

## bioinformatics Multi-Property Time Petri Net Conclusion

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

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## bioinformatics Multi-Property Time Petri Net Conclusion

### Outline

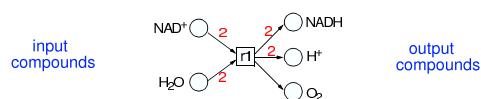
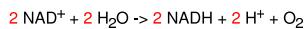
Definitions  
Petri Net  
Time Petri Net  
Main Property  
State Space Reduction  
Applications  
Reachability Graph  
T-Invariants  
Time Paths in unbounded TPNs  
Time Paths in bounded TPNs  
Time PN and Timed PN  
Conclusion

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## BIONETWORKS, BASICS

PN & Systems Biology

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



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## BIONETWORKS, INTRO

r1: A → B



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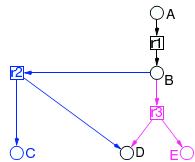
## BIONETWORKS, INTRO

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## BIONETWORKS, INTRO

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r1: A → B  
r2: B → C + D  
r3: B → D + E

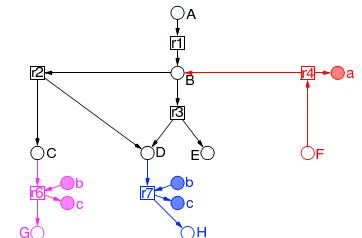


-> alternative reactions

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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

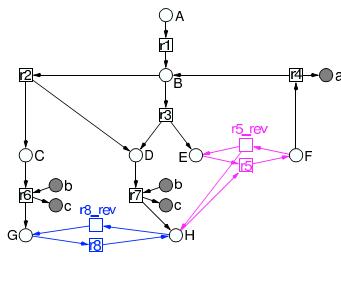
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## BIONETWORKS, INTRO

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- r4: F → B + a
- r5: E + H <-> F
- r6: C + b → G + c
- r7: D + b → H + c
- r8: H <-> G



> reversible reactions

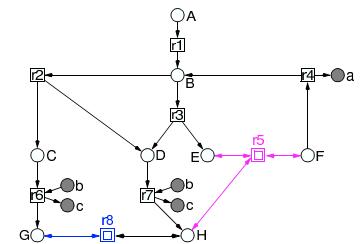
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## BIONETWORKS, INTRO

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> reversible reactions  
- hierarchical nodes

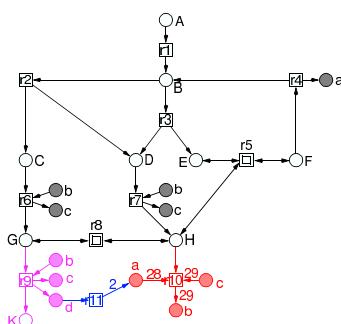
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- r7: D + b → H + c
- r8: H <-> G
- r9: G + b → K + c + d
- r10: H + 28a + 29c → 29b
- r11: d → 2a



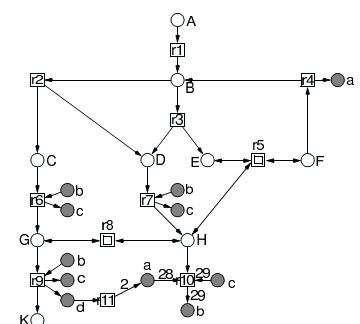
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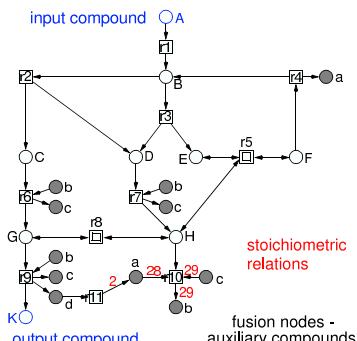
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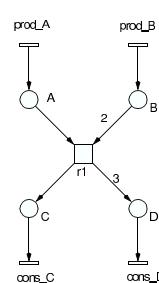


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## TRANSFORMATION, EX1

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> properties as time-less net

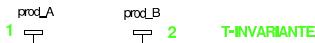
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N	Y	N	Y	N	Y	Y	N	Y	N	X	X	N	N	Y	N	Y
CPL	CTI	B	SB	REV	DST	BSR	DT	GCF	L	LV	L&S	Y	Y	Y	Y	Y

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## TRANSFORMATION, Ex1

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T-INvariante

-> properties as time-less net

INR																	
ORD	HOM	NBM	PUR	CSV	SCF	CON	SC	Ft0	tF0	pF0	pF0	MG	SM	FC	EFC	ES	
N	Y	N	Y	N	Y	Y	N	Y	N	Y	N	Y	N	Y	Y	Y	
CPI	CTI	B	SB	REV	DSt	BSt	DTx	DFx	L	LV	L&S						
N	Y	N	Y	N	Y	N	?	N	Y	Y	N	Y	N	Y	Y	Y	

## TRANSFORMATION, Ex1

PN & Systems Biology



T-INvariante

-> properties as time net

INR																	
ORD	HOM	NBM	PUR	CSV	SCF	CON	SC	Ft0	tF0	pF0	pF0	MG	SM	FC	EFC	ES	
N	Y	N	Y	N	Y	Y	N	Y	N	Y	N	Y	N	Y	Y	Y	
CPI	CTI	B	SB	REV	DSt	BSt	DTx	DFx	L	LV	L&S						
N	Y	N	Y	N	Y	N	?	N	Y	Y	N	Y	N	Y	Y	Y	

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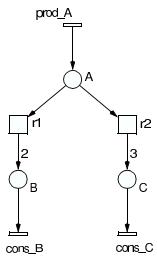
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## TRANSFORMATION, Ex2

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-> properties as time-less net

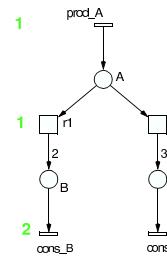
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CPI	CTI	B	SB	REV	DSt	BSt	DTx	DFx	L	LV	L&S						
N	Y	N	Y	N	Y	N	?	N	Y	Y	N	Y	N	Y	Y	Y	

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## TRANSFORMATION, Ex2

PN & Systems Biology



T-INvariante1  
T-INvariante2

-> properties as time-less net

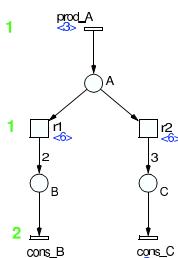
INR																	
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N	Y	N	Y	N	Y	Y	N	Y	N	Y	N	Y	N	Y	Y	Y	
CPI	CTI	B	SB	REV	DSt	BSt	DTx	DFx	L	LV	L&S						
N	Y	N	Y	N	Y	N	?	N	Y	Y	N	Y	N	Y	Y	Y	

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## TRANSFORMATION, Ex2

PN & Systems Biology



-> properties as time net

INR																	
ORD	HOM	NBM	PUR	CSV	SCF	CON	SC	Ft0	tF0	pF0	pF0	MG	SM	FC	EFC	ES	
N	Y	N	Y	N	Y	Y	N	Y	N	Y	N	Y	N	Y	Y	Y	
CPI	CTI	B	SB	REV	DSt	BSt	DTx	DFx	L	LV	L&S						
N	Y	N	Y	N	Y	N	?	N	Y	Y	N	Y	N	Y	Y	Y	

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Petri Net  
Multi-Places  
Time Petri Net  
Time Place Net

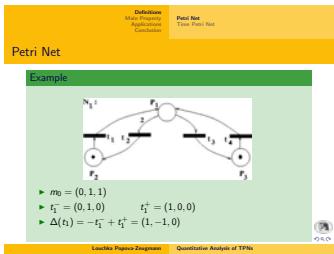
### Petri Net

#### Definition (Petri Net)

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

- $P, T$  are finite sets,
- $P$  - set of places
- $T$  - set of transitions
- $P \cap T = \emptyset$ ,  $P \cup T \neq \emptyset$ ,
- $F$  - set of edges (arcs)
- $F \subseteq (P \times T) \cup (T \times P)$  and  $\text{dom}(F) \cup \text{cod}(F) = P \cup T$
- $V : F \longrightarrow \mathbb{N}^+$  (weights of edges)
- $m_0 : P \longrightarrow \mathbb{N}$  (initial marking)

NetLogo Petri Diagrams Quantitative Analysis of Petri Nets



**Firing transition**

Definitions  
Marking  
Application  
Conclusion

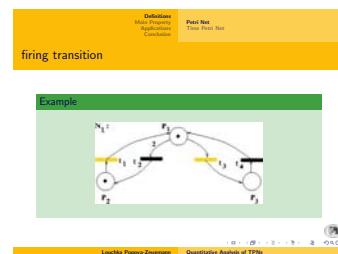
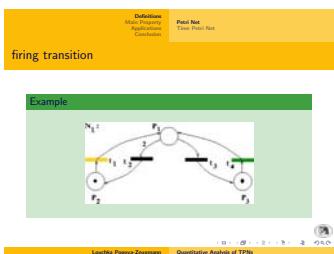
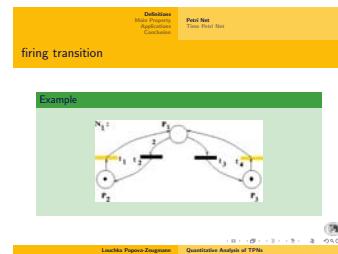
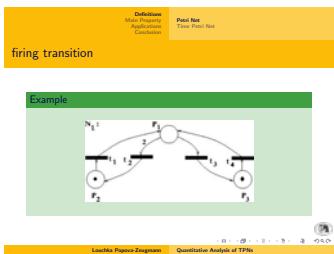
Petri Net  
Time Petri Net

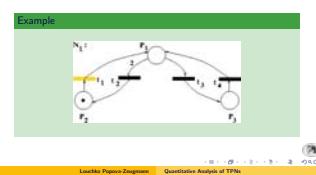
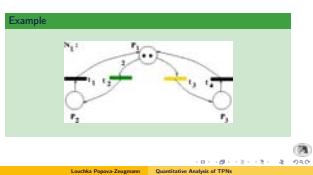
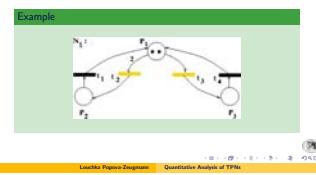
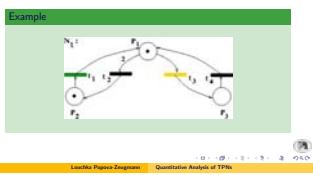
**Definition**

- A transition  $t \in T$  is **enabled (may fire)** at a marking  $m$  iff all input-places of  $t$  have enough tokens e.g.  $t^- \leq m$
- When an enabled transition  $t$  at a marking  $m$  fires, a successor marking  $m'$  is reached given by  $m' := m + \Delta t$

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

Locality Petri Diagram Quantitative Analysis of TPNs





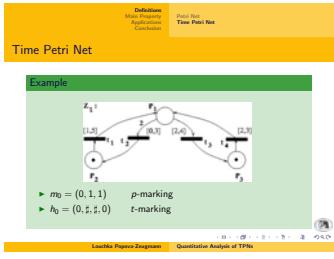
**Definition (Time Petri net)**  
The structure  $Z = (P, T, F, V, m_0, I)$  is called a **Time Petri net (TPN)** iff:

- $S(Z) := (P, T, F, V, m_0)$  is a PN (skeleton of  $Z$ )
- $I: T \longrightarrow Q_0^+ \times (Q_0^+ \cup \{\infty\})$  and  
 $h_i(t) \leq b_i(t)$  for each  $t \in T$ , where  $I(t) = (h(t), b(t))$ .



**Definition (FTPN)**  
A TPN is called finite Time Petri net (FTPN) iff  
 $I: T \longrightarrow Q_0^+ \times Q_0^+$ .





Definitions  
Marking  
Application  
Conclusion

Petri Net  
Time Petri Net

**state**

**Definition (state)**

Let  $Z = (P, T, F, V, m_0, h)$  be a TPN and  $h : T \rightarrow \mathbb{R}_0^+ \cup \{\#\}$ .  
 $z = (m, h)$  is called a **state** in  $Z$  iff:

- $m$  is a p-marking in  $Z$ , e.g.  $m$  is a marking in  $S(Z)$ .
- $h$  is a t-marking in  $Z$ , e.g.

$\forall t (t \in T \wedge t^- \leq m) \longrightarrow (h(t) \in \mathbb{R}_0^+ \wedge h(t) \leq h(t))$ ,  
and  
 $\forall t (t \in T \wedge t^- \leq m) \longrightarrow h(t) = \#$ .

Loadable Petri Diagram Quantitative Analysis of TPNs

Definitions  
Marking  
Application  
Conclusion

Petri Net  
Time Petri Net

**Definition (state changing)**

Let  $Z = (P, T, F, V, m_0, h)$  be a TPN,  
 $\hat{t}$  be a transition in  $T$  and  
 $z = (m, h), z' = (m', h')$  be two states.  
Then

- the transition  $\hat{t}$  is **ready** to fire in the state  $z = (m, h)$ , denoted by  $z \xrightarrow{\hat{t}} z'$ , iff
  - $t^- \leq m$  and
  - $ef(\hat{t}) \leq h(\hat{t})$ .

Loadable Petri Diagram Quantitative Analysis of TPNs

Definitions  
Marking  
Application  
Conclusion

Petri Net  
Time Petri Net

**state changing**

**Definition (state changing)**

(b) the state  $z = (m, h)$  is **changed** into the state  $z' = (m', h')$  by **firing the transition**  $\hat{t}$ , denoted by  $z \xrightarrow{\hat{t}} z'$ , iff

- $t$  is ready to fire in the state  $z = (m, h)$
- $m' = m + \Delta t$  and
- $\forall t (t \in T \wedge t^- \leq m') \longrightarrow$

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

Loadable Petri Diagram Quantitative Analysis of TPNs

state changing

Definitions  
Marking  
Application  
Conclusion

Petri Net  
Time Petri Net

**Definition (state changing)**

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

- $m' = m$  and
- $\forall t (t \in T \wedge h(t) \neq \#) \longrightarrow m(t) + \tau \leq h(t)$  i.e. the time elapsing  $\tau$  is possible, and
- $\forall t (t \in T \longrightarrow h'(t) := \begin{cases} h(t) + \tau & \text{iff } t^- \leq m' \\ \# & \text{iff } t^- \geq m' \end{cases})$ .

Loadable Petri Diagram Quantitative Analysis of TPNs

Definitions  
Marking  
Application  
Conclusion

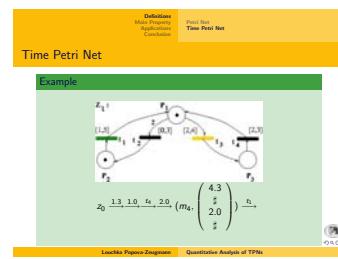
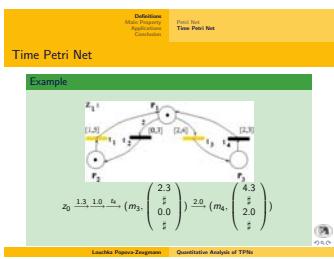
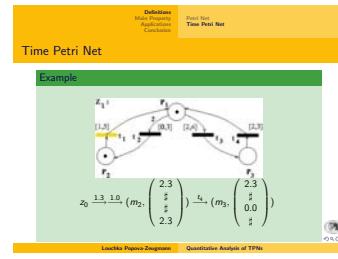
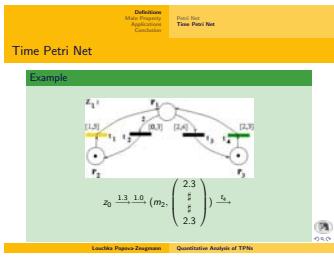
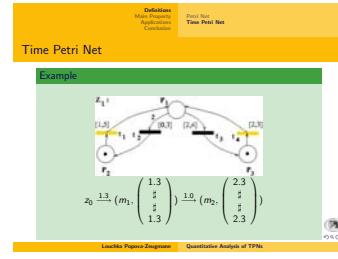
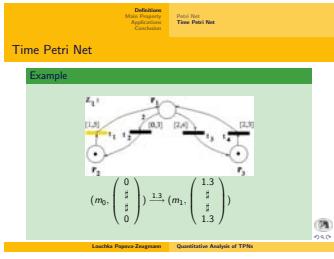
Petri Net  
Time Petri Net

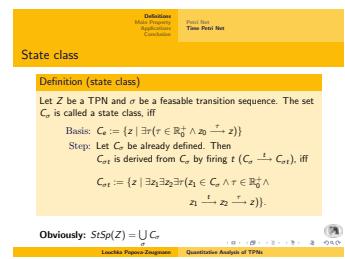
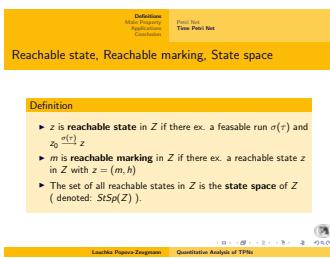
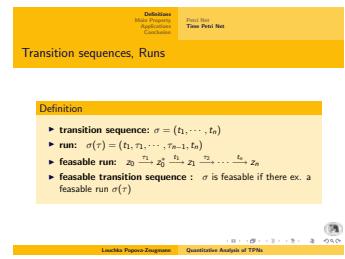
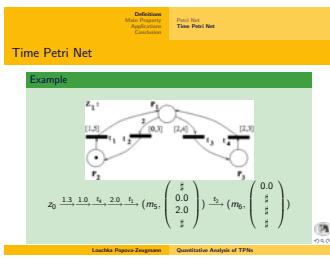
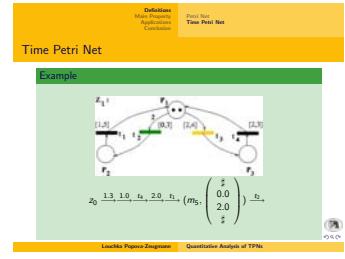
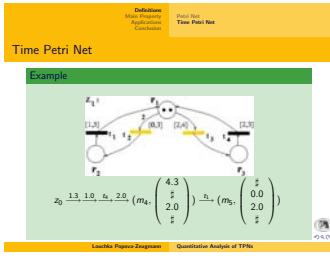
**Time Petri Net**

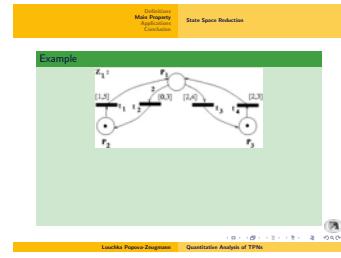
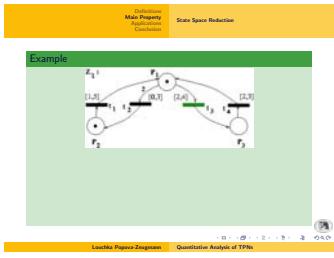
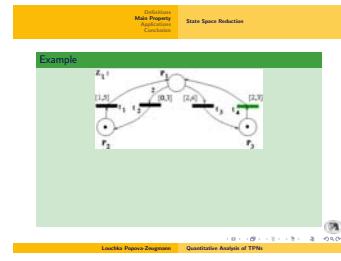
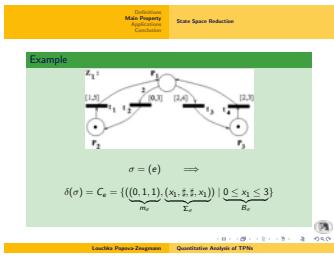
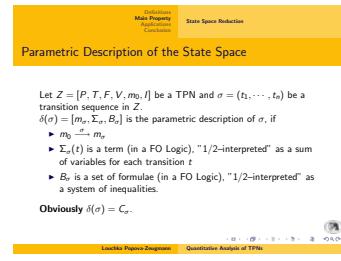
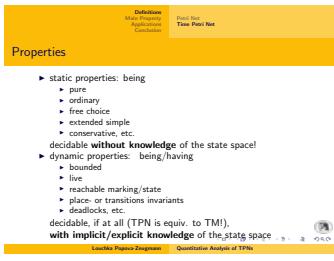
**Example**

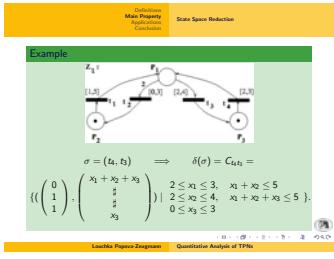
$(m_0, \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix})$

Loadable Petri Diagram Quantitative Analysis of TPNs









Main Property  
Continuation

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.

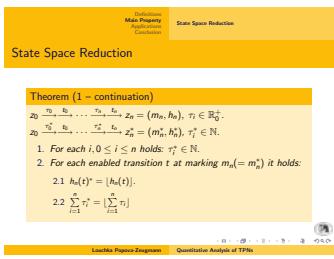
$$z_0 \xrightarrow{\tau_0} t_0 \xrightarrow{\tau_1} \dots \xrightarrow{\tau_n} t_n \xrightarrow{\tau_{n+1}} z_n = (m_n, h_n),$$

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

$$z_0 \xrightarrow{\tau_0^*} t_0 \xrightarrow{\tau_1^*} \dots \xrightarrow{\tau_n^*} t_n \xrightarrow{\tau_{n+1}^*} z_n^* = (m_n^*, h_n^*),$$

such that

Labels: Petri Diagram Quantitative Analysis of TPNs



Main Property  
Continuation

State Space Reduction

**Theorem (2 – similar to 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.

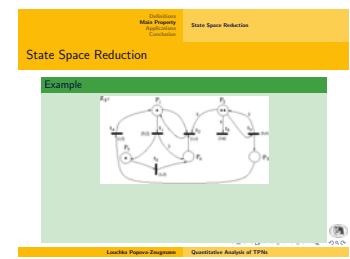
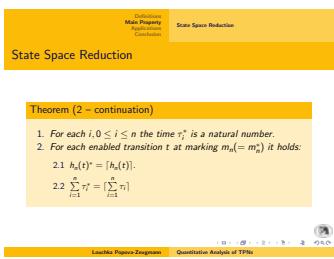
$$z_0 \xrightarrow{\tau_0} t_0 \xrightarrow{\tau_1} \dots \xrightarrow{\tau_n} t_n \xrightarrow{\tau_{n+1}} z_n = (m_n, h_n),$$

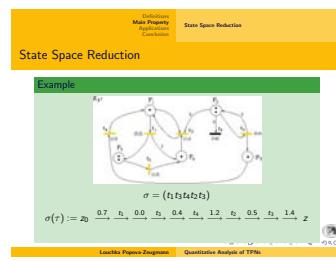
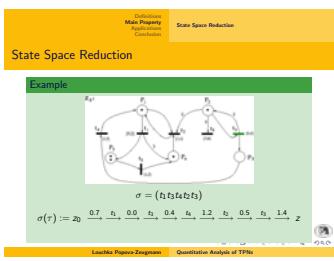
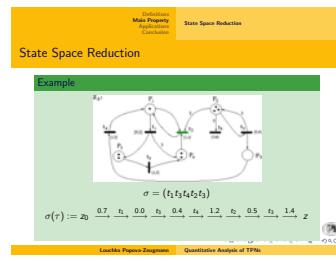
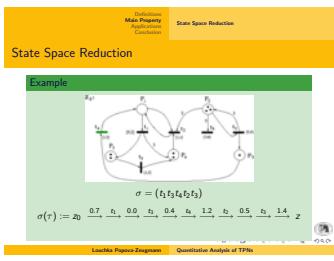
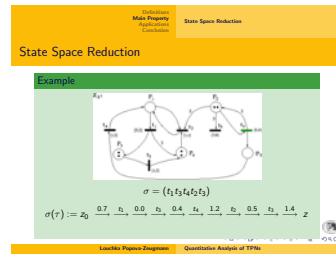
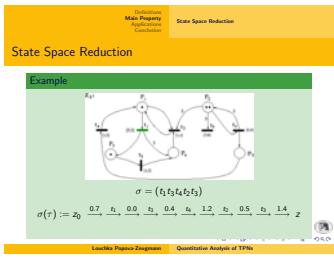
and all  $\tau_j \in \mathbb{R}_0^+$ . Then, there exists a further feasible run  $\sigma(\tau^*)$  of  $\sigma$  with

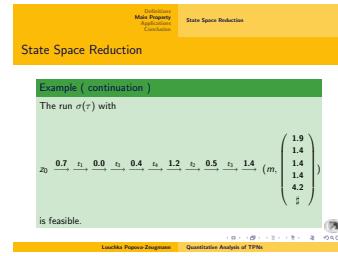
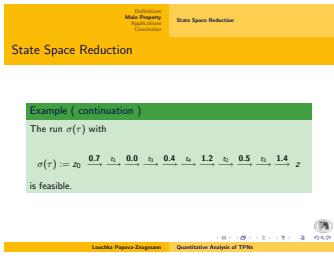
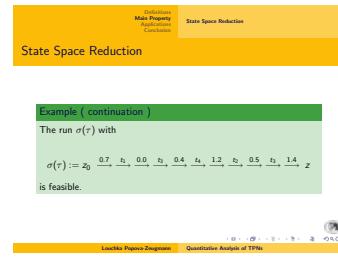
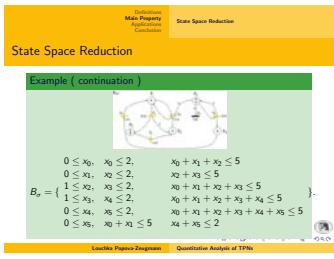
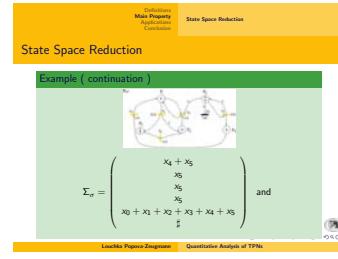
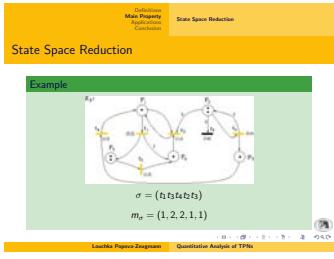
$$z_0 \xrightarrow{\tau_0^*} t_0 \xrightarrow{\tau_1^*} \dots \xrightarrow{\tau_n^*} t_n \xrightarrow{\tau_{n+1}^*} z_n^* = (m_n^*, h_n^*),$$

such that

Labels: Petri Diagram Quantitative Analysis of TPNs







State Space Reduction						
Redundant Markings Elimination				State Space Reduction		
Example ( continuation )						
$\beta$	$x_0$	$x_1$	$x_2$	$x_3$	$x_4$	$x_5$
$\beta_0$	0.7	0.0	0.4	1.2	0.5	1.4
$\beta_1$	0.7	0.0	0.4	1.2	0.5	1
$\beta_2$	0.7	0.0	0.4	1.2	0	1
$\beta_3$	0.7	0.0	0.4	1	0	1
$\beta_4$	0.7	0.0	0.4	1	0	1
$\beta_5$	0.7	0.0	0.4	1	0	1
$\beta_6$	1	0	1	1	0	1
						4.0

State Space Reduction						
	Markov Application Condition			State Space Reduction		
Example ( continuation )	$x_0$	$x_1$	$x_2$	$x_3$	$x_4$	$x_5$
$\beta =$	$b_0$	0.0	0.0	0.4	1.5	0.4
	$b_0$	0.7	0.0	0.4	1.5	2
	$b_2$	0.7	0.0	0.4	1.2	0
	$b_3$	0.7	0.0	0.4	0	2
	$b_4$	0.7	0.0	0.4	0	1
	$b_5$	0.7	0.0	0.4	0	1
	$b_6$	0.7	0.0	0.4	0	1
	$b_7$	0.7	0.0	0.4	0	1
	$b_8$	1	0	1	1	0
					1.9	1.4
					2.0	4.8
					2.0	4.3
						5.1
						4.7
						4.7
						5.0

**State Space Reduction**

**Example ( continuation )**

Hence, the runs

$$\sigma(z_1^*) := z_0 \xrightarrow{1} n_1 \xrightarrow{0} n_2 \xrightarrow{1} n_3 \xrightarrow{1} n_4 \xrightarrow{2} n_5 \xrightarrow{0} n_6 \xrightarrow{1} [Z]$$

and

$$\sigma(z_2^*) := z_0 \xrightarrow{1} n_1 \xrightarrow{0} n_2 \xrightarrow{0} n_3 \xrightarrow{2} n_4 \xrightarrow{2} n_5 \xrightarrow{0} n_6 \xrightarrow{2} [Z]$$

are feasible in  $Z$ , too.

State Space Reduction	State Space Reduction
<p><b>Corollary</b></p> <ul style="list-style-type: none"> <li>▶ Each feasible t-sequence <math>\sigma</math> in <math>Z</math> can be realized with an “integer” run.</li> <li>▶ Each reachable marking in <math>Z</math> can be found using “integer” run only.</li> <li>▶ If <math>z</math> is reachable in <math>Z</math>, then <math> z </math> and <math>[z]</math> are reachable in <math>Z</math>, too.</li> <li>▶ The length of the shortest and longest time path between two arbitrary states are natural numbers.</li> </ul>	

**State Space Reduction**

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

**Theorem (3 )**  
 $\text{Let } Z \text{ be a FFTP.}$   
 $\text{The set of all reachable integer states in } Z \text{ is finite}$   
 $\text{if and only if}$   
 $\text{the set of all reachable markings in } Z \text{ is finite.}$

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

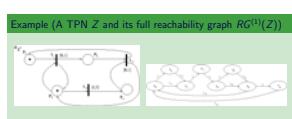
Reachability Graph

**Definition**

**Basic**)  
 $z_0 \in RG(Z)$

**Step**)  
 Let  $z$  be in  $RG(Z)$  already.  
 1. for  $i=1$  to  $|Z|$  do  
     if  $z \xrightarrow{A_i} z'$  possible in  $Z$  then  $z' \in RG(Z)$  end  
 2. if  $z \xrightarrow{A_i} z'$  possible in  $Z$  then  $z' \in RG(Z)$

==> The reachability graph is a weighted directed graph.

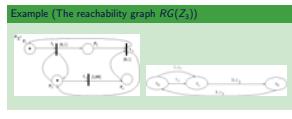


Lecture Petri Diagrams Quantitative Analysis of TPNs



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

Lecture Petri Diagrams Quantitative Analysis of TPNs



Lecture Petri Diagrams Quantitative Analysis of TPNs



**Definition**  
The transition sequence  $\sigma$  is a **feasible T-invariant** in a TPN  $Z$  if for each marking  $m$  in  $Z$  holds:  $m \xrightarrow{\sigma} m$ .  
**For timeless PN:**  $\sigma$  is a feasible T-invariant iff  
 $m = m + C \cdot \psi(\sigma)$  and  $\psi(\sigma)$  - the Pankhi-vektor of  $\sigma$ .  
→ easy to be found.

Lecture Petri Diagrams Quantitative Analysis of TPNs



**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  $Z = (P, T, F, V, I, m_0)$  be a TPN.  
Then the following problems can be decided/computed without knowledge of its RG.

**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  $Z = (P, T, F, V, I, m_0)$  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  $Z = (P, T, F, V, I, m_0)$  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  $Z = (P, T, F, V, I, m_0)$  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  $\sigma(\tau) \leq \lambda\tau$ .  
**Solution:** Solve a linear program in  $\mathbb{Q}_0^+$ .



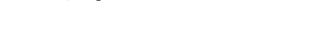
#### Result 5:

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

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



Let  $Z = (P, T, F, V, I, m_0)$  be a bounded TPN. Additionally the following problems can be decided/computed with the knowledge of its RG, amongst others:



Let  $Z = (P, T, F, V, I, m_0)$  be a bounded TPN. Additionally the following problems can be decided/computed with the knowledge of its RG, amongst others:

#### 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  $O(|V| \cdot |E|)$ ) and  $RG(Z) = (V, E)$ )





Let  $Z = (P, T, F, V, I, m_0)$  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, e.g. Bellman-Ford algorithm (polyn. running time). 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)



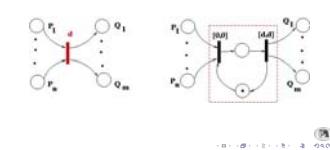
#### Result 9.

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

**Output:**

- 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)



- theoretical approach  
 $BN \implies \text{modelling} \implies PN \implies \text{modelling of steady state} \implies DPN \implies \text{analysing} \implies TPN$

- experimental approach  
 $BN \implies \text{modelling \& analysing} \implies TPN$

