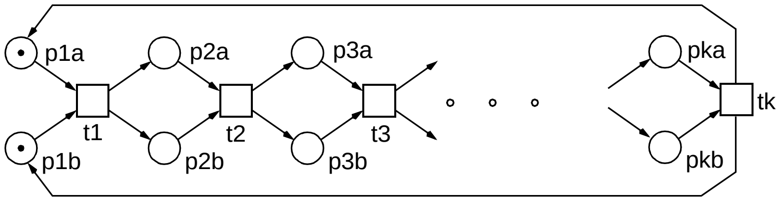
INVARIANT ANALYSIS - EXAMPLES

INDEX

[STARKE 121]



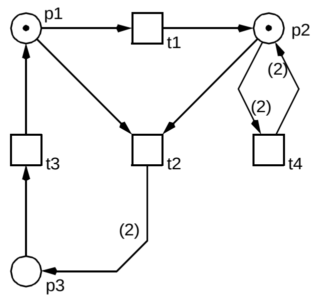
- k = 4, 2^4 = 16 minimal P-invariants:

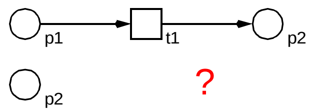
  (p1a, p2a, p3a, p4a), (p1b, p2a, p3a, p4a),
  (p1a, p2a, p3a, p4b), (p1b, p2a, p3a, p4b),
  (p1a, p2a, p3b, p4a), (p1b, p2a, p3b, p4a),
  (p1a, p2a, p3b, p4b), (p1b, p2a, p3b, p4b),
  (p1a, p2b, p3a, p4a), (p1b, p2b, p3a, p4a),
  (p1a, p2b, p3a, p4b), (p1b, p2b, p3a, p4b),
  (p1a, p2b, p3b, p4a), (p1b, p2b, p3b, p4a),
  (p1a, p2b, p3b, p4b), (p1b, p2b, p3b, p4b)

  -> *generally* 2^k P-invariants

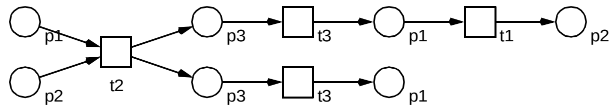
- analogously for T-invariants

[STARKE, P. 111]





t-invariant= {t1, t2, t3, t3}



INA:

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

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

[STARKE, P. 111], INVARIANTS

- incidence matrix

$$C = \begin{bmatrix} -1 & -1 & 1 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 2 & -1 & 0 \end{bmatrix}$$

-> *side conditions, here p2 for t4, are not reflected in C*

- CPI
  - -> *the only P-invariant (p1, p2, p3) covers the net*

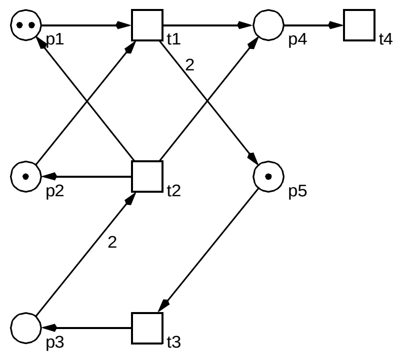
- CTI
  - -> *T-inv1: (1, 1, 2, 0) -> (t1, t2, 2 t3) -> {t1, t2, t3, t3}*
  - -> *T-inv2: (t4)*

- but not live
  - -> *t4 - the only live transition*

- state equation, counter example
  - -> *m0 = (1, 0, 0), m1 = (0, 0, 1)*
    m1 = m0 + Cx
    Cx = m1 - m0
    Cx = (-1, 0, 1)
  - -> *x = (t1, t2, t3)*
  - -> *BUT, no permutation of t1, t2, t3 can be fired*
    (t2 needs two tokens)

[PRIESE 2003, P. 80]

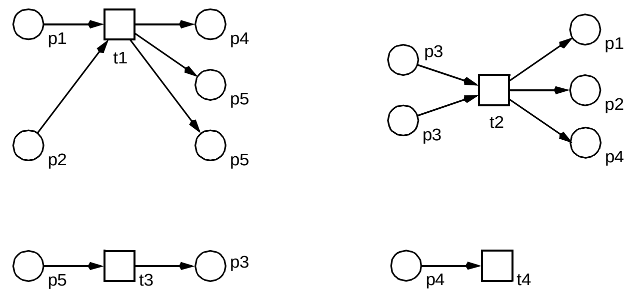
- the system



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	N	Y	N	N	N	N	Y	Y	Y

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

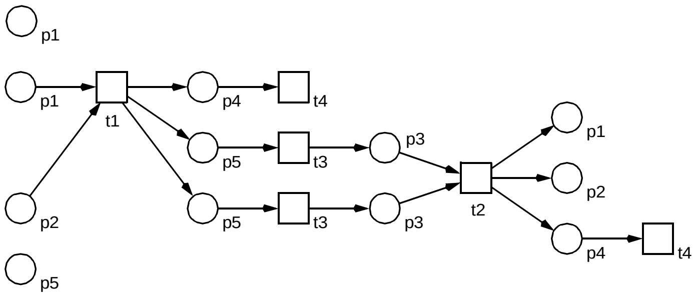
- its basic steps

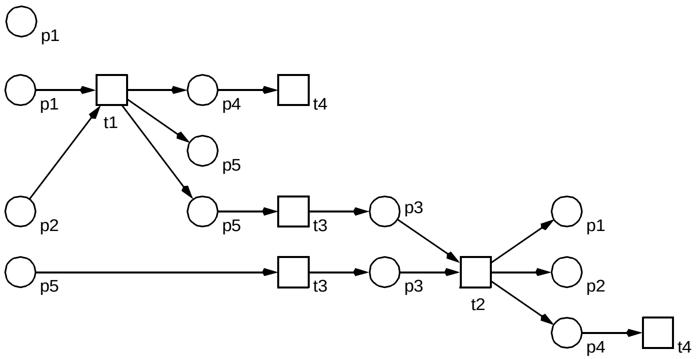


[PRIESE 2003, P. 80], T-INVARIANTS

- The net is covered by one minimal T-invariants.
  t-inv = (1, 1, 2, 2) = {t1, t2, t3, t3, t4, t4}

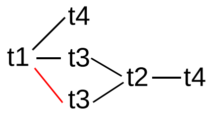
- two possible runs

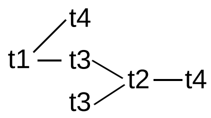




[PRIESE 2003, P. 80], T-INVARIANTS

- possible runs,
  short notation



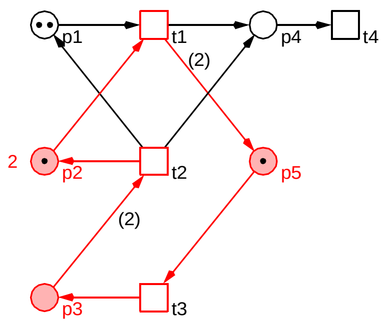


- required terminus ?!
  -> *“maximally unordered”*

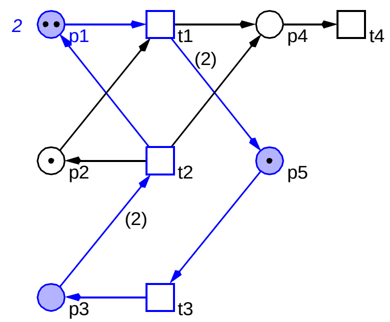
[PRIESE 2003, P. 80], P-INVARIANTS

- The net is NOT covered by semipositive P-invariants.
  Covered places: p1, p2, p3, p5,
  - -> *semipositive place invariants =*

1 | p2 : 2, | p3 : 1, | p5 : 1



2 | p1 : 2, | p3 : 1, | p5 : 1

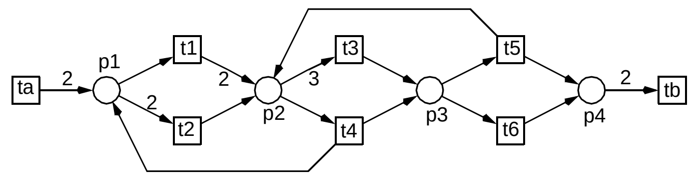


- Karp-Millller graph
  - -> *18 nodes*
  - -> *capacities needed:*

p1	p2	p3	p4	p5
2	1	3	oo	3

LAUTENBACH'S MIRACLE

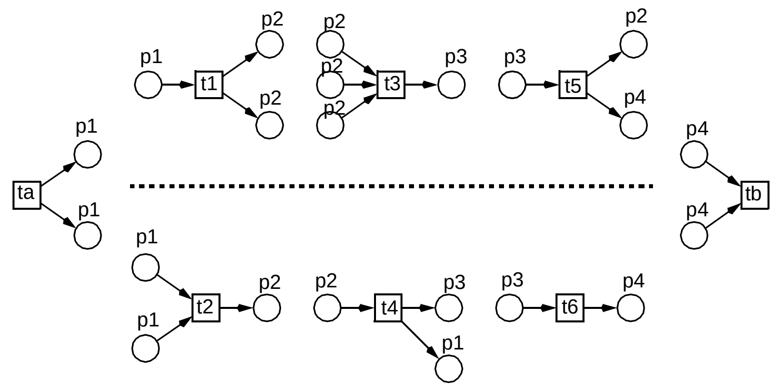
- the system



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

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

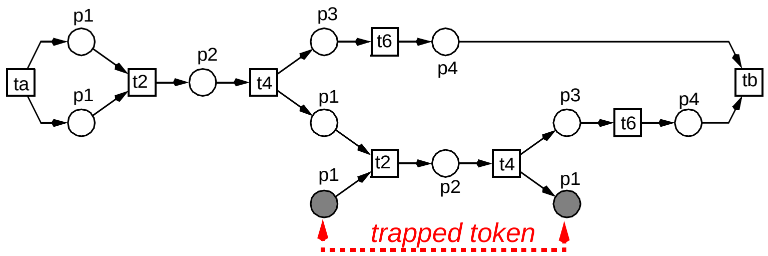
- its basic steps

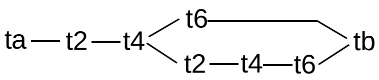


LAUTENBACH'S MIRACLE

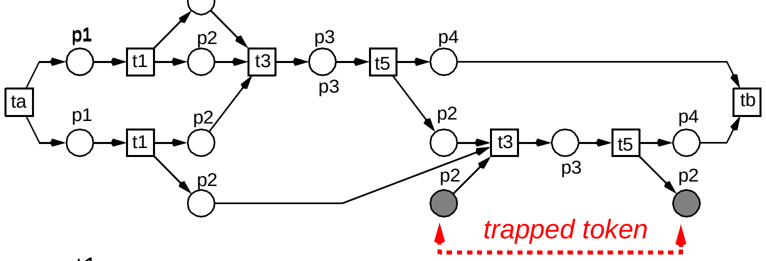
- two minimal T-invariants
  - -> *not realizable under the empty marking*
  - -> *not reproducing the empty marking*
- unique runs

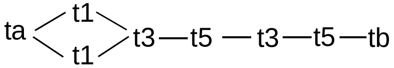
t-inv1 = {ta, t2, t2, t4, t4, t6, t6, tb}





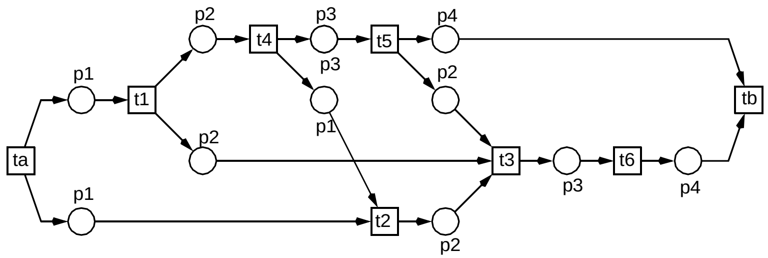
t-inv2 = {ta, t1, t1, t3, t3, t5, t5, tb}

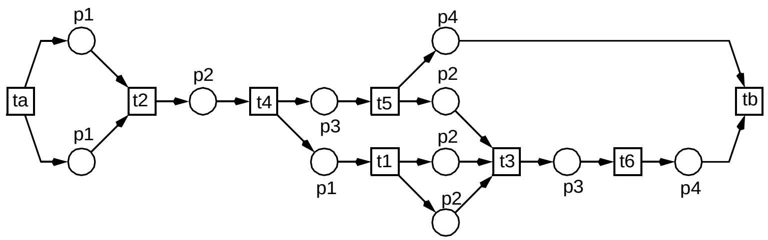




LAUTENBACH'S MIRACLE

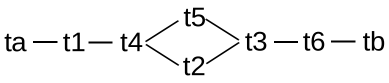
- a non-minimal T-invariant
  - -> *covering the net*
  - -> *reproducing the empty marking*
- T-inv3 = {ta, t1, t2, t3, t4, t5, t6, tb}
  - -> *T-inv3 = (T-inv1 + T-inv2) / 2*
  - -> *non-negative linear combination of minimal ones*
- two possible runs

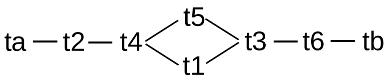




LAUTENBACH'S MIRACLE

- short notation of the two possible runs



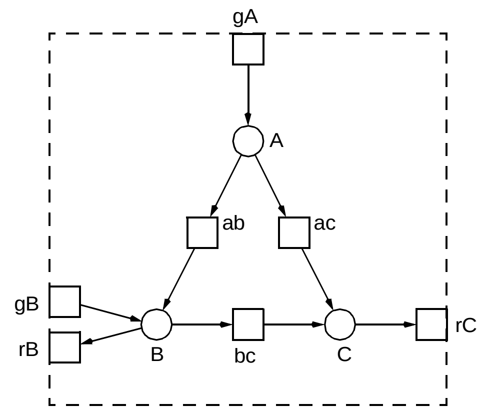


- comparison ?

- guess
  -> *no chance for uniqueness of non-minimal T-invariants'runs*

PATHWAY ANALYSIS

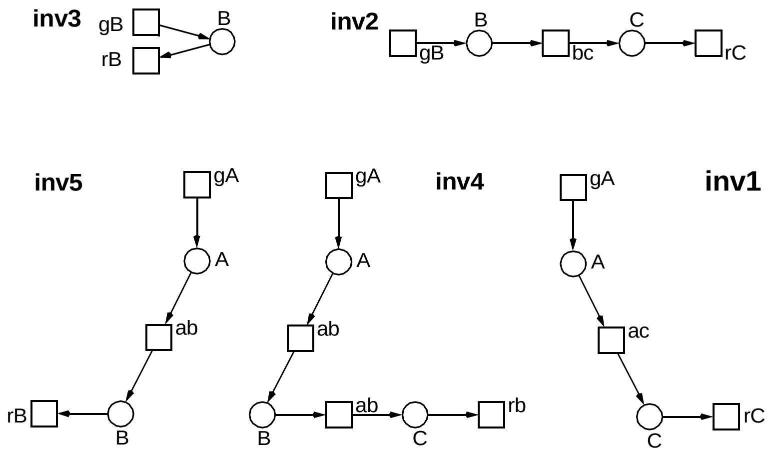
- substances involved
  -> *input substance A*
  -> *output substance C*
  -> *auxiliary substance B*



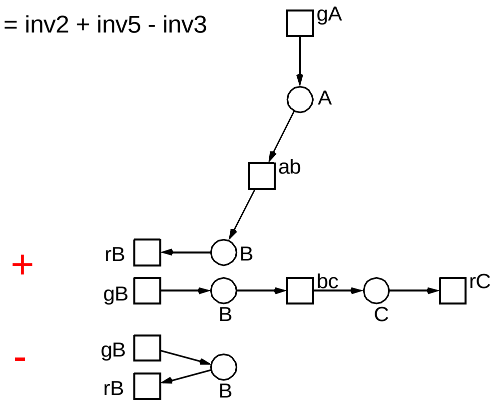
- steady state substance flows
  -> *T-invariants*

- all flow behaviour under the steady state assumption
  -> *non-negative linear combination of minimal T-invariants*

T-INVARIANTS AND EXTREME PATHWAYS

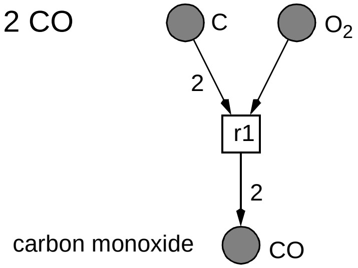


inv4 = inv2 + inv5 - inv3

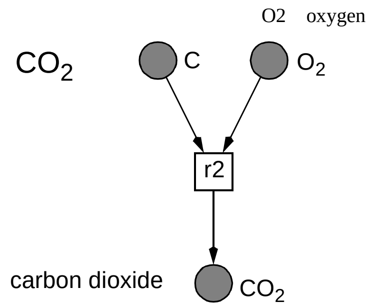


CARBON OXIDATION, BASIC REACTIONS

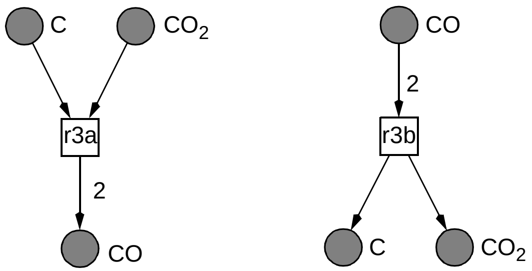
r1) $2\ C + O_2$ --> $2\ CO$



r2) $C + O_2$ --> CO_2

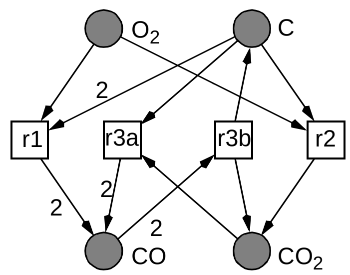


r3) $C + CO_2$ <--> $2\ CO$



CARBON OXIDATION, COMPOSITION

BASIC MODEL

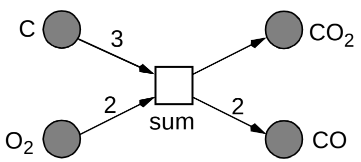


SYSTEM'S TOTAL EQUATION

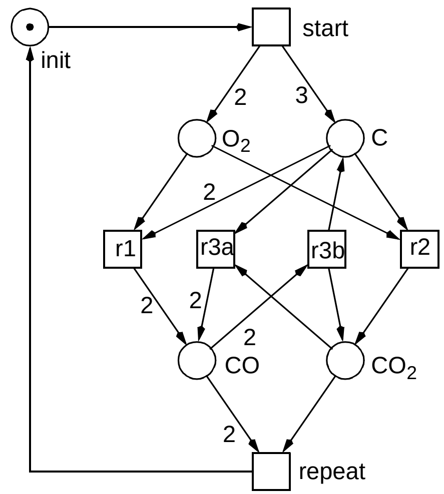
1) $2\,C + O_2 \rightarrow 2\,CO$
2) $C + O_2 \rightarrow CO_2$
[3) $C + CO_2 \leftrightarrow 2\,CO$]

$$3\,C + 2\,O_2 \rightarrow 2\,CO + CO_2$$

MODEL OF THE SYSTEM'S TOTAL EQUATION



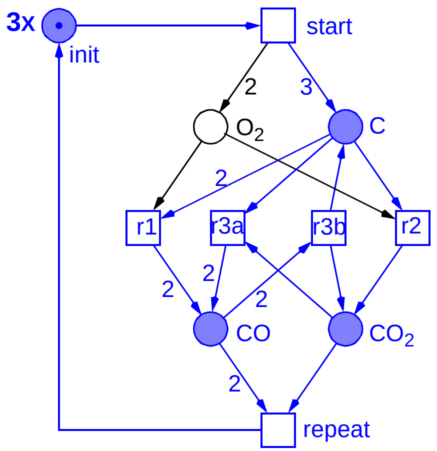
CARBON/BND, INCIDENCE MATRIX



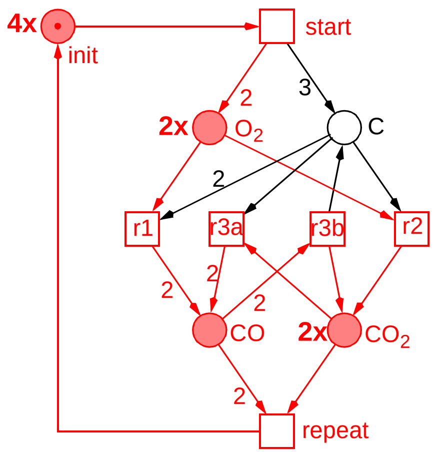
P \ T	r1	r2	r3a	r3b	start	repeat
O_2	-1	-1	0	0	+2	0
C	-2	-1	-1	+1	+3	0
CO	+2	0	2	-2	0	-2
CO_2	0	+1	-1	+1	0	-1
init	0	0	0	0	-1	+1

CARBON/BND, P-INVARIANTS

P-inv1 = (3 init, C, CO, CO_2) -> carbon preservation

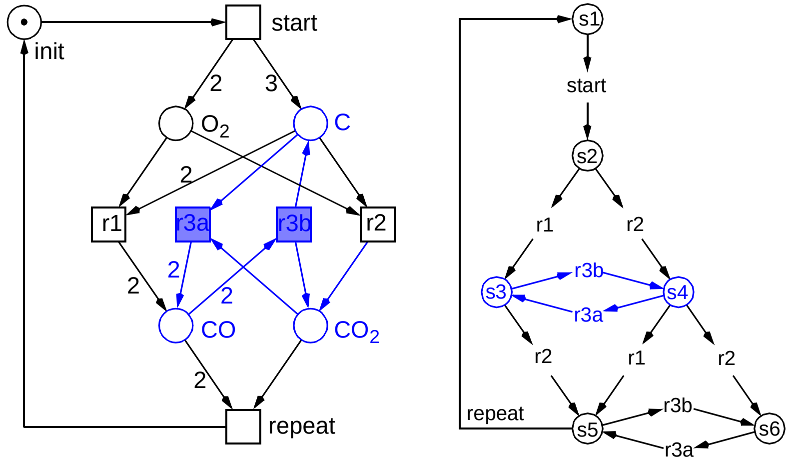


P-inv2 = (4 init, 2 O_2, CO, 2 CO_2) -> oxygen preservation

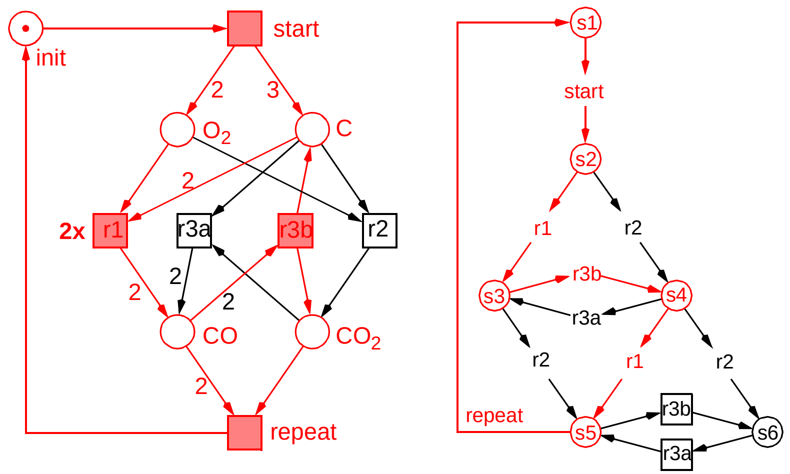


CARBON/BND, T-INVARIANTS 1, 2

T-inv1 = (r3a, r3b) -> inner cycle

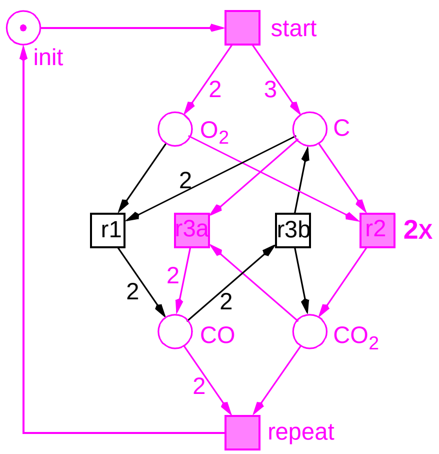


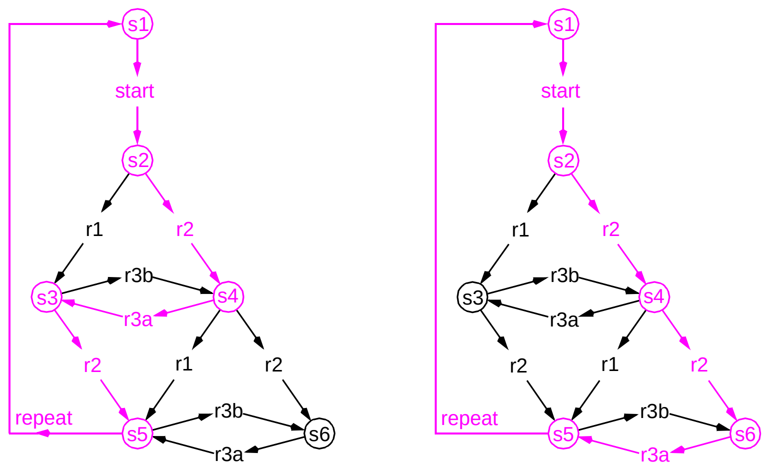
T-inv2 = (start, 2 r1, r3b, repeat) -> input/output cycle



CARBON/BND, T-INVARIANTS 3

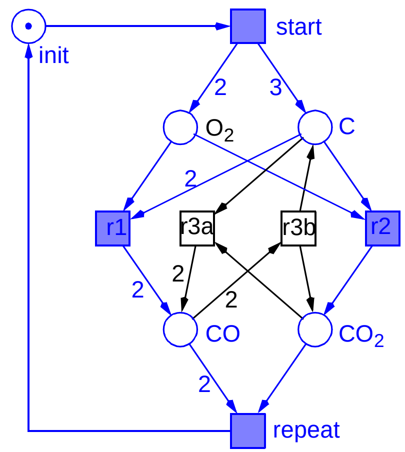
T-inv3 = (start, 2 r2, r3a, repeat) → start – r2 < r2, r3a > repeat

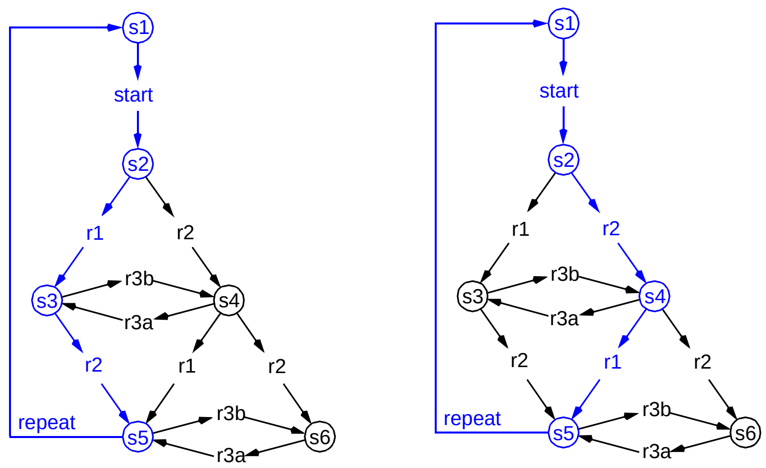




CARBON/BND, T-INVARIANTS 4

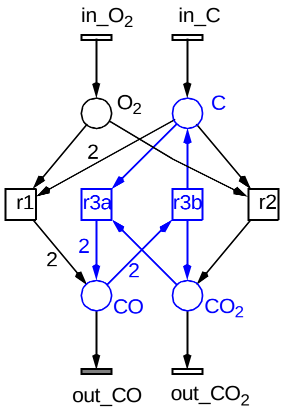
T-inv4 = (start, r1, r2, repeat) → start < r1, r2 > repeat



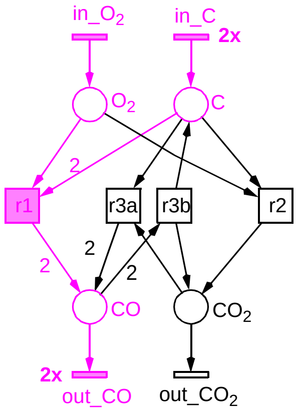


CARBON/UNBOUNDED, T-INVARIANTS 1 - 3

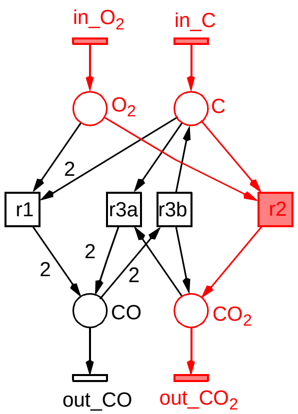
T-inv1 = (r3a, r3b)



T-inv2 = (in_O_2 , 2 in_C, r1, 2 out_CO)

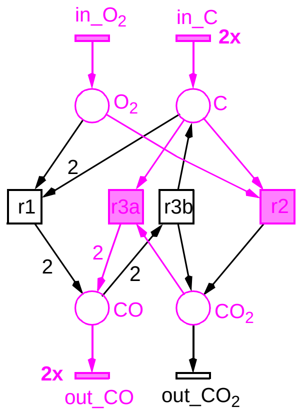


T-inv3 = (in_O_2, in_C, r2, out_CO_2)

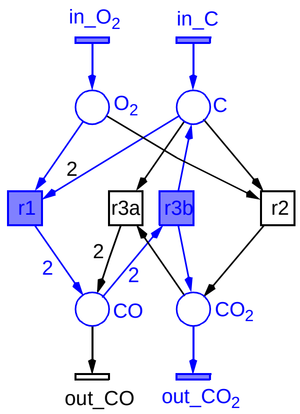


CARBON/UNBOUNDED, T-INVARIANTS 4, 5

T-inv4 = (in_O_2, 2 in_C, r2, r3a, 2 out_CO)



T-inv5 = (in_O_2, in_C, r1, r3b, out_CO_2)



CARBON/UNBOUNDED, T-INVARIANTS, INTERPRETATION

- steady state = constant token distribution

- preservation of
  a given system state under continuous firing
  requires
  - -> *relative transition firing rates*
    = T-invariant's entries
  - -> *ex T-inv2: a given state is preserved,*
    if in_C and out_CO fire twice as often as
    in_O_2 and r1;

- the in- / out-components of the T-invariant
  - -> *sum equation of the*
    T-invariants remaining transitions

T-inv1: --
    -> inner cycle

T-inv2: O_2 + 2 C -> 2 CO
    -> stoichiometric equation of r1

T-inv3: C + O_2 -> CO_2
    -> stoichiometric equation of r2

T-inv4: 2 C + O_2 -> 2 CO
    -> sum of the stoichiometric equations of r2, r3a

T-inv5: C + O2 -> CO2
    -> sum of the stoichiometric equations of r1, r3b

T-INVARIANTS, SUMMARY

TWO INTERPRETATIONS

- state-reproducing transition sequence (partial order)
  of transitions occuring one after the other

- relative transition firing rates
  of transitions occuring permanently & concurrently

BASIC TYPES IN BIO NETWORKS

- trivial minimal T-invariants
  - -> *boundary transitions of*
    auxiliary compounds
  - -> *reversible reactions*

- non-trivial minimal T-invariants
  - -> *i/o-T-invariants*
    covering boundary transitions of
    input / output compounds
  - -> *inner cycles*

PROBLEM

- given
  - -> *(minimal) T-invariant*
- wanted
  - -> *partial order run, according to net structure*
- purpose
  - -> *visualization*
  - -> *decision on realizability*
  - -> *looking for a minimal marking, making the invariant realizable*
- questions
  - -> *unique solution ?*
  - -> *preconditions, e. g. minimal T-invariants ?*
  - -> *required termini ?*
- preliminary remark
  - -> *obviously, there is no unique solution for an interleaving sequence of concurrent transitions*

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