (denoted: $StSp(Z)$).

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Obviously: $StSp(Z) = \bigcup_\sigma C_\sigma$

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  - ordinary
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Parametric Description of the State Space

Let $Z = [P, T, F, V, m_0, I]$ be a TPN and $\sigma = (t_1, \cdots, t_n)$ be a transition sequence in Z.
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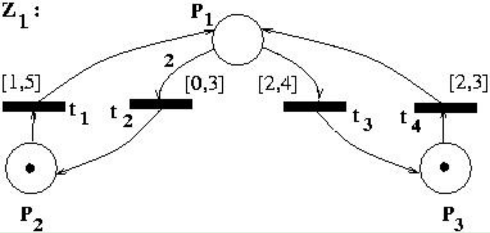
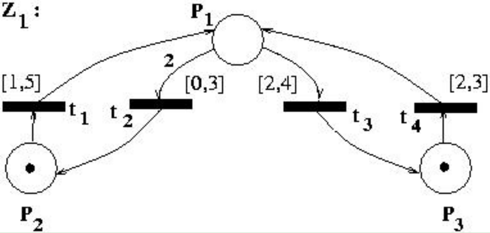
Obviously $\delta(\sigma) = C_\sigma$.

Example



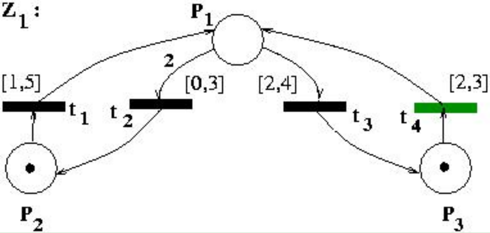
Example



$$\sigma = (e) \qquad \Longrightarrow$$

$$\delta(\sigma) = C_e = \{(\underbrace{(0,1,1)}_{m_\sigma}, \underbrace{(x_1, \sharp, \sharp, x_1)}_{\Sigma_\sigma}) \mid \underbrace{0 \leq x_1 \leq 3}_{B_\sigma}\}$$

Example



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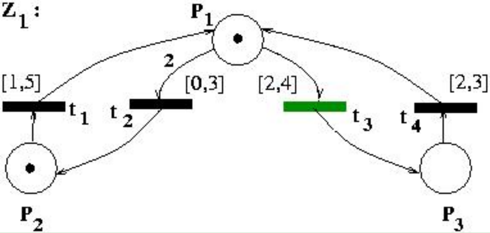

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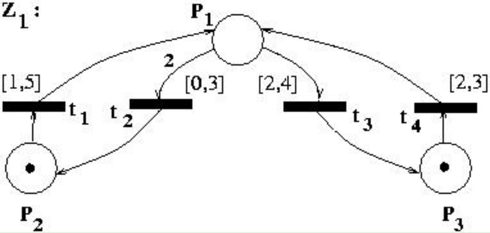

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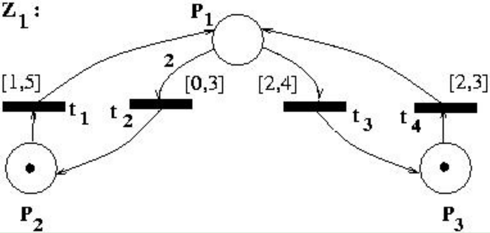
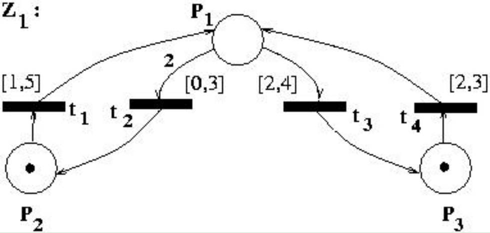


$$\sigma = (t_4, t_3)$$

Example



$$\sigma = (t_4, t_3) \quad \Longrightarrow \quad \delta(\sigma) = C_{t_4 t_3} =$$

$$\{ (\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}, \begin{pmatrix} x_1 + x_2 + x_3 \\ \sharp \\ \sharp \\ x_3 \end{pmatrix}) \mid \begin{array}{ll} 2 \leq x_1 \leq 3, & x_1 + x_2 \leq 5 \\ 2 \leq x_2 \leq 4, & x_1 + x_2 + x_3 \leq 5 \\ 0 \leq x_3 \leq 3 & \end{array} \}.$$

State Space Reduction

Theorem (1)

Let Z be a TPN and $\sigma = (t_1, \cdots, t_n)$ be a feasible transition sequence in Z, with a run $\sigma(\tau)$ as an execution of σ, i.e.

$$z_0 \xrightarrow{\tau_0} \xrightarrow{t_0} \cdots \xrightarrow{\tau_n} \xrightarrow{t_n} z_n = (m_n, h_n),$$

and all $\tau_i \in \mathbb{R}_0^+$.
Then, there exists a further feasible run $\sigma(\tau^*)$ of σ with

$$z_0 \xrightarrow{\tau_0^*} \xrightarrow{t_0} \cdots \xrightarrow{\tau_n^*} \xrightarrow{t_n} z_n^* = (m_n^*, h_n^*).$$

such that

State Space Reduction

Theorem (1 – continuation)

$$z_0 \xrightarrow{\tau_0} \xrightarrow{t_0} \cdots \xrightarrow{\tau_n} \xrightarrow{t_n} z_n = (m_n, h_n), \ \tau_i \in \mathbb{R}_0^+.$$

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State Space Reduction

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$z_0 \xrightarrow{\tau_0^*} \xrightarrow{t_0} \cdots \xrightarrow{\tau_n^*} \xrightarrow{t_n} z_n^* = (m_n^*, h_n^*)$

1. *For each* $i, 0 \leq i \leq n$ *holds:* $\tau_i^* \in \mathbb{N}$.

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1. *For each* $i, 0 \leq i \leq n$ *holds:* $\tau_i^* \in \mathbb{N}$.
2. *For each enabled transition* t *at marking* $m_n (= m_n^*)$ *it holds:*

   2.1 $h_n(t)^* = \lfloor h_n(t) \rfloor$.

   2.2 $\sum_{i=1}^{n} \tau_i^* = \lfloor \sum_{i=1}^{n} \tau_i \rfloor$

State Space Reduction

Theorem (2 – similar to 1)

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Theorem (2 – continuation)

1. *For each* $i, 0 \leq i \leq n$ *the time* τ_i^* *is a natural number.*
2. *For each enabled transition* t *at marking* $m_n (= m_n^*)$ *it holds:*

    2.1 $h_n(t)^* = \lceil h_n(t) \rceil$.

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State Space Reduction

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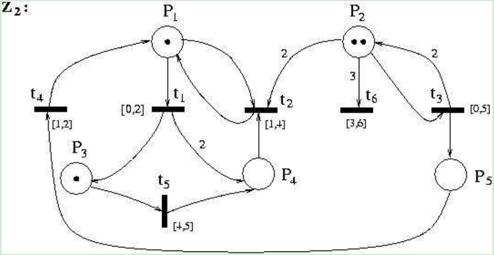

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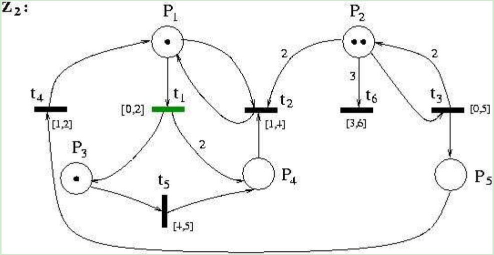

$$\sigma = (t_1 t_3 t_4 t_2 t_3)$$

$$\sigma(\tau) := z_0 \xrightarrow{0.7} \xrightarrow{t_1} \xrightarrow{0.0} \xrightarrow{t_3} \xrightarrow{0.4} \xrightarrow{t_4} \xrightarrow{1.2} \xrightarrow{t_2} \xrightarrow{0.5} \xrightarrow{t_3} \xrightarrow{1.4} z$$

State Space Reduction

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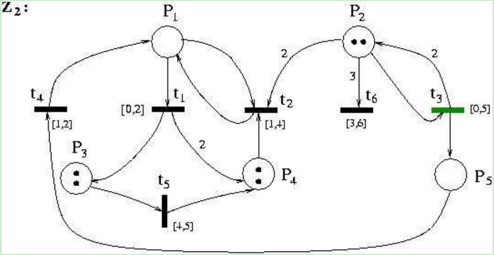

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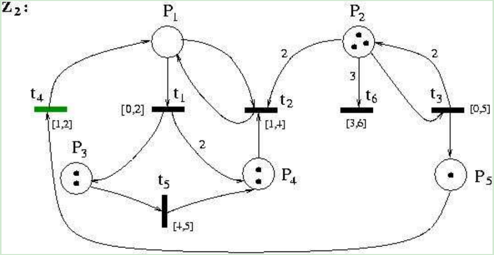
$$\sigma(\tau) := z_0 \xrightarrow{0.7} \xrightarrow{t_1} \xrightarrow{0.0} \xrightarrow{t_3} \xrightarrow{0.4} \xrightarrow{t_4} \xrightarrow{1.2} \xrightarrow{t_2} \xrightarrow{0.5} \xrightarrow{t_3} \xrightarrow{1.4} z$$

State Space Reduction

Example



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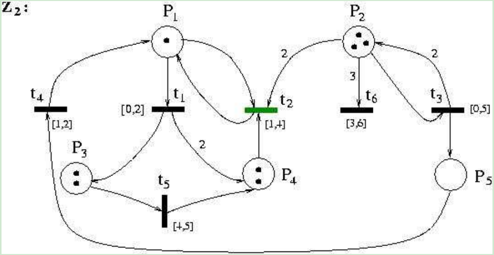

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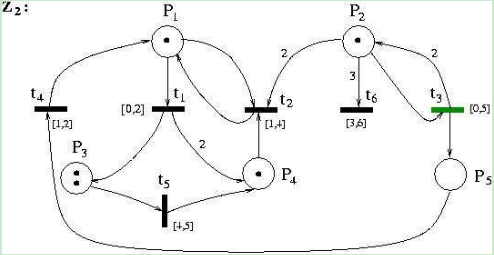

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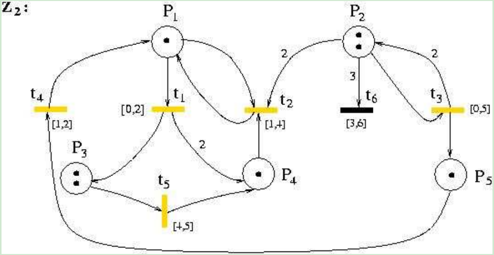

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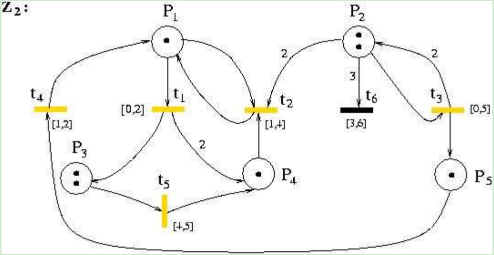
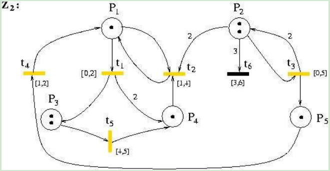


$$\sigma = (t_1 t_3 t_4 t_2 t_3)$$

$$m_\sigma = (1, 2, 2, 1, 1)$$

State Space Reduction

Example (continuation)



$$\Sigma_\sigma = \begin{pmatrix} x_4 + x_5 \\ x_5 \\ x_5 \\ x_5 \\ x_0 + x_1 + x_2 + x_3 + x_4 + x_5 \\ \sharp \end{pmatrix} \quad \text{and}$$

State Space Reduction

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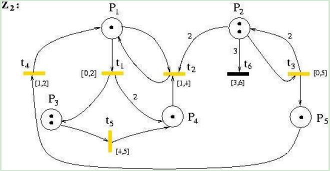

$$B_\sigma = \left\{ \begin{array}{lll} 0 \le x_0, & x_0 \le 2, & x_0 + x_1 + x_2 \le 5 \\ 0 \le x_1, & x_2 \le 2, & x_2 + x_3 \le 5 \\ 1 \le x_2, & x_3 \le 2, & x_0 + x_1 + x_2 + x_3 \le 5 \\ 1 \le x_3, & x_4 \le 2, & x_0 + x_1 + x_2 + x_3 + x_4 \le 5 \\ 0 \le x_4, & x_5 \le 2, & x_0 + x_1 + x_2 + x_3 + x_4 + x_5 \le 5 \\ 0 \le x_5, & x_0 + x_1 \le 5 & x_4 + x_5 \le 2 \end{array} \right\}.$$

State Space Reduction

Example (continuation)

The run $\sigma(\tau)$ with

$$\sigma(\tau) := z_0 \xrightarrow{0.7} \xrightarrow{t_1} \xrightarrow{0.0} \xrightarrow{t_3} \xrightarrow{0.4} \xrightarrow{t_4} \xrightarrow{1.2} \xrightarrow{t_2} \xrightarrow{0.5} \xrightarrow{t_3} \xrightarrow{1.4} z$$

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is feasible.

State Space Reduction

Example (continuation)

		x_0	x_1	x_2	x_3	x_4	x_5	$\Sigma_\sigma(t_1)$	$\Sigma_\sigma(t_2)$	$\Sigma_\sigma(t_5)$
$\hat{\beta}$ =	β_0	0.7	0.0	0.4	1.2	0.5	1.4	1.9	1.4	4.2
	β_1	0.7	0.0	0.4	1.2	0.5	**1**	1.5	1.0	3.8
	β_2	0.7	0.0	0.4	1.2	**0**	1	1.0		3.3
	β_3	0.7	0.0	0.4	**1**	0	1			3.1
	β_4	0.7	0.0	**1**	1	0	1			3.7
	β_5	0.7	**0**	1	1	0	1			3.7
	β_6	**1**	0	1	1	0	1			4.0

State Space Reduction

Example (continuation)

		x_0	x_1	x_2	x_3	x_4	x_5	$\Sigma_\sigma(t_1)$	$\Sigma_\sigma(t_2)$	$\Sigma_\sigma(t_5)$
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	β_2	0.7	0.0	0.4	1.2	**0**	1	2.0		4.3
	β_3	0.7	0.0	0.4	**2**	0	1			5.1
	β_4	0.7	0.0	**0**	1	0	1			4.7
	β_5	0.7	**0**	1	1	0	1			4.7
	β_6	**1**	0	1	1	0	1			5.0

State Space Reduction

Example (continuation)

Hence, the runs

$$\sigma(\tau_1^*) := z_0 \xrightarrow{\mathbf{1}} \xrightarrow{t_1} \xrightarrow{\mathbf{0}} \xrightarrow{t_3} \xrightarrow{\mathbf{1}} \xrightarrow{t_4} \xrightarrow{\mathbf{1}} \xrightarrow{t_2} \xrightarrow{\mathbf{0}} \xrightarrow{t_3} \xrightarrow{\mathbf{1}} \lfloor z \rfloor$$

and

$$\sigma(\tau_2^*) := z_0 \xrightarrow{\mathbf{1}} \xrightarrow{t_1} \xrightarrow{\mathbf{0}} \xrightarrow{t_3} \xrightarrow{\mathbf{0}} \xrightarrow{t_4} \xrightarrow{\mathbf{2}} \xrightarrow{t_2} \xrightarrow{\mathbf{0}} \xrightarrow{t_3} \xrightarrow{\mathbf{2}} \lceil z \rceil$$

are feasible in Z, too.

State Space Reduction

Corollary

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- *Each reachable marking in Z can be found using "integer" runs only.*
- *If z is reachable in Z, then $\lfloor z \rfloor$ and $\lceil z \rceil$ are reachable in Z, too.*
- *The length of the shortest and longest time path between two arbitrary states are natural numbers.*

State Space Reduction

Definition

A state $z = (m, h)$ in a TPN is **integer** one iff
for all enabled transitions t at m holds: $h(t) \in \mathbb{N}$.

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Remark: Theorem 3 can be generalized for all TPNs (applying a further reduction).

Reachability Graph

Definition

Basis)

$z_0 \in RG(Z)$

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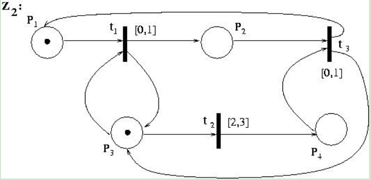
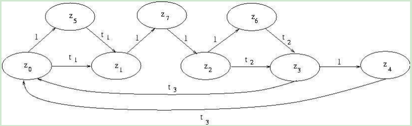
$\Longrightarrow$ The reachability graph is a weighted directed graph.

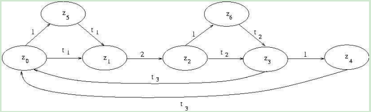
A TPN and its full Reachability Graph

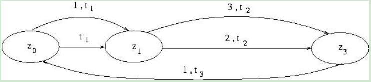
Example (A TPN Z and its full reachability graph $RG^{(1)}(Z)$)



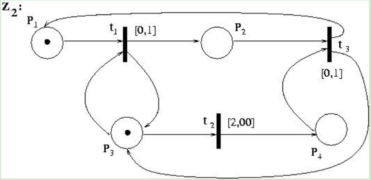


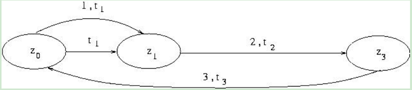
Example (The reduced reachability graphs $RG^{(2)}(Z)$ and $RG(Z)$)





Example (The reachability graph $RG(Z_3)$)





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For **timeless PN:** σ is a feasible T-invariant iff
$m = m + C \cdot \psi(\sigma)$ and $\psi(\sigma)$ - the Parikh-vektor of σ.
$\Longrightarrow$ easy to be found.

Lemma

Let Z be a TPN, $S(Z)$ be the skeleton of Z and σ be a feasible T-invariant in $S(Z)$.
σ is a feasible T-invariant in Z **iff** *B_σ has a solution.*

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Computing the T-invariants of a Z:

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Computing the T-invariants of a Z:

- Solve the linear system of equations $C \cdot x = 0$ for $x \in \mathbb{N}$.
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- If σ is feasible, then solve the linear system of inequalities B_σ in $\mathbb{R}_0^+$.

Remark: The reachability graph of a TPN is not used for computing the feasible T-invariants of Z

$$\Longrightarrow$$

feasible T-invariants for **unbounded** nets can be computed!

Let $Z = (P, T, F, V, I, m_o)$ be a TPN.
Then the following problems can be decided/computed without knowledge of its RG:

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Result 1:

Input:	The time function I is fixed, σ is an arbitrary transition sequence.
Output:	Feasibility of σ in Z?
Solution:	Solve a linear system of inequalities in $\mathbb{R}_0^+$.

Let $Z = (P, T, F, V, I, m_o)$ be a TPN.
Then the following problems can be decided/computed without knowledge of its RG:

Result 2:

Input:	The time function I is not fixed, σ is an arbitrary transition sequence.
Output:	Feasibility of σ in Z for a fixed I?
Solution:	Solve a linear system of inequalities in $\mathbb{Q}_0^+$.

Let $Z = (P, T, F, V, I, m_o)$ be a TPN.
Then the following problems can be decided/computed without knowledge of its RG:

Result 3:

Input:	The time function I is fixed, σ is an arbitrary transition sequence.
Output:	min / max-length of σ.
Solution:	Solve a linear program in $\mathbb{R}_0^+$. (Actually, the solution is in $\mathbb{N}$.)

Let $Z = (P, T, F, V, I, m_o)$ be a TPN.
Then the following problems can be decided/computed without knowledge of its RG:

Result 4:

Input: The time function I is not fixed,
σ is an arbitrary transition sequence,
λ is an arbitrary real number.

Output: Existence of a fixed I and a run $\sigma(\tau)$ in Z and the length of $\sigma(\tau) \leq \lambda$?

Solution: Solve a linear program in $\mathbb{Q}_0^+$.

Result 5:

Input: The time function I is not fixed,
$\sigma_1 = (\sigma, t')$ is a arbitrary t-sequence and
$\sigma_2 = (\sigma, t'')$ is a arbitrary t-sequence.

Output: Existence of a fixed I so that σ_1 is feasible in Z and σ_2 is not feasible in Z?

Solution: Solve

$$\underbrace{\max\{< c', x >| \ A' \cdot x \leq b'\}}_{\text{linear program in } \mathbb{Q}_0^+} < \underbrace{\min\{< c'', x >| \ A'' \cdot x \leq b''\}}_{\text{linear program in } \mathbb{Q}_0^+}.$$

Let $Z = (P, T, F, V, I, m_o)$ be a bounded TPN. Additionally the following problems can be decided/computed with the knowledge of its RG, amongst others:

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Result 6:

Input: z and z' - two states (in Z).

Output: – Is there a path between z and z' in $RG(Z)$?
– If yes, compute the path with the shortest time length.

Solution: By means of prevalent methods of the graph theory, e.g. Bellman-Ford algorithm (the running time is $\mathcal{O}(|V| \cdot |E|)$ and $RG(Z) = (V, E)$)

Let $Z = (P, T, F, V, I, m_o)$ be a bounded TPN. Additionally the following problems can be decided/computed with the knowledge of its RG, amongst others:

Result 7:

Input: m and m' - two markings (in Z).

Output:
- Is there a path between m and m' in $RG(Z)$?
- If yes, compute the path with the shortest time length.

Solution: By means of prevalent methods of the graph theory, for computing all-pairs shortest paths.
The running time is polynomial, too.

Definition

The **longest path** between two states (vertices in $RG(Z)$) z and z' is $lp(z, z')$ with

$$lp(z,z') := \begin{cases} \infty & \text{, if a cycle is reachable starting on } z \\ \max \sum\limits_{\sigma(\tau)} \tau_i & \text{, if } z \xrightarrow{\sigma(\tau)} z' \end{cases}$$

Result 8:

Input: z and z' - two states (in Z).

Output:
– Is there a path between z and z' in $RG(Z)$?
– If yes, compute the path with the longest time length.

Solution: By means of prevalent methods of the graph theory, e.g. Bellman-Ford algorithm (polyn. running time). or by computing all strongly connected components of $RG(Z)$. (linear running time)

Result 9:

Input: m and m' - two states (in Z).

Output:
– Is there a path between z and z' in $RG(Z)$?
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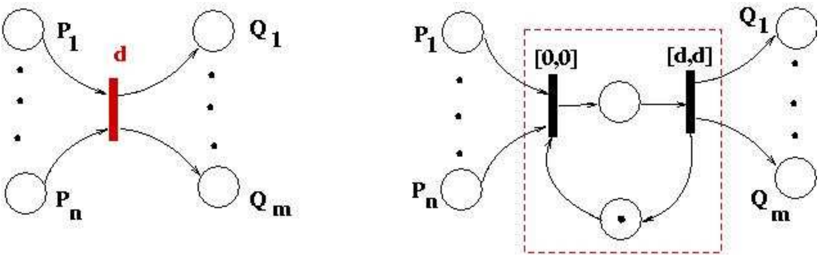
Transformation Timed PN $\longrightarrow$ Time PN



Conclusion

- theoretical approach

  BN $\Longrightarrow$ *modelling* $\Longrightarrow$ PN $\Longrightarrow$ *modelling of steady state* $\Longrightarrow$

  DPN $\Longrightarrow$ *analysing* $\Longrightarrow$ TPN

- experimental approach

  BN $\Longrightarrow$ *modelling & analysing* $\Longrightarrow$ TPN