

# Quantitative Analysis of Time Petri Nets Used for Modelling Biochemical Networks

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# Outline

## Definitions

Petri Net

Time Petri Net

## Main Property

State Space Reduction

## Applications

Reachability Graph

T-Invariants

Time Paths in unbounded TPNs

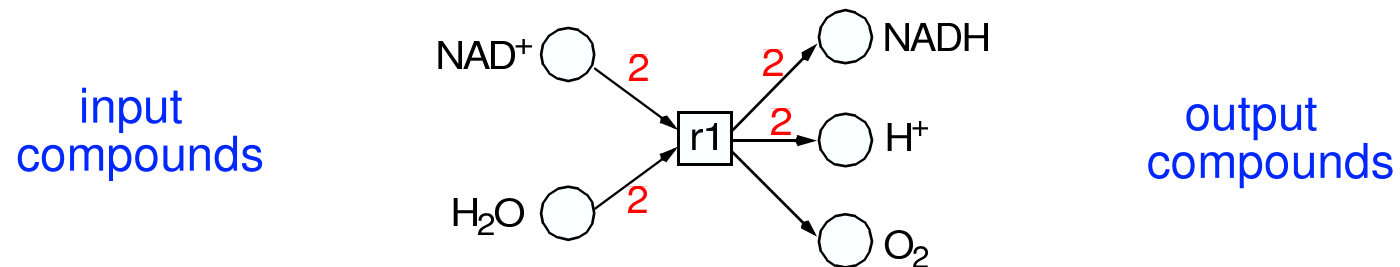
Time Paths in bounded TPNs

Time PN and Timed PN

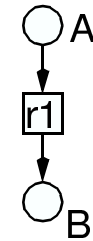
## Conclusion



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



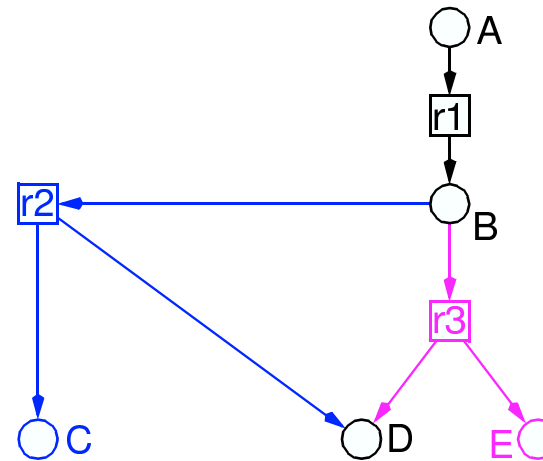
r1: A -> B



r1: A -> B

r2: B -> C + D

r3: B -> D + E



-> *alternative reactions*

r1:  $A \rightarrow B$

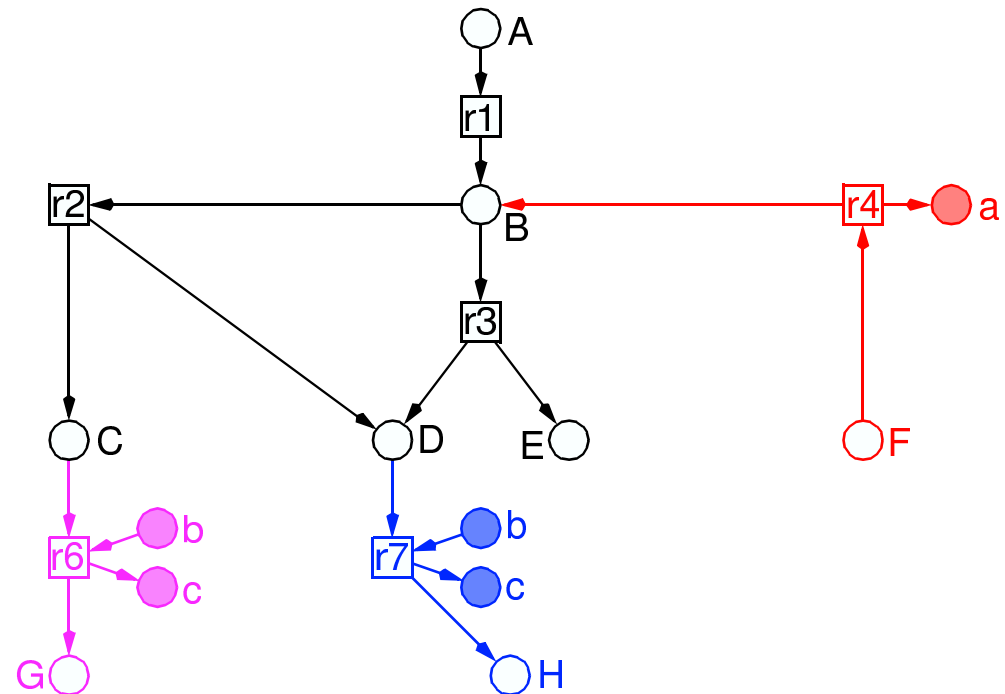
r2:  $B \rightarrow C + D$

r3:  $B \rightarrow D + E$

r4:  $F \rightarrow B + a$

r6:  $C + b \rightarrow G + c$

r7:  $D + b \rightarrow H + c$



-> concurrent reactions

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r3:  $B \rightarrow D + E$

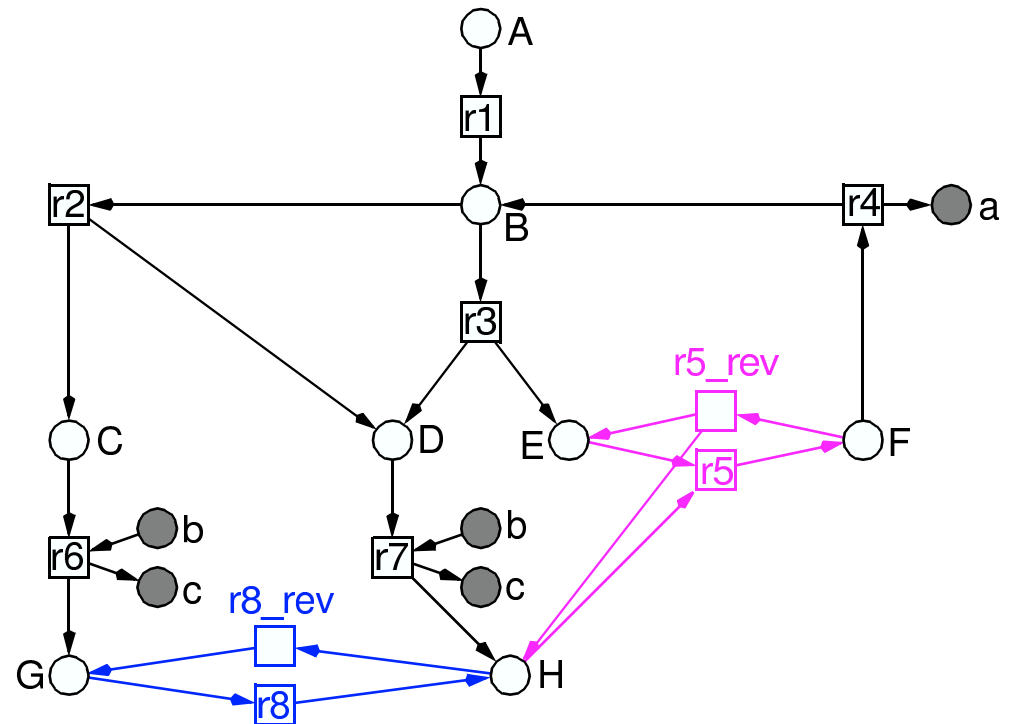
r4:  $F \rightarrow B + a$

r5:  $E + H \rightleftharpoons F$

r6:  $C + b \rightarrow G + c$

r7:  $D + b \rightarrow H + c$

r8:  $H \rightleftharpoons G$



*-> reversible reactions*

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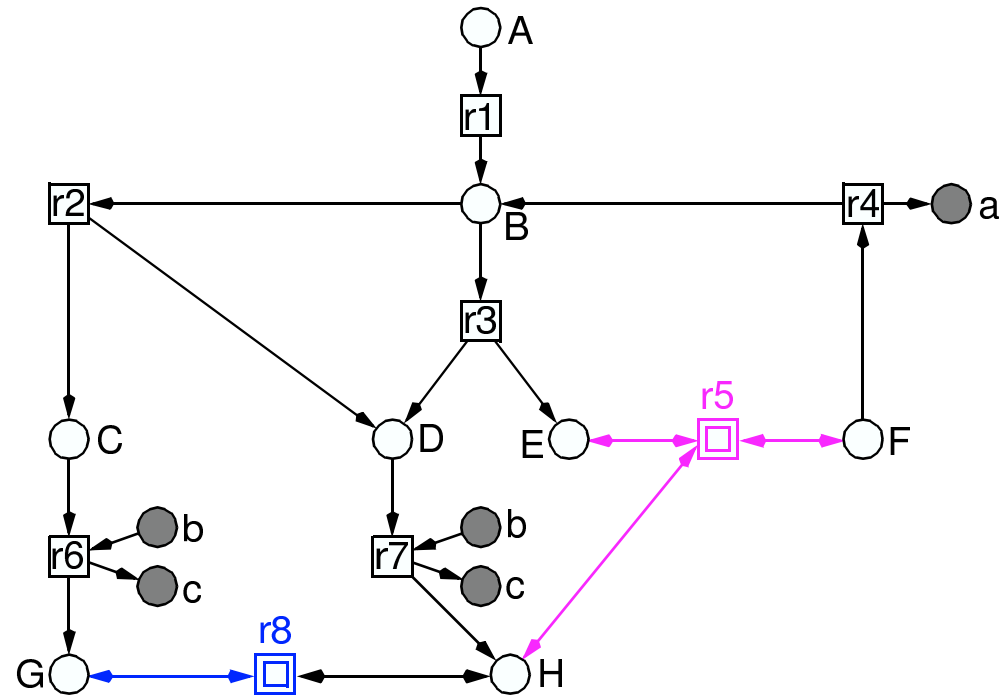
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-> reversible reactions  
- hierarchical nodes



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r4:  $F \rightarrow B + a$

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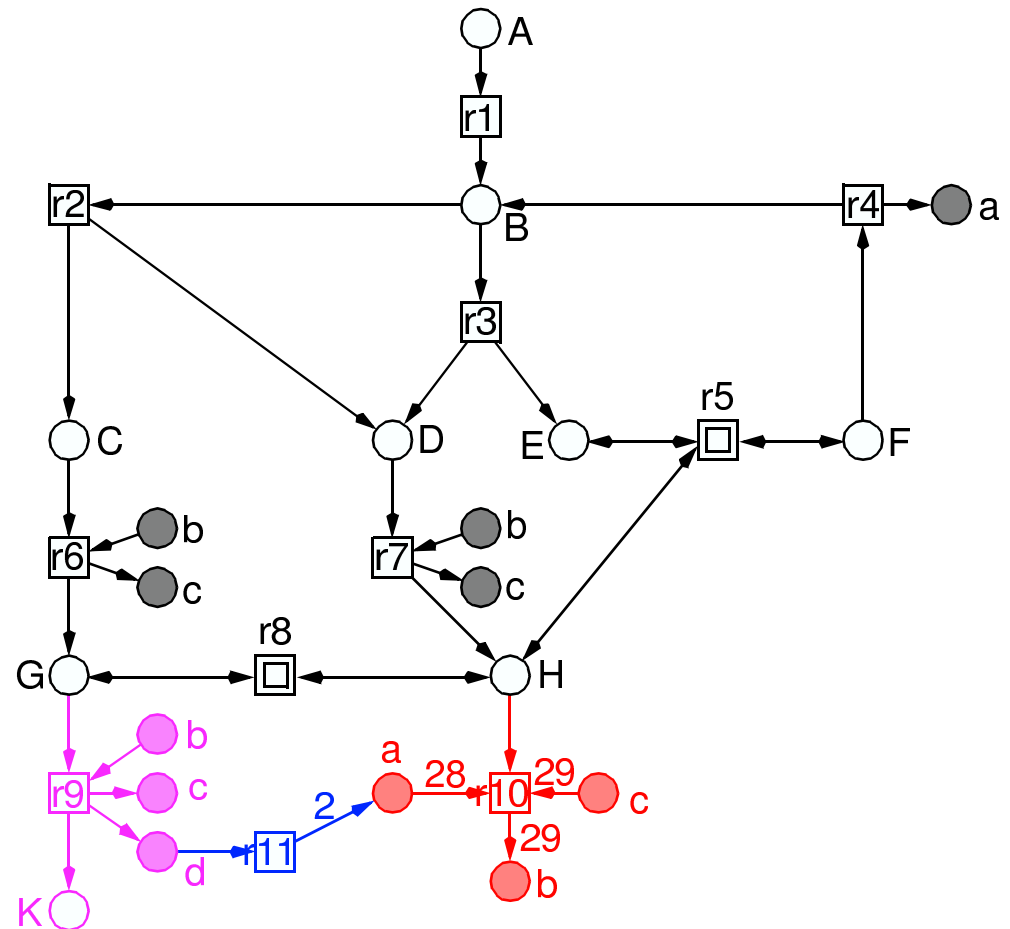
r7:  $D + b \rightarrow H + c$

r8:  $H \leftrightarrow G$

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r10:  $H + 28a + 29c \rightarrow 29b$

r11:  $d \rightarrow 2a$



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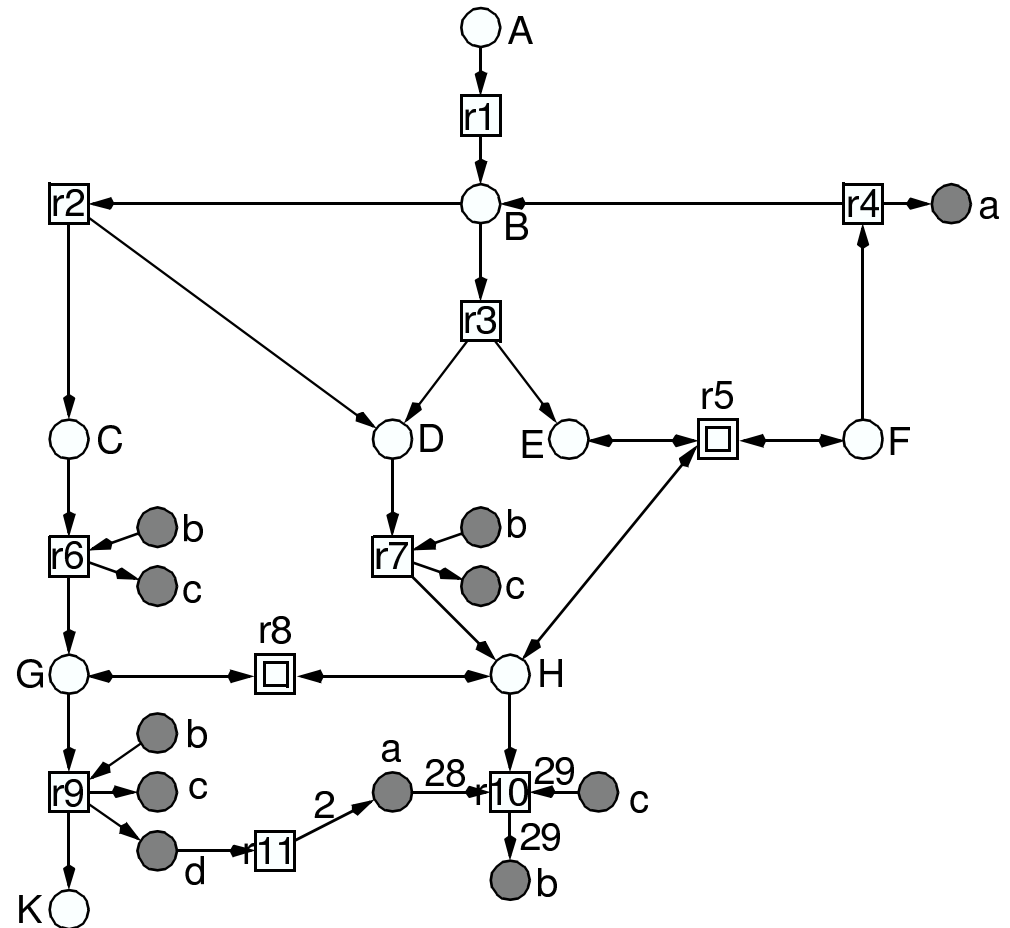
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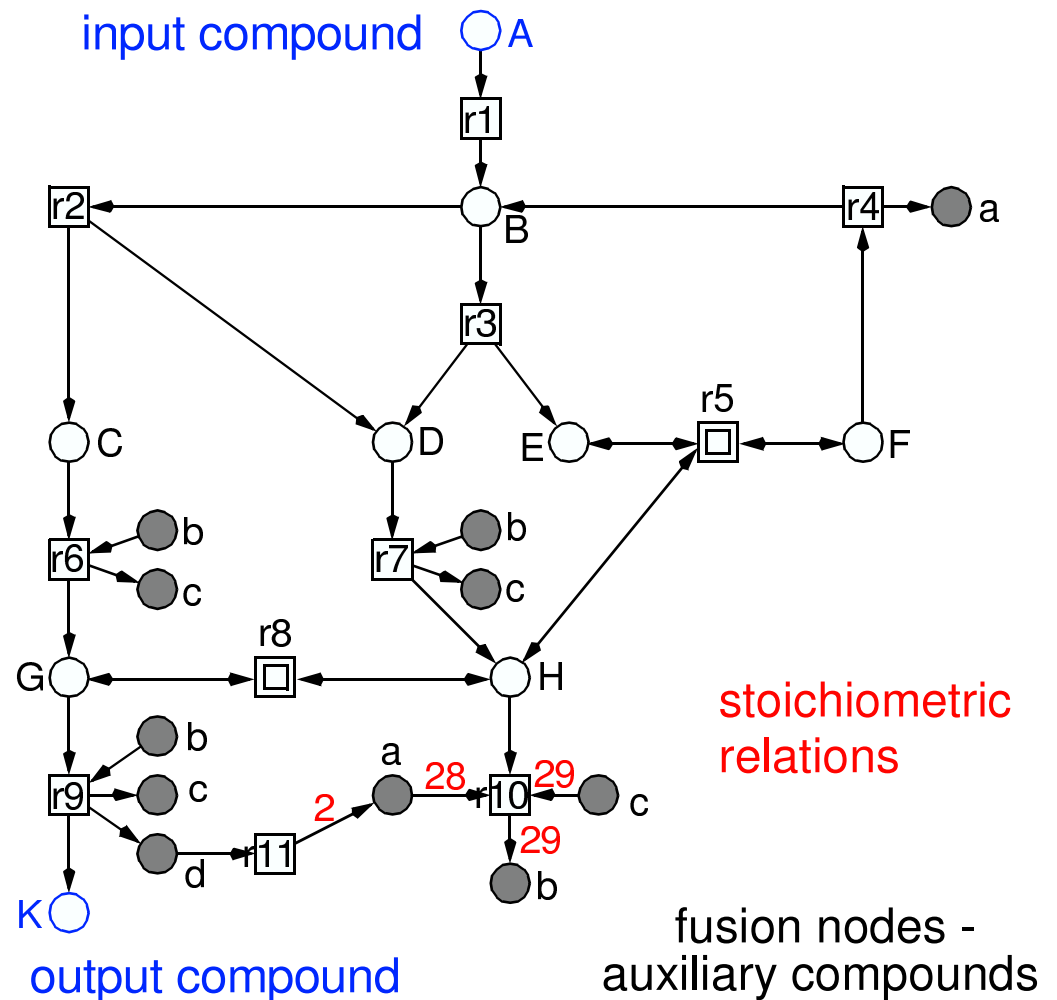
r9:  $G + b \rightarrow K + c + d$

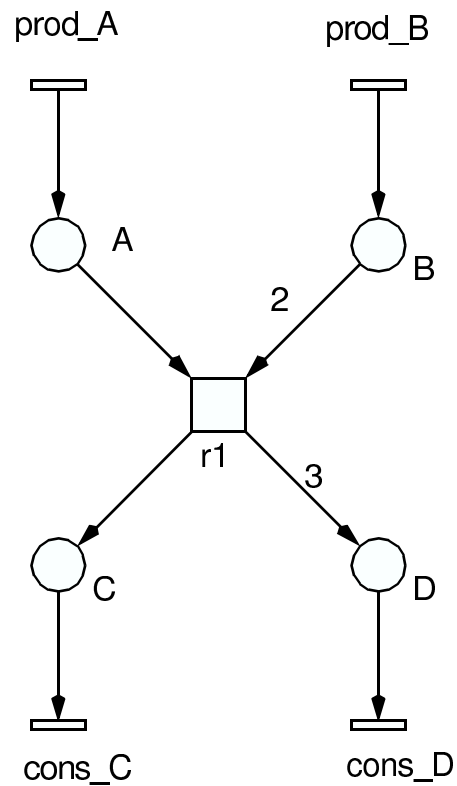
r10:  $H + 28a + 29c \rightarrow 29b$

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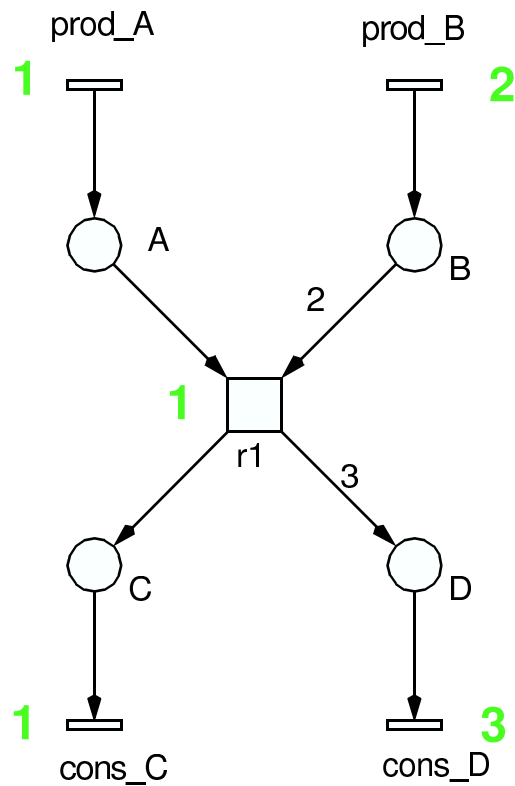




-> properties as time-less net

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					

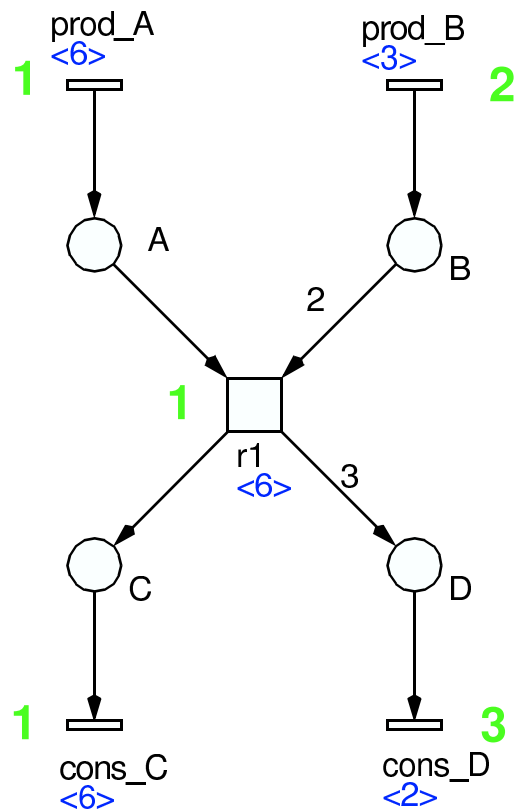


T-INVARIANTE

-> 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					

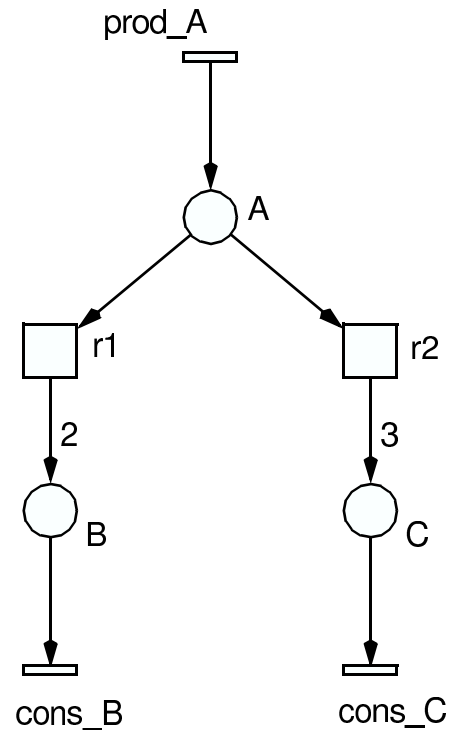


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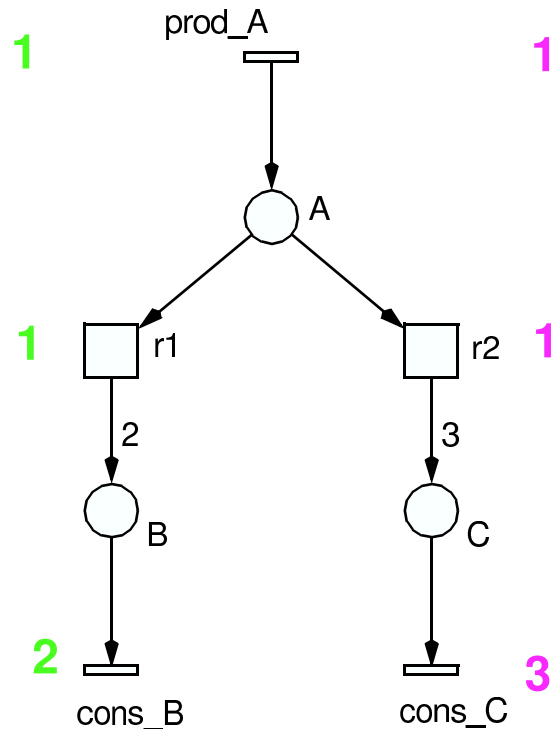
ORD	HOM	NBM	PUR	CSV	SCF	CON	SC	Ft0	tF0	Fp0	pF0	MG	SM	FC	EFC	ES
N	Y	N	Y	N	Y	Y	N	Y	Y	N	N	Y	N	Y	Y	Y
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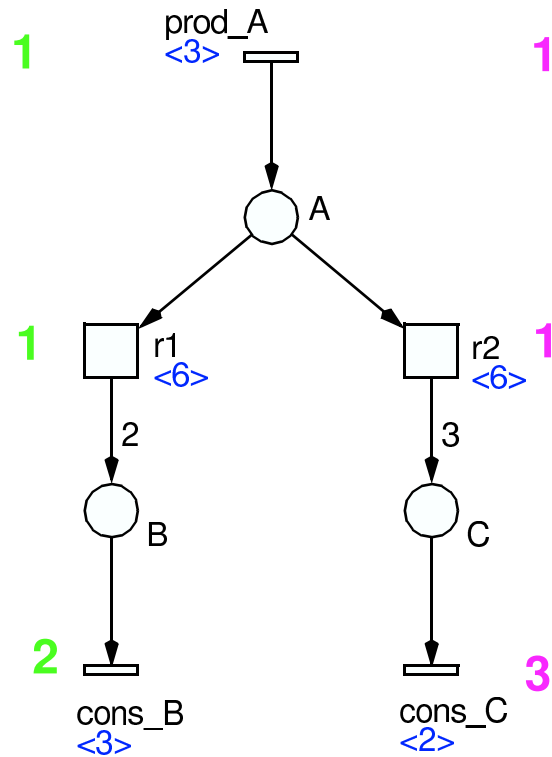
T-INVARIANTE1  
T-INVARIANTE2

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





T-INVARIANTE1  
T-INVARIANTE2

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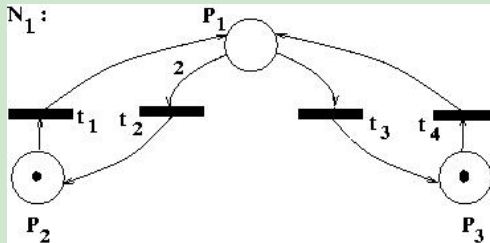
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- ▶  $V : F \longrightarrow \mathbb{N}^+$  (weights of edges)
- ▶  $m_0 : P \longrightarrow \mathbb{N}$  (initial marking)

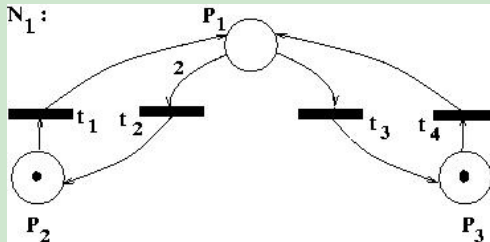
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## Example



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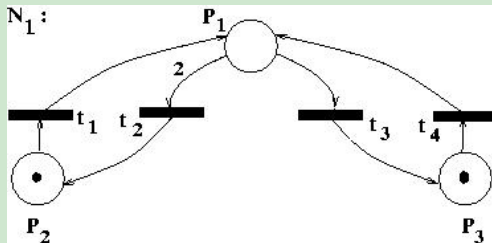
## Example



►  $m_0 = (0, 1, 1)$

# Petri Net

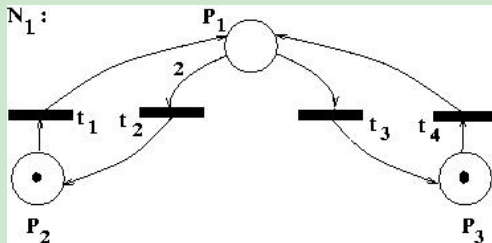
## Example



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

# Petri Net

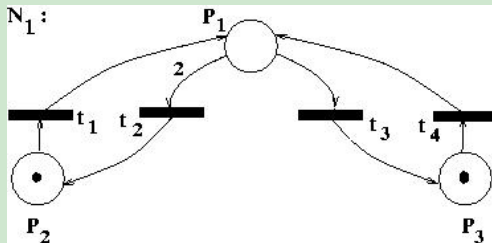
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# Petri Net

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



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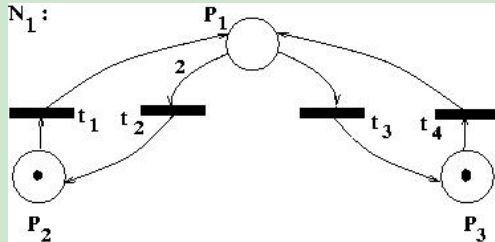
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denoted by  $m \xrightarrow{t} m'$ .



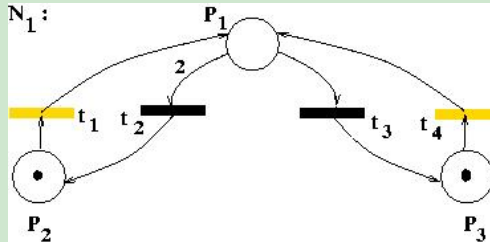
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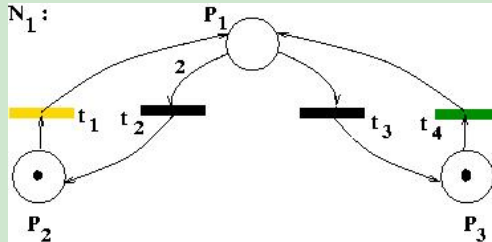
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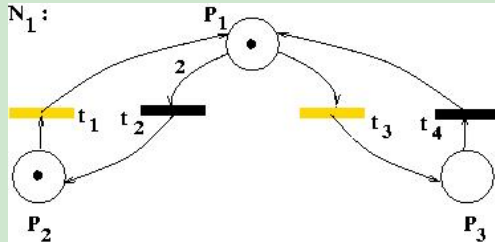
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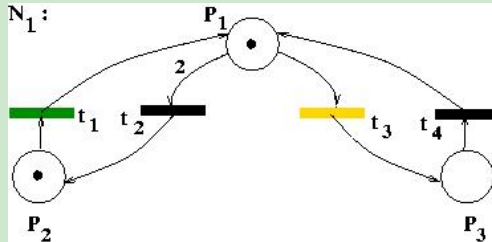
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## Example



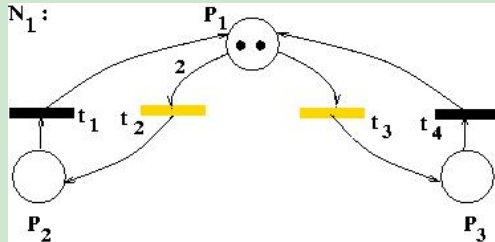
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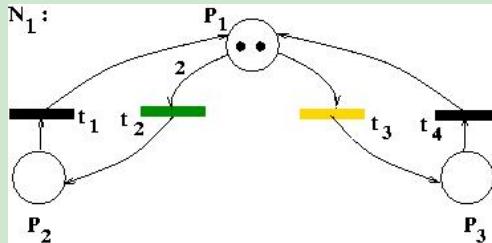
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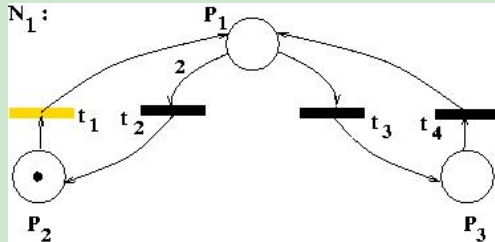
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- ▶  $I : T \longrightarrow \mathbb{Q}_0^+ \times (\mathbb{Q}_0^+ \cup \{\infty\})$  and  
 $l_1(t) \leq l_2(t)$  for each  $t \in T$ , where  $I(t) = (l_1(t), l_2(t))$ .



# Time Petri Net

## Definition (FTPN)

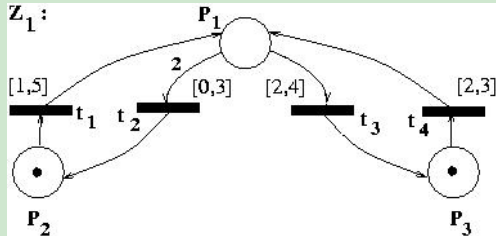
A TPN is called finite Time Petri net (FTPN) iff

$$I : T \longrightarrow \mathbb{Q}_0^+ \times \mathbb{Q}_0^+.$$



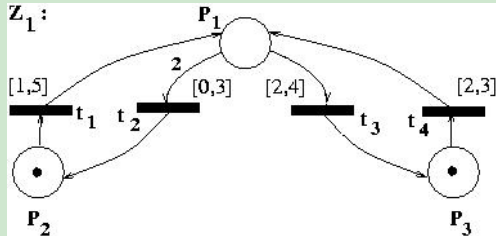
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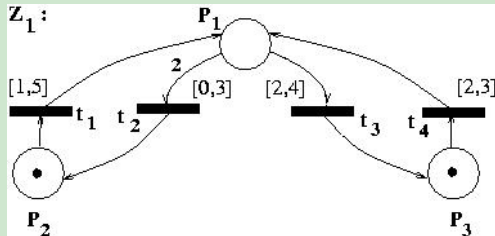


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# Time Petri Net

## Example



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



# state

## Definition (state)

Let  $Z = (P, T, F, V, m_o, I)$  be a TPN and  $h : T \longrightarrow \mathbb{R}_0^+ \cup \{\#\}$ .  
 $z = (m, h)$  is called a **state** in  $Z$  iff:



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$$\forall t \left( (t \in T \wedge t^- \leq m) \longrightarrow (h(t) \in \mathbb{R}_0^+ \wedge h(t) \leq lft(t)) \right),$$



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 $\forall t \ ( (t \in T \wedge t^- \leq m) \longrightarrow (h(t) \in \mathbb{R}_0^+ \wedge h(t) \leq lft(t)))$ ,  
 and  
 $\forall t \ ( (t \in T \wedge t^- \not\leq m) \longrightarrow h(t) = \#).$



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- (i)  $\hat{t}^- \leq m$  and
  - (ii)  $\text{eft}(\hat{t}) \leq h(\hat{t})$ .



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



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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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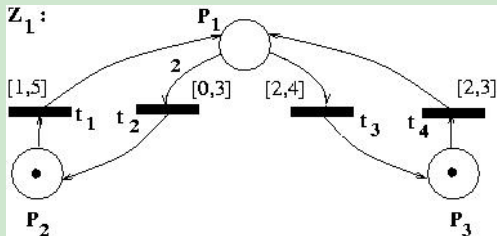
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  - (iii)  $\forall t ( t \in T \longrightarrow h'(t) := \begin{cases} h(t) + \tau & \text{iff } t^- \leq m' \\ \# & \text{iff } t^- \not\leq m' \end{cases} )$ .



# Time Petri Net

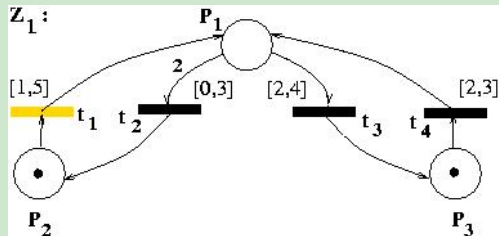
## Example



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

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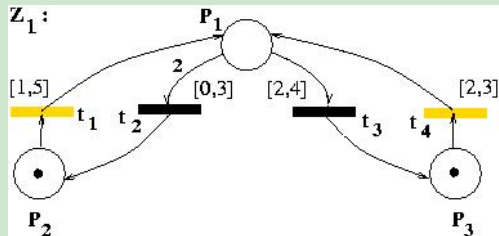


$$(m_0, \begin{pmatrix} 0 \\ \# \\ \# \\ 0 \end{pmatrix}) \xrightarrow{1.3} (m_1, \begin{pmatrix} 1.3 \\ \# \\ \# \\ 1.3 \end{pmatrix})$$



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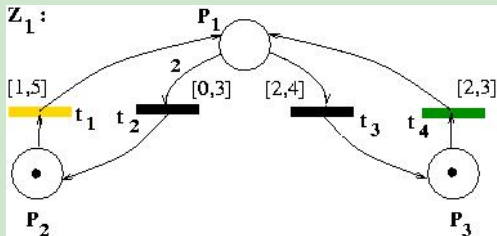
## Example



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

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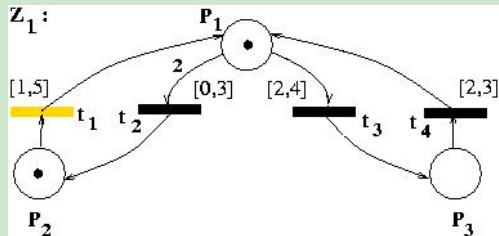
## Example



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

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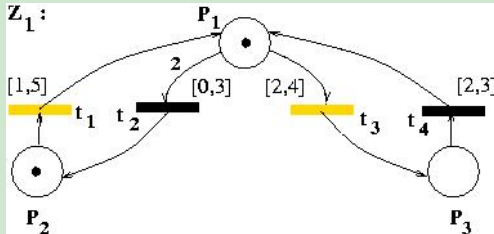
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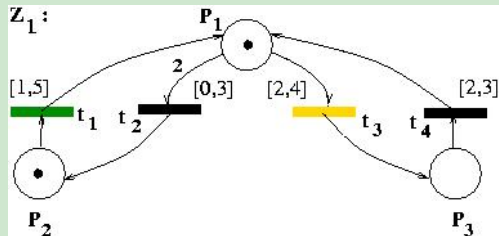
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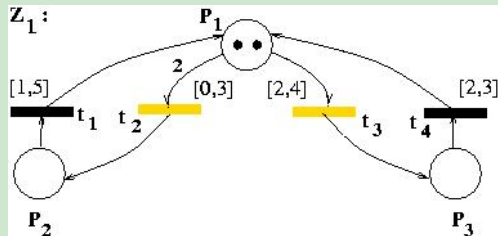
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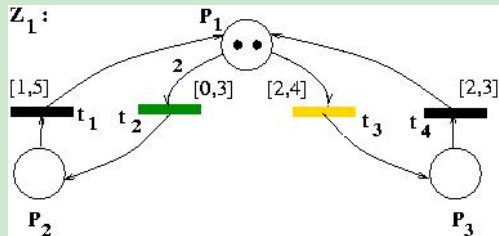
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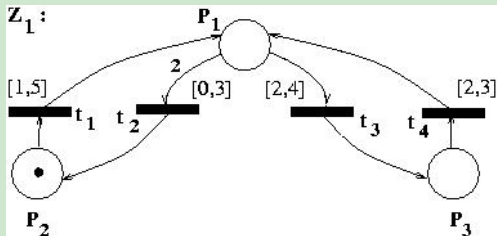
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- ▶ The set of all reachable states in  $Z$  is the **state space** of  $Z$  ( denoted:  $StSp(Z)$  ).



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



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# Parametric Description of the State Space

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

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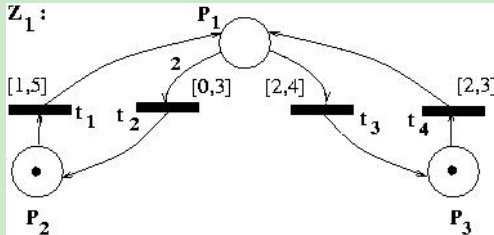
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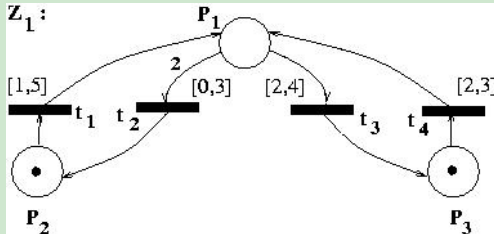
**Obviously**  $\delta(\sigma) = C_\sigma$ .



## Example



## Example

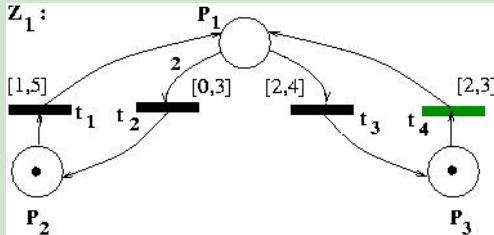


$$\sigma = (e) \quad \Rightarrow$$

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

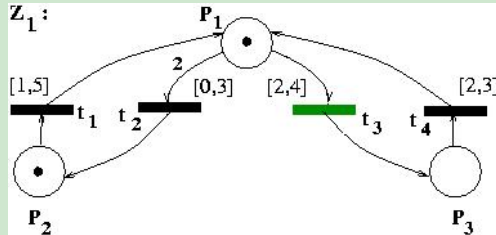


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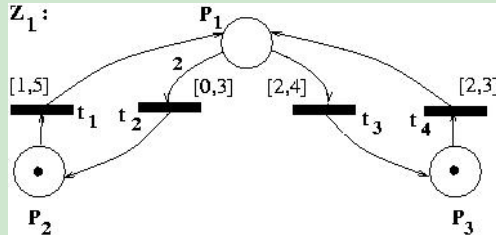




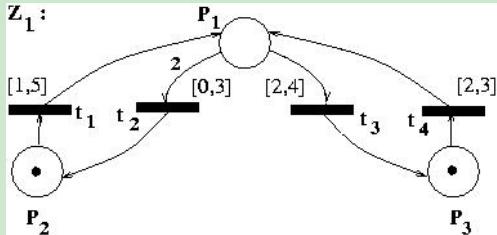
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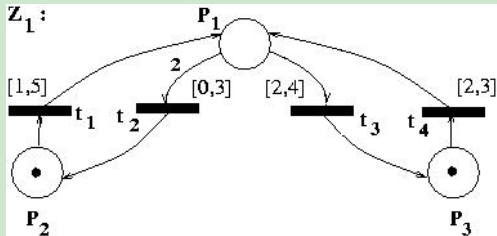


## Example



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

## Example



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

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



# State Space Reduction

## Theorem (1)

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

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

*and all  $\tau_i \in \mathbb{R}_0^+$ .*

*Then, there exists a further feasible run  $\sigma(\tau^*)$  of  $\sigma$  with*

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

*such that*



# State Space Reduction

## Theorem (1 – continuation)

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

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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:

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

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



# State Space Reduction

## Theorem (2 – similar to 1)

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# State Space Reduction

## Theorem (2 – continuation)

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

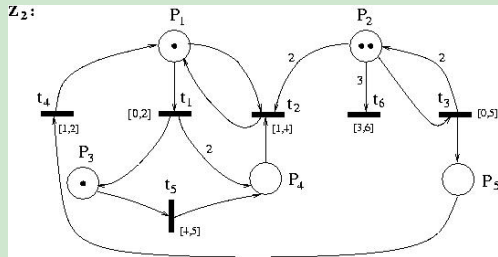
$$2.1 \quad h_n(t)^* = \lceil h_n(t) \rceil.$$

$$2.2 \quad \sum_{i=1}^n \tau_i^* = \lceil \sum_{i=1}^n \tau_i \rceil$$



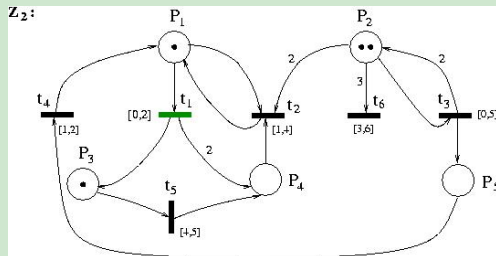
# State Space Reduction

## Example



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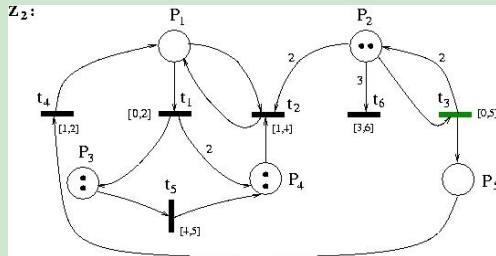
$$\sigma = (t_1 t_3 t_4 t_2 t_3)$$

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



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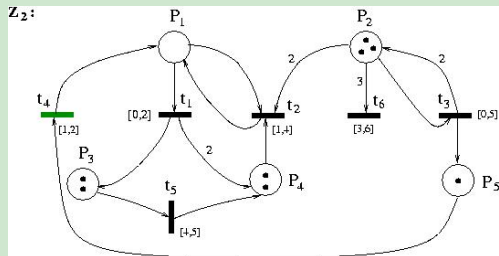
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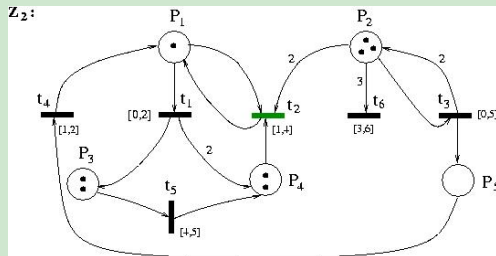
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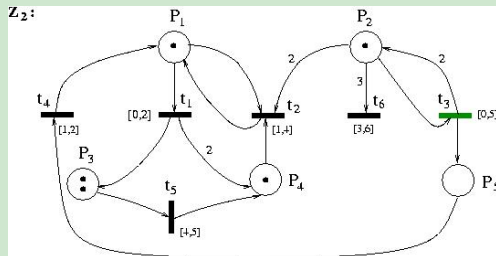
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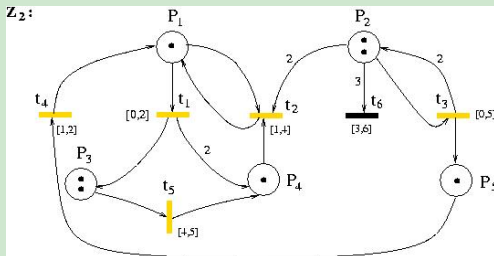
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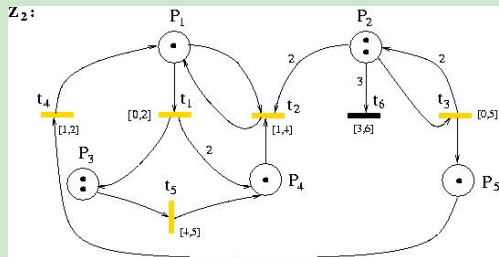
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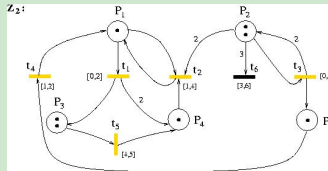
$$\sigma = (t_1 t_3 t_4 t_2 t_3)$$

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



# State Space Reduction

## Example ( continuation )

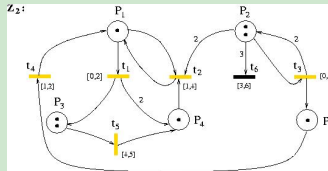


$$\Sigma_{\sigma} = \begin{pmatrix} x_4 + x_5 \\ x_5 \\ x_5 \\ x_5 \\ x_0 + x_1 + x_2 + x_3 + x_4 + x_5 \\ \# \end{pmatrix} \text{ and}$$



# State Space Reduction

## Example ( continuation )



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



# State Space Reduction

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The run  $\sigma(\tau)$  with

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is feasible.





# State Space Reduction

## Example ( continuation )

	$x_0$	$x_1$	$x_2$	$x_3$	$x_4$	$x_5$	$\Sigma_\sigma(t_1)$	$\Sigma_\sigma(t_2)$	$\Sigma_\sigma(t_5)$
$\hat{\beta} = \beta_0$	0.7	0.0	0.4	1.2	0.5	1.4	1.9	1.4	4.2
$\beta_1$	0.7	0.0	0.4	1.2	0.5	<b>1</b>	1.5	1.0	3.8
$\beta_2$	0.7	0.0	0.4	1.2	<b>0</b>	1	1.0		3.3
$\beta_3$	0.7	0.0	0.4	<b>1</b>	0	1			3.1
$\beta_4$	0.7	0.0	<b>1</b>	1	0	1			3.7
$\beta_5$	0.7	<b>0</b>	1	1	0	1			3.7
$\beta_6$	<b>1</b>	0	1	1	0	1			4.0



# State Space Reduction

## Example ( continuation )

	$x_0$	$x_1$	$x_2$	$x_3$	$x_4$	$x_5$	$\Sigma_\sigma(t_1)$	$\Sigma_\sigma(t_2)$	$\Sigma_\sigma(t_5)$
$\hat{\beta} = \beta_0$	0.7	0.0	0.4	1.2	0.5	1.4	1.9	1.4	4.2
$\beta_1$	0.7	0.0	0.4	1.2	0.5	<b>2</b>	2.5	2.0	4.8
$\beta_2$	0.7	0.0	0.4	1.2	<b>0</b>	1	2.0		4.3
$\beta_3$	0.7	0.0	0.4	<b>2</b>	0	1			5.1
$\beta_4$	0.7	0.0	<b>0</b>	1	0	1			4.7
$\beta_5$	0.7	<b>0</b>	1	1	0	1			4.7
$\beta_6$	<b>1</b>	0	1	1	0	1			5.0



# State Space Reduction

## Example ( continuation )

Hence, the runs

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

and

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

are feasible in  $Z$ , too.



# State Space Reduction

## Corollary

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- ▶ *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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## Theorem ( 3 )

*Let  $Z$  be a FTPN.*

*The set of all reachable integer states in  $Z$  is finite*

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



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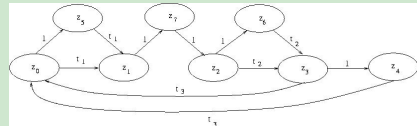
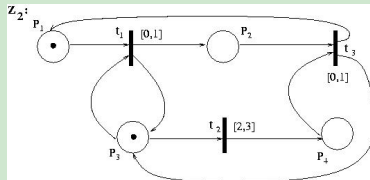
2. if  $z \xrightarrow{1} z'$  possible in  $Z$  then  $z' \in RG(Z)$

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



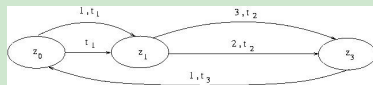
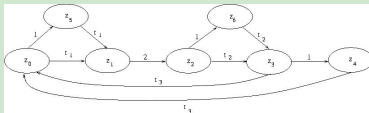
# A TPN and its full Reachability Graph

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

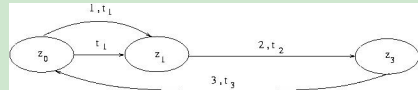
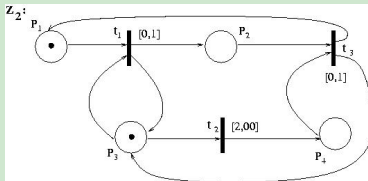




## Example (The reduced reachability graphs $RG^{(2)}(Z)$ and $RG(Z)$ )



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



## Definition

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



## Lemma

*Let  $Z$  be a TPN,  $S(Z)$  be the skeleton of  $Z$  and  $\sigma$  be a feasible  $T$ -invariant in  $S(Z)$ .*

*$\sigma$  is a feasible  $T$ -invariant in  $Z$  iff  $B_\sigma$  has a solution.*



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- ▶ If  $\sigma$  is feasible, then solve the linear system of inequalities  $B_\sigma$  in  $\mathbb{R}_0^+$ .





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



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



Let  $Z = (P, T, F, V, I, m_o)$  be a TPN.

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### Result 1:

- Input:** The time function  $I$  is fixed,  
 $\sigma$  is an arbitrary transition sequence.
- Output:** Feasibility of  $\sigma$  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,  
 $\sigma$  is an arbitrary transition sequence.

**Output:** Feasibility of  $\sigma$  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,  
 $\sigma$  is an arbitrary transition sequence.

**Output:** min / max-length of  $\sigma$ .

**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,  
 $\sigma$  is an arbitrary transition sequence,  
 $\lambda$  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  $\sigma_1$  is feasible in  $Z$   
and  $\sigma_2$  is not feasible in  $Z$ ?
- Solution:** Solve

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



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

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



## 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  $Z$ ).

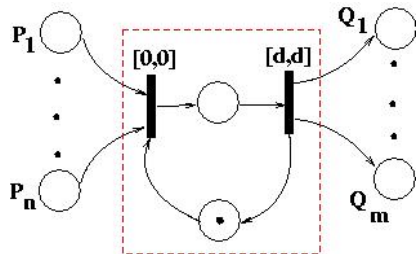
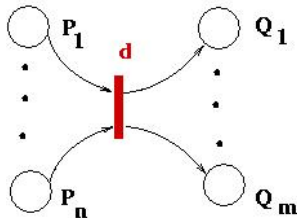
**Output:**

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## Transformation Timed PN $\longrightarrow$ Time PN



# Conclusion

- theoretical approach

$BN \Rightarrow \textit{modelling} \Rightarrow PN \Rightarrow \textit{modelling of steady state} \Rightarrow$

$DPN \Rightarrow \textit{analysing} \Rightarrow TPN$

- experimental approach

$BN \Rightarrow \textit{modelling \& analysing} \Rightarrow TPN$

