CONSISTENCY EXAMPLES

(Ref. THERMODYN. CONSISTENCY OF AUTOCAT. CYCLES)

LET'S STUDY AN EXAMPLE WHERE CONES <u>SHARE A REACTION</u>, BUT THEY USE IT OPPOSITELY TO FORM AUTOCATALYSIS

$$Y_1 \underset{2}{\overset{1}{\rightleftarrows}} Y_2$$

$$Y_3 \underset{4}{\overset{3}{\rightleftarrows}} Y_1 + Y_2$$

$$X_3 + Y_2 \underset{6}{\overset{5}{\rightleftarrows}} 2Y_3$$

$$Y_4 + Y_5 \underset{8}{\overset{7}{\rightleftarrows}} Y_6$$

$$2Y_5 \underset{10}{\overset{9}{\rightleftarrows}} Y_4 + Y_6$$

$$Y_6 \underset{12}{\overset{11}{\rightleftarrows}} Y_4$$

12 IRREVERSIBLE REACTIONS OR 6 REVERSIBLE REACTIONS

REACTIONS (7) AND (8) (NAMELY J_{+4} AND J_{-4}) ARE INCOHERENT, THE 2 CONES USE A REACTION IN AN OPPOSITE WAY

$\Rightarrow$ CONES ARE:

$$\left[\begin{array}{l} Y_4 + Y_5 \xrightarrow{7} Y_6 \\ Y_4 + Y_6 \xrightarrow{10} 2Y_5 \end{array}\right]$$

$$\left[\begin{array}{l} Y_3 \xrightarrow{3} Y_1 + Y_2 \\ X_3 + Y_2 \xrightarrow{5} 2Y_3 \end{array}\right]$$

$$\left[\begin{array}{l} Y_6 \xrightarrow{8} Y_4 + Y_5 \\ 2Y_5 \xrightarrow{9} Y_4 + Y_6 \\ Y_4 \xrightarrow{12} Y_6 \end{array}\right]$$

(2) IF WE SIMULATE THE DYNAMICS AND MEASURE THE CURRENTS, WE CAN SEE THE DIRECTION OF THE NET ONES

$Y_1 \overset{\circ}{\sim} Y_2$ → CURRENTS IS NØ AT S.S.

$Y_3 \overset{\circ}{\sim} Y_1 + Y_2$ →

$X_3 + Y_2 \overset{\circ}{\sim} 2Y_3$ ↗

$Y_4 + Y_5 \leftarrow Y_6$ ← SHARED REACTION

$2Y_5 \rightarrow Y_4 + Y_6$

$Y_6 \leftarrow Y_4$ SHARING A CURRENT ✓

WHICH MEANS THAT THE 2 CORES WILL HAVE SUCH NET CURRENTS:

$Y_4 + Y_5 \leftarrow Y_6$

$Y_4 + Y_6 \leftarrow 2Y_5$

COHERENT CURRENTS ✓

$Y_6 \rightarrow Y_4 + Y_5$

~~$X_3 + Y_2 \rightarrow 2Y_3$~~

$2Y_5 \rightarrow Y_4 + Y_6$

$Y_4 \rightarrow Y_6$

COHERENT CURRENTS ✓

SO AS PROVEN IN THE PAPER, CORES MAINTAIN COHERENT DIRECTION OF CURRENTS AT STEADY STATE:

THE SECOND CORE IS WINNING AND PUSHES THE FLOW OF CURRENTS IN ITS DIRECTION

THE FIRST LOSES, HAVING ITS CURRENTS GOING

BACKWARDS, BUT THEY ARE STILL COHERENT WITH EACH OTHER!

WHAT WOULD HAPPEN IF 2 CONES SHARE INSTE

(2) REACTIONS BUT <u>INCOHERENT</u> TO EACH OTHER

IN FACT, NOW THE 2 CONES FOUND AN AGREEMENT ON THE DIRECTION OF REACTION (RED AR

BUT WHAT IF THEY CANNOT?

EXAMPLE:

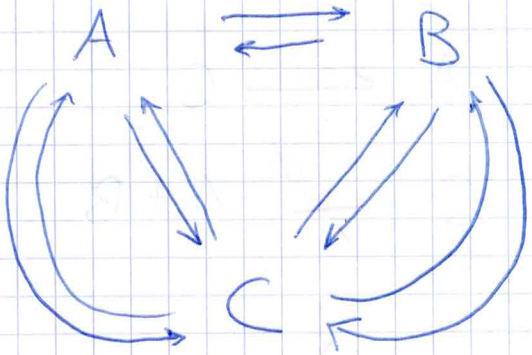
$A \rightleftarrows B$

$B \rightleftarrows C$

$A \rightleftarrows C$

$C \rightleftarrows A+B$

$\Rightarrow$

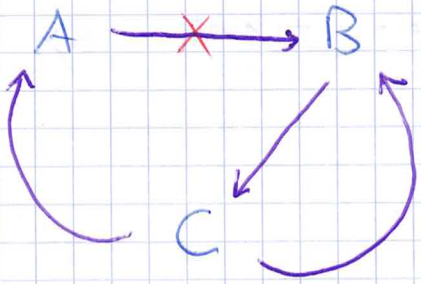


LET'S CONSIDER THE 2 CONES IN THE NETWOR

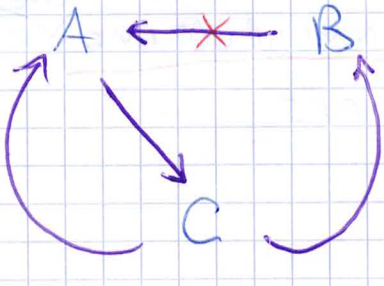
1	$A \rightarrow B$	1	$B \rightarrow A$
2	$B \rightarrow C$	2	$A \rightarrow C$
3	$C \rightarrow A+B$	3	$C \rightarrow A+B$

THEY SHARE REACTION 3, AND THEY SHARE REACTION 1 BUT OPPOSITELY → THEY CAN'T FIND AN AGREEMENT!

CONE 1

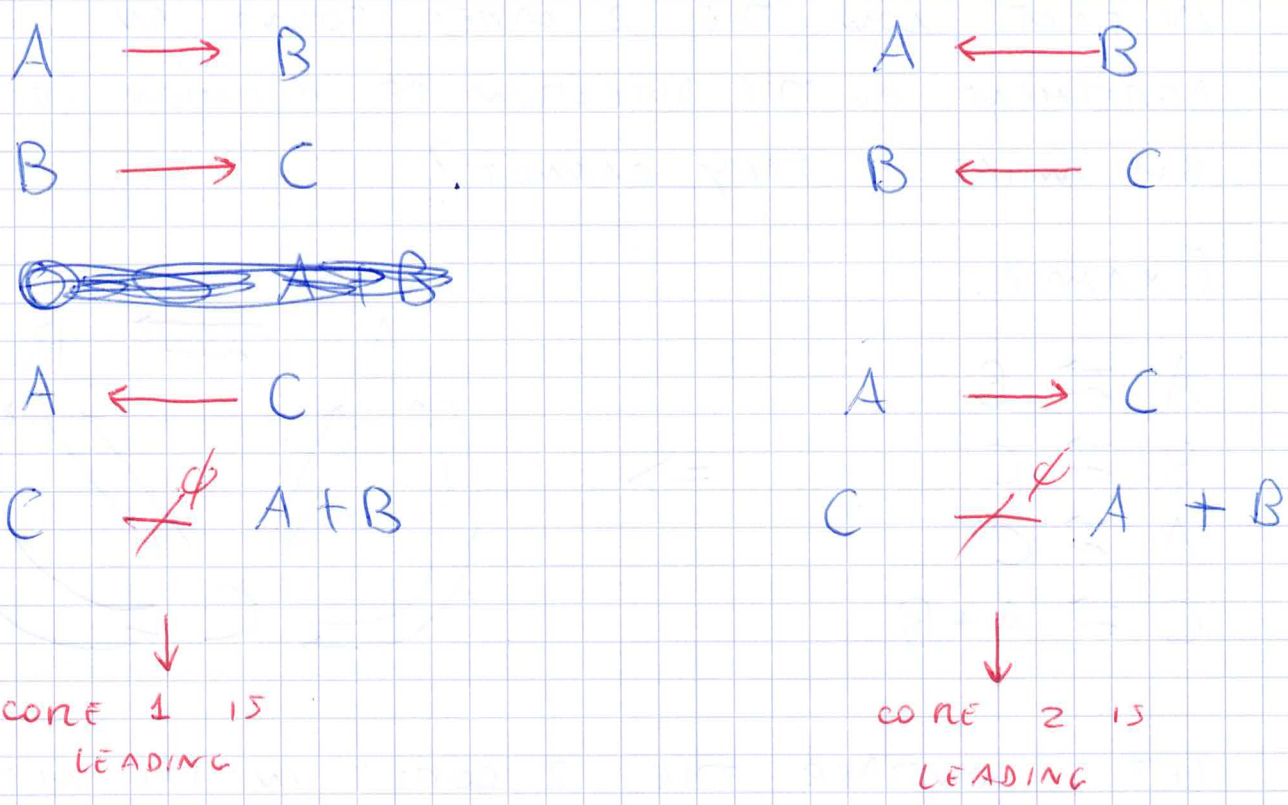


CONE 2



(4) DEPENDING ON THE RANDOM PARAMETER CHOICE YOU CAN END UP WITH 2 COMPLEMENTARY SITUATIONS AT STEADY STATE

(OBTAINED FROM DYNAMICAL SIMULATIONS)



WHAT HAPPENS IS, AS EXPECTED, NO MATTER THE CONFIGURATION (DEPENDING ON $\vec{k}$), REACTION 4 IS ALWAYS NOT USED, AND IT WILL REACH LOCAL EQUILIBRIUM. THIS IS DUE TO FRUSTRATION. THE EXISTENCE OF 2 ≠ CORES INCOHERENT WITH EACH OTHER DOESN'T ALLOW THE DISTRIBUTION OF THE NET CURRENTS AT STEADY STATE TO FOLLOW AND BE COHERENT WITH BOTH CORES, RESULTING IN ANNIHILATING ONE OF THE CURRENTS SHARED BY THE CORES