Shapes of dependencies in reaction systems ♻️⛓️🌼

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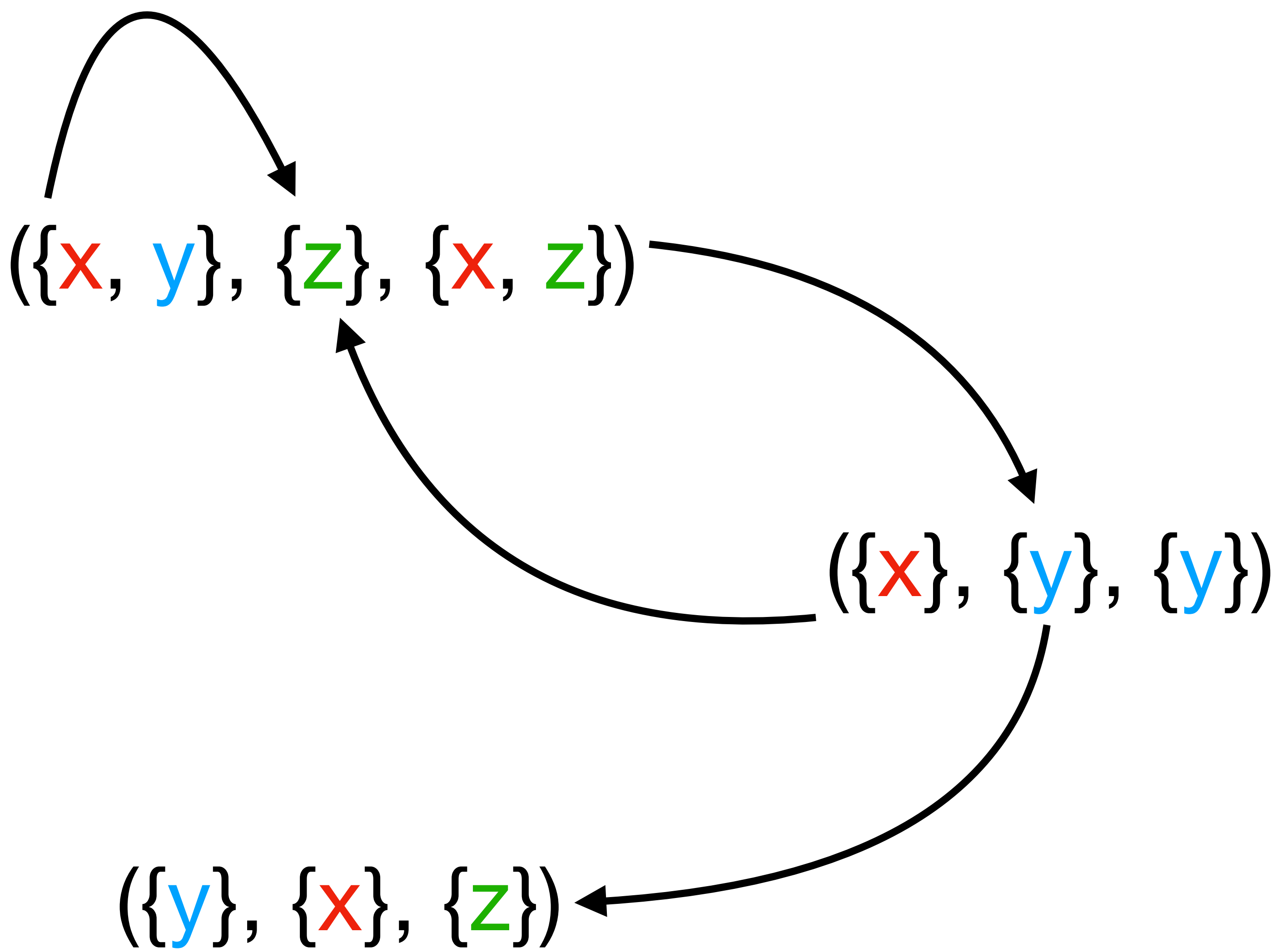
Structure vs behaviour

- What are the consequences of structural restrictions on the behaviour of RS?
- Example: minimal RS cannot compute all result functions
- But, for each RS $\mathcal{A}$ there exists a minimal RS $\mathcal{B}$ such that $\mathrm{res}_{\mathcal{A}}{}^{k}(T) = \mathrm{res}_{\mathcal{B}}{}^{2k}(T)$ for all $k \in \mathbf{N}$ and state T of $\mathcal{A}$

Positive dependency graph

- Vertices = set of reactions A
- There is an oriented edge $a \to b$ iff at least one product of reaction a is a reactant of reaction b

Positive dependency graph

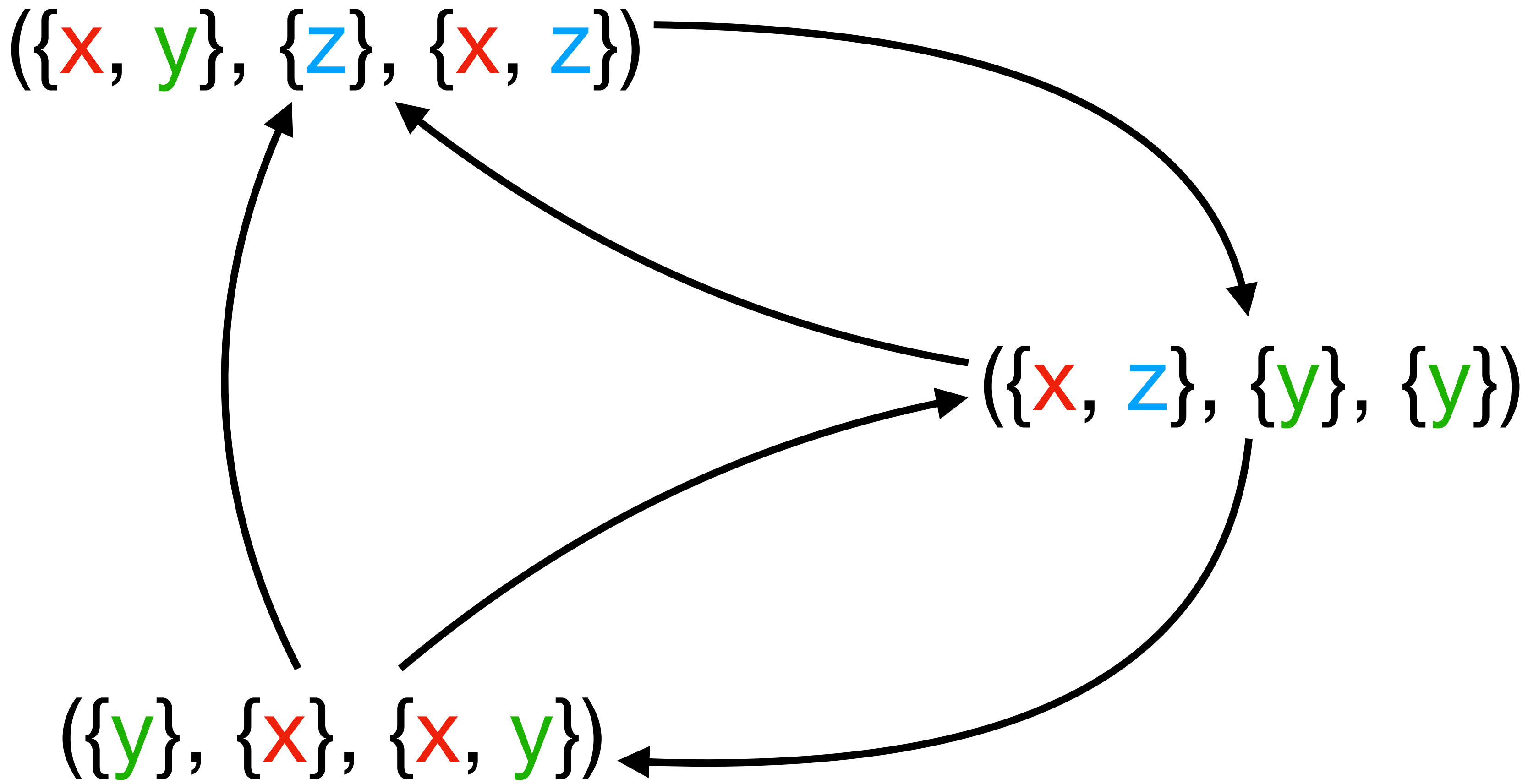


Self-sustaining cycle ♻️

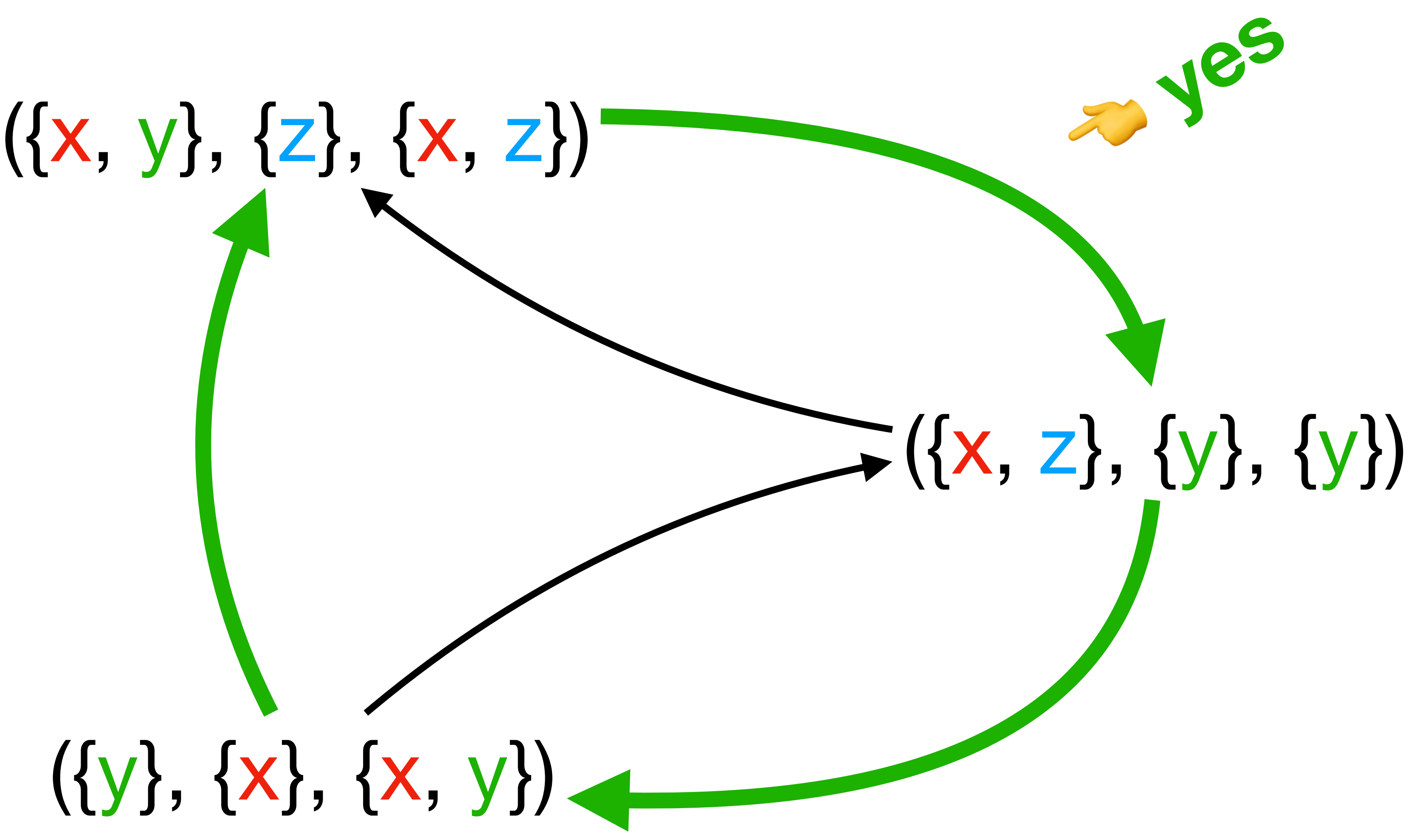
A path in the (positive) dependency graph
such that for each edge $a \rightarrow b$ we have:

- Reaction a produces all reactants of b: $R_b \subseteq P_a$
- Reaction a doesn't produce any inhibitor for b: $P_a \cap I_b = \varnothing$

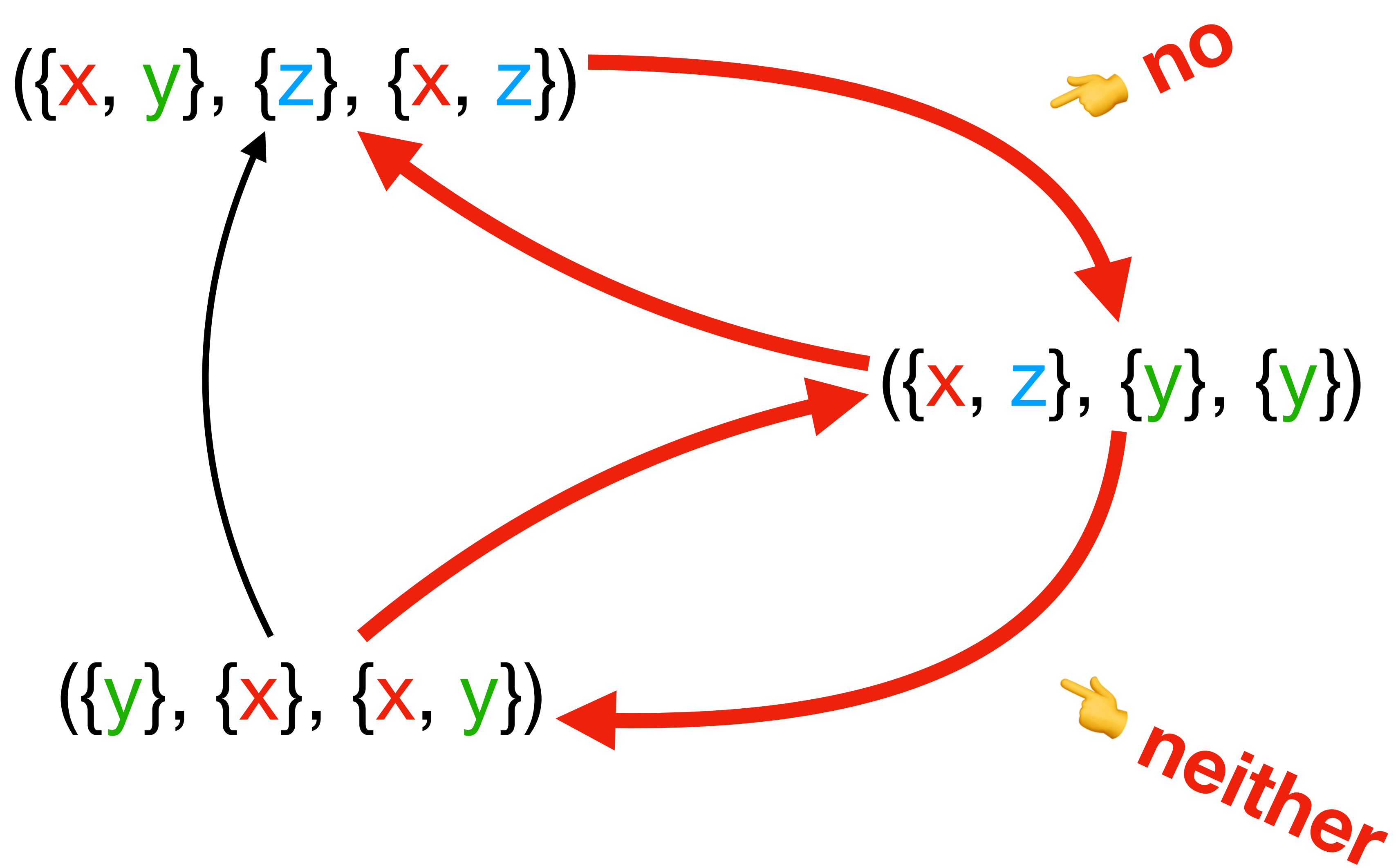
Self-sustaining cycle ♻️



Self-sustaining cycle ♻️



Self-sustaining cycle ♻️

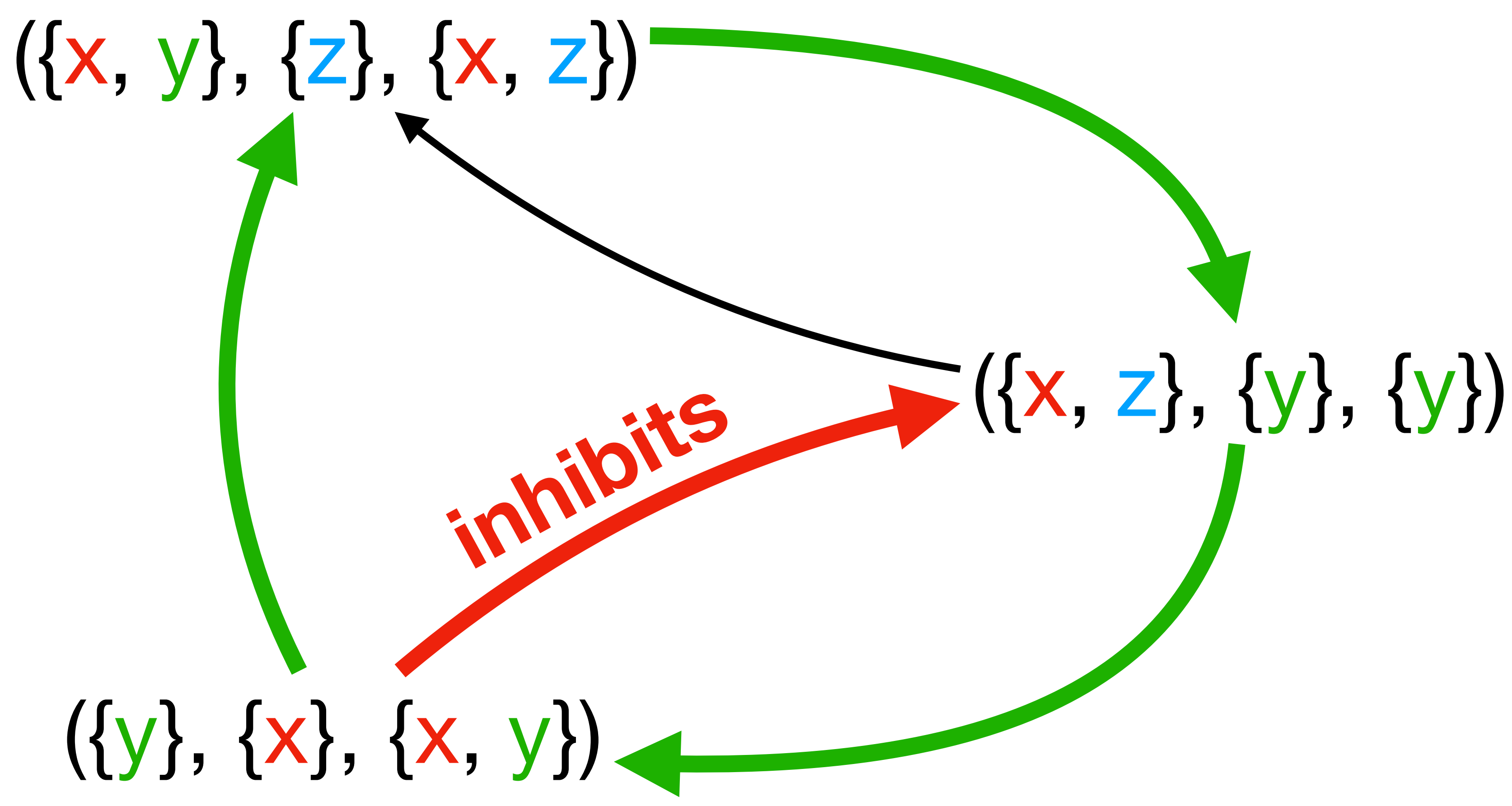


Non self-inhibiting reactions

A set of reactions $\{a_1, a_2, \ldots, a_n\}$ such that no reaction produces inhibitors for any other reaction in the set:
$P_i \cap P_j = \varnothing$ for all i, j belonging to the set

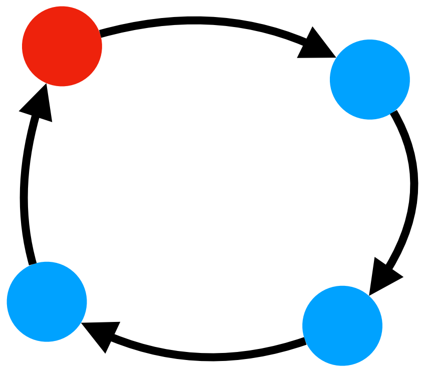
Otherwise, the set is called self-inhibiting

Self-sustaining but also self-inhibiting cycle



Simple cyclical dependencies

RS with a single self-sustaining, non self-inhibiting dependency cycle



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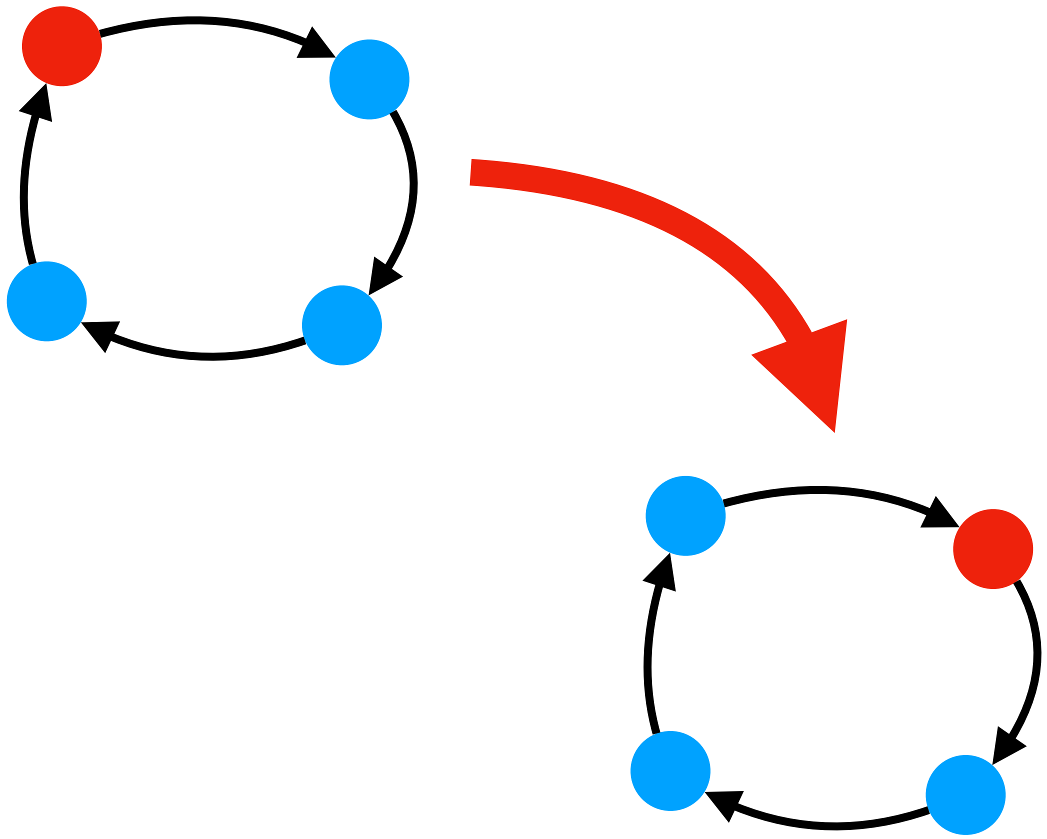

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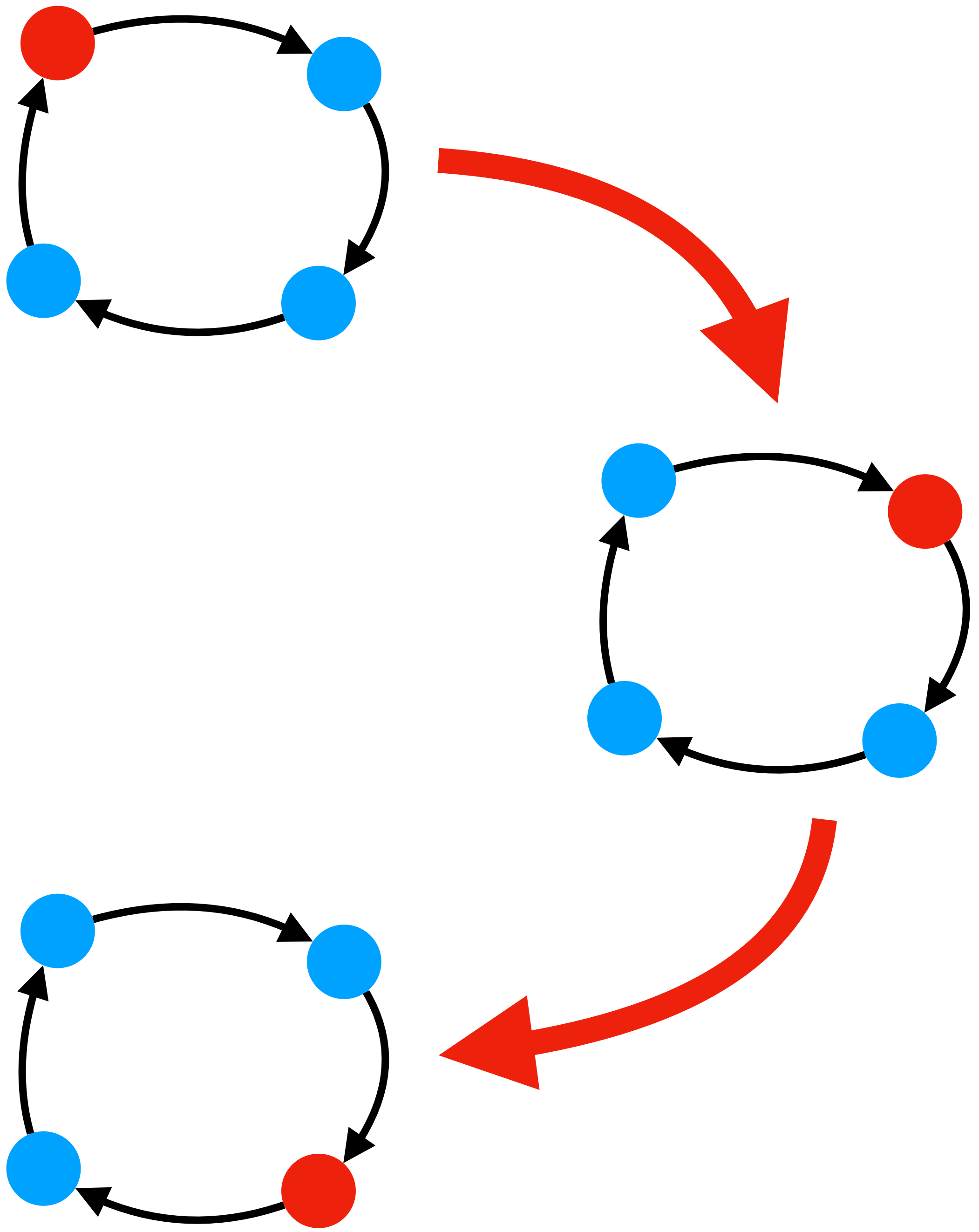

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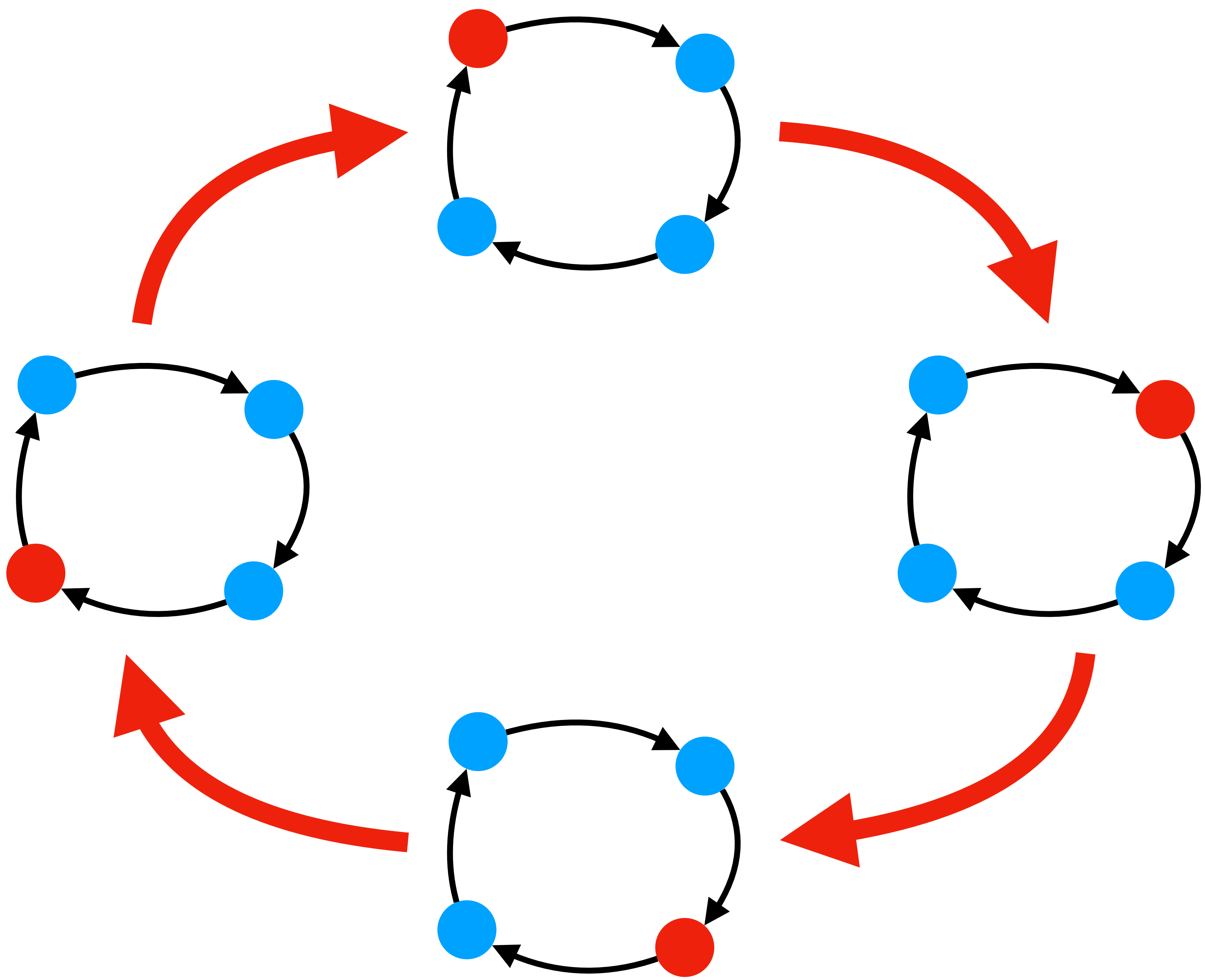

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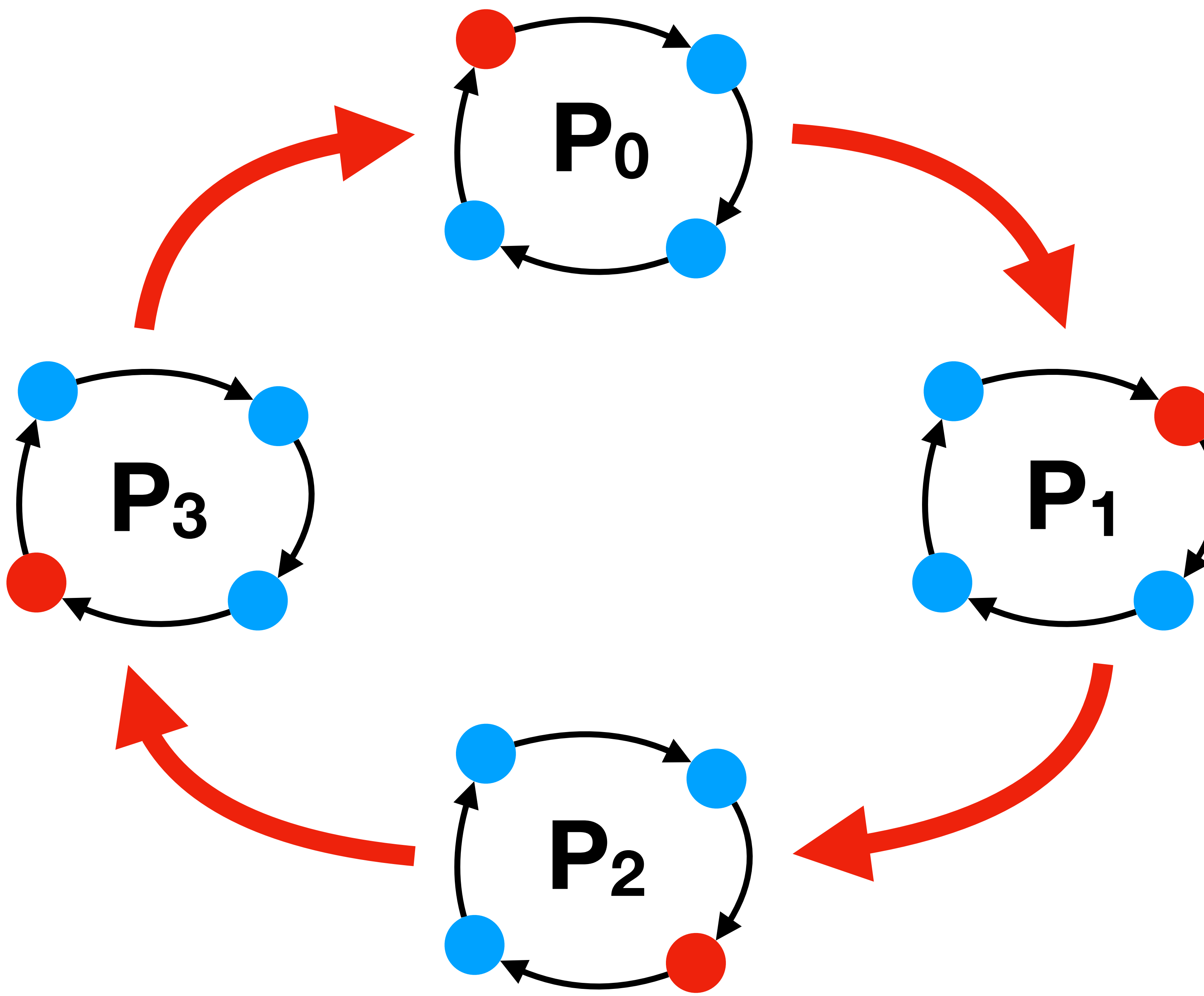


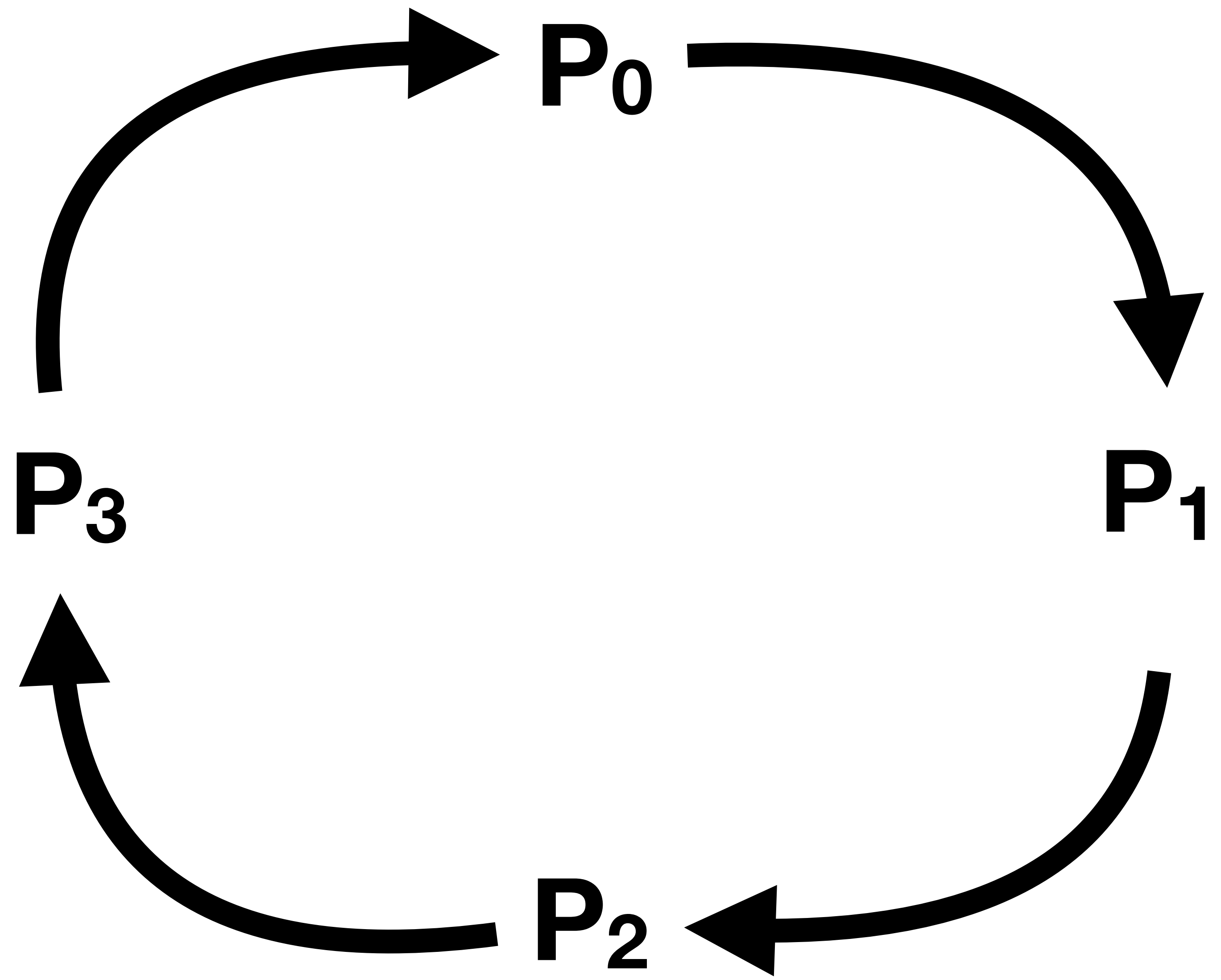
RS with a single self-sustaining, non self-inhibiting dependency cycle

P_0

P_3 P_1

P_2

RS with a single self-sustaining, non self-inhibiting dependency cycle



Rotations and cycles

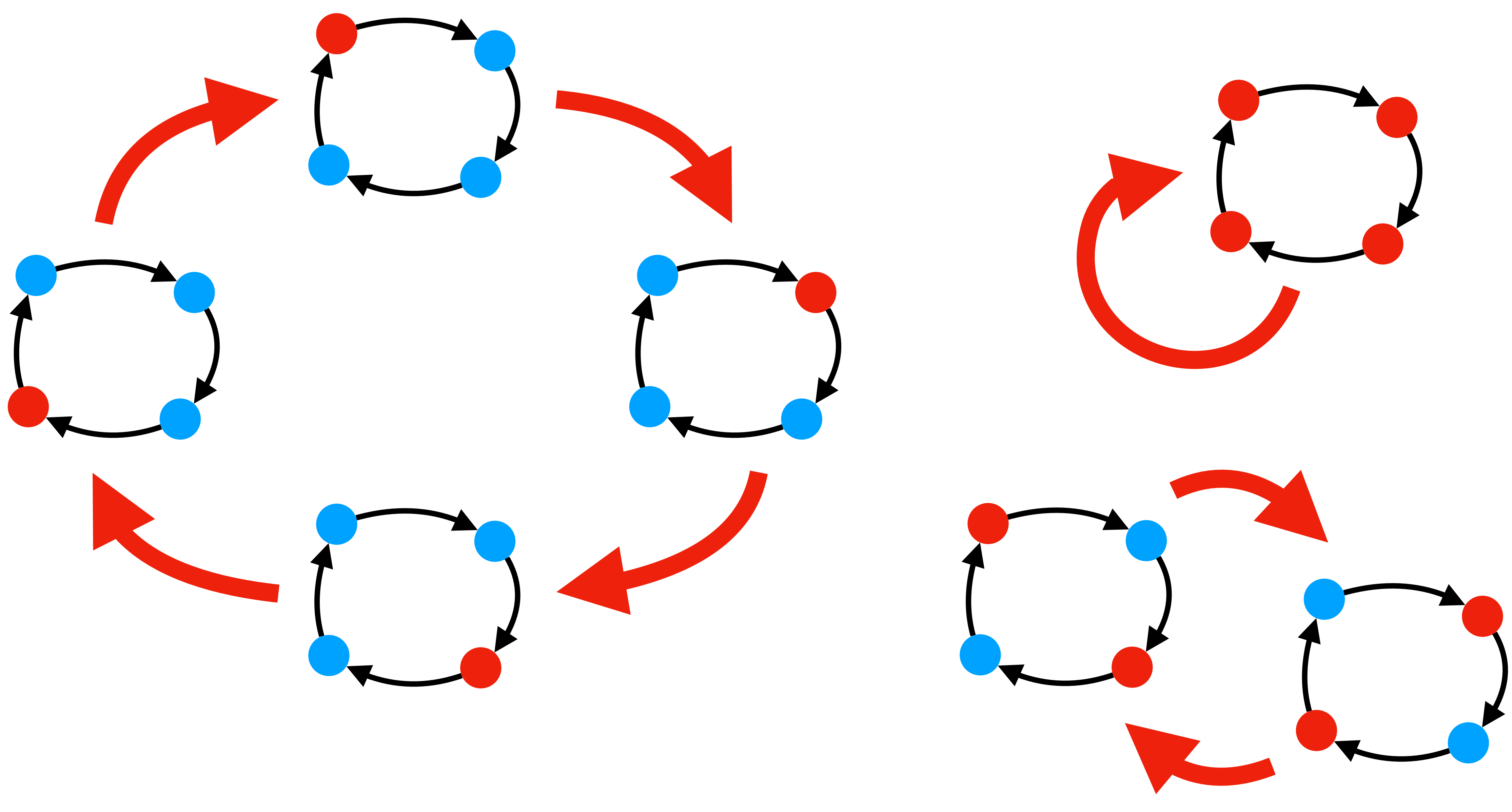
The rotations of active reactions along the (unique) cycle in the dependency graph (starting from a given configuration) correspond to transitions in the graph of the dynamics.

♻️ Theorem

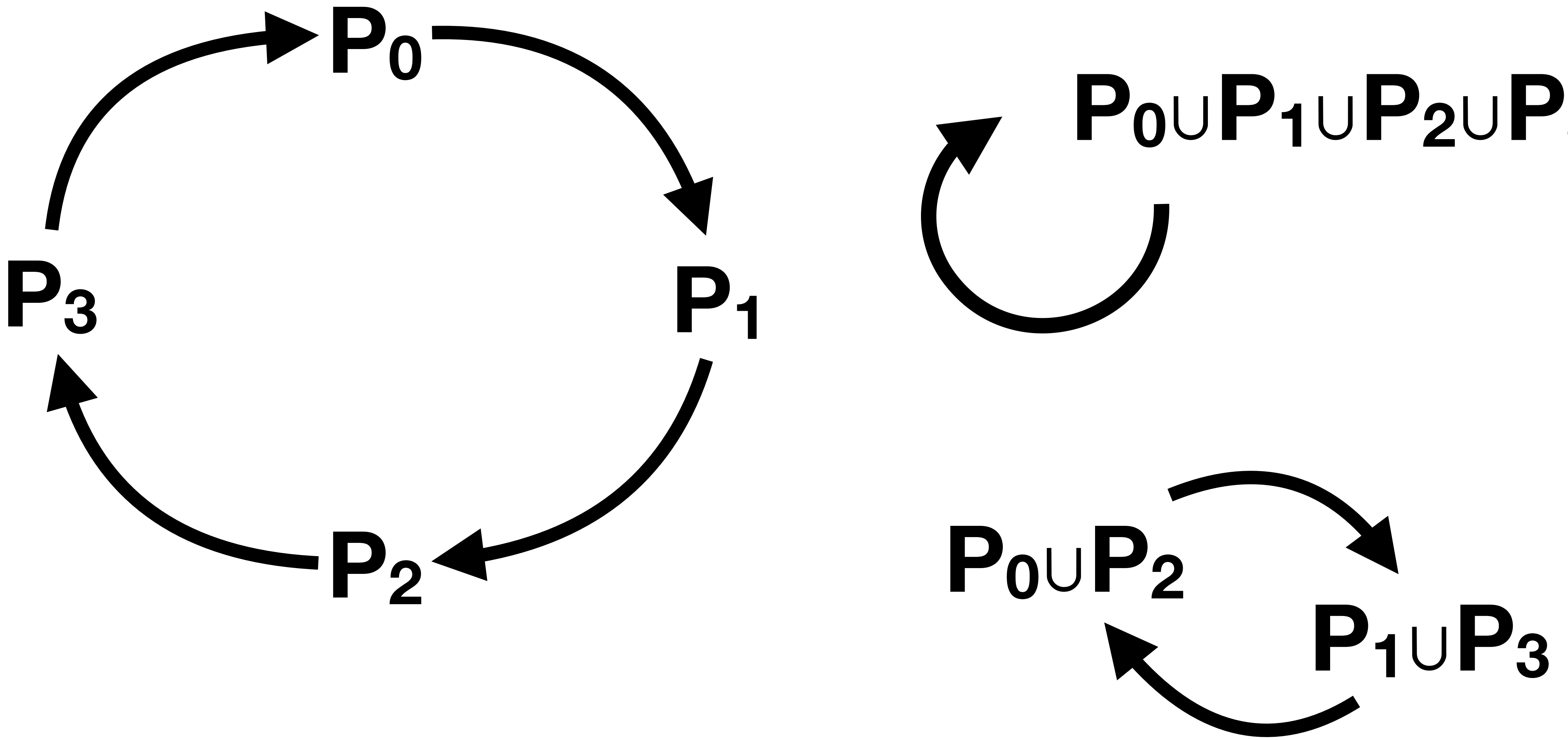
IF the dependency graph of a RS consists only one self-sustaining, non-self-inhibiting cycle of length n

THEN the dynamics of the RS only contains cycles of length dividing n, and there is at least one such cycle for each divisor of n.

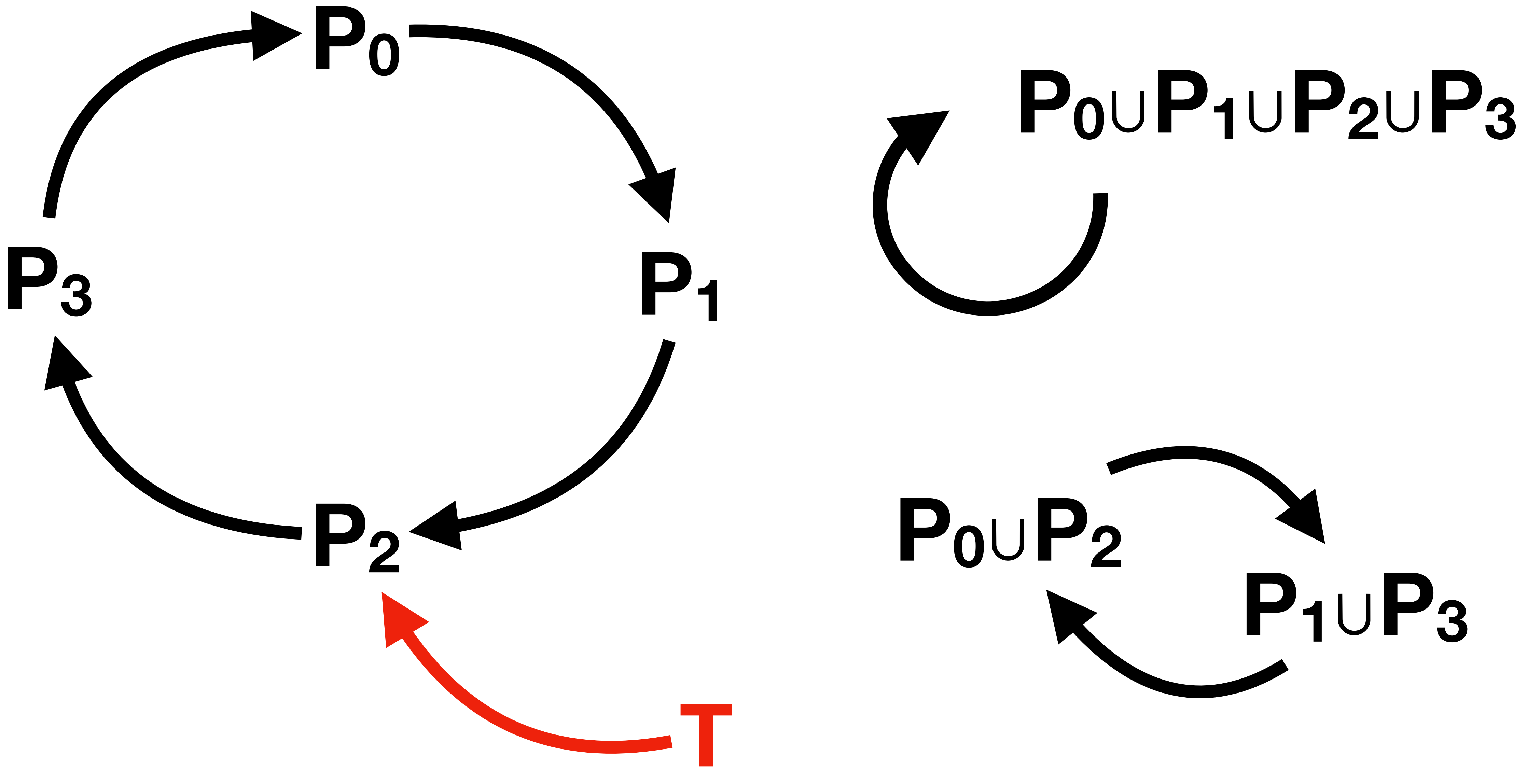
Length of the cycles



Length of the cycles

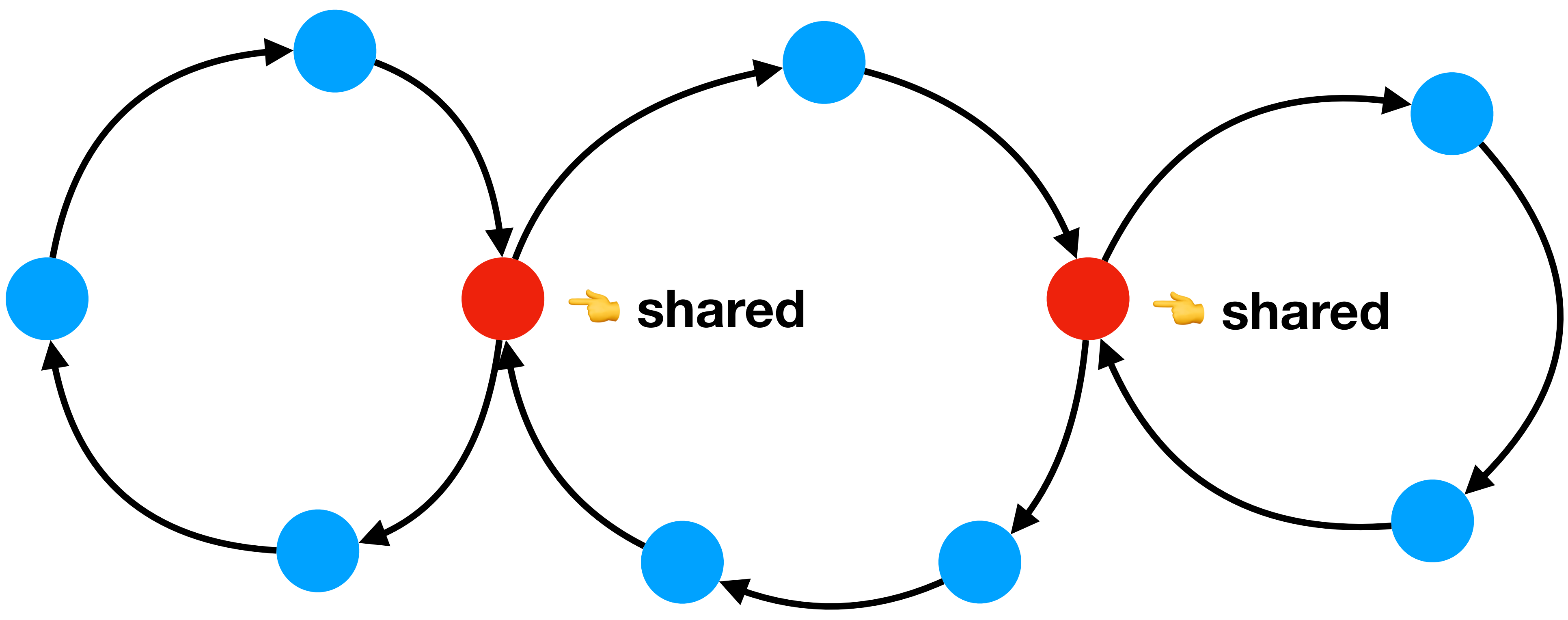


Length of the cycles



Chains of dependency

Chains ⛓️

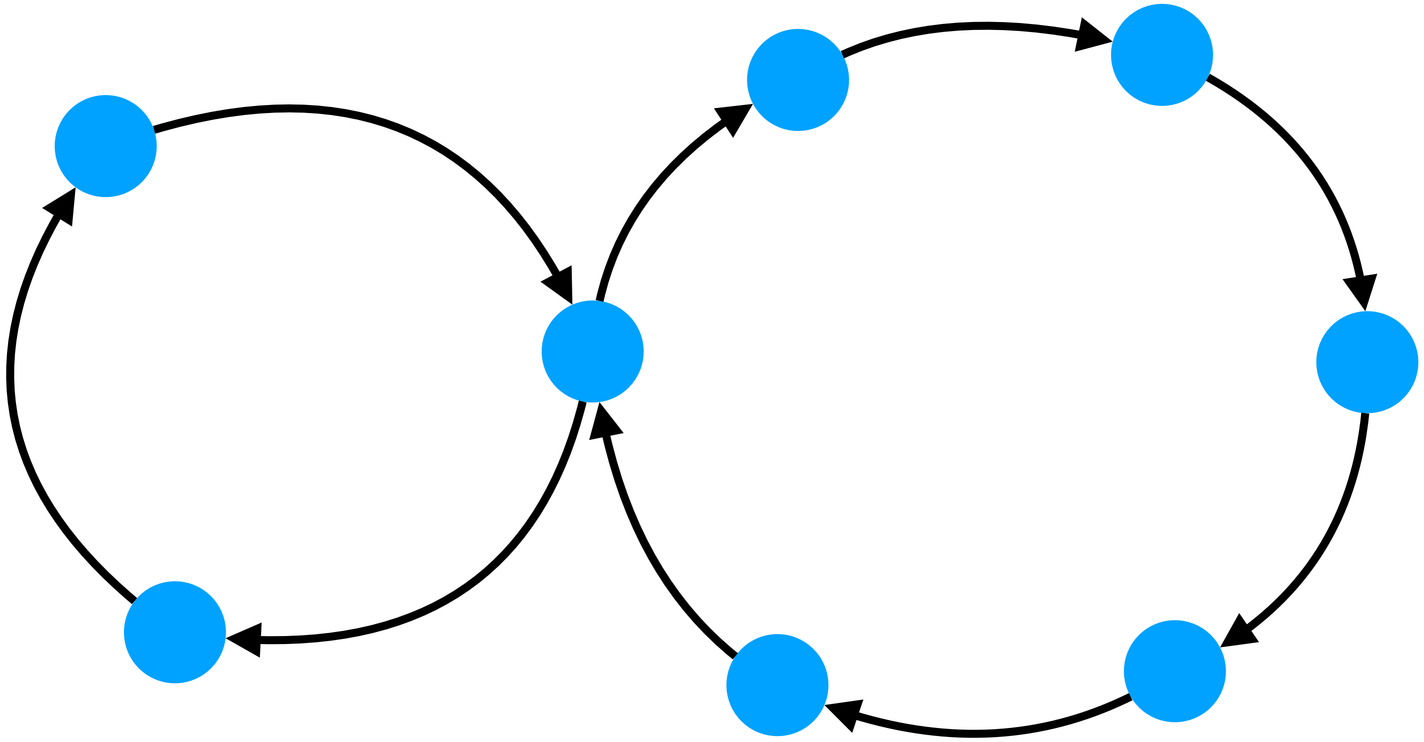


🗝 Lemma

IF the dependency graph of a RS contains a chain of two self-sustaining, non self-inhibiting cycles of length m and n

THEN when starting from a configuration where at least one reaction involved in the cycles is enabled, eventually all the reactions will be enabled once every $\gcd(m, n)$ steps.

🗝️ Lemma in action



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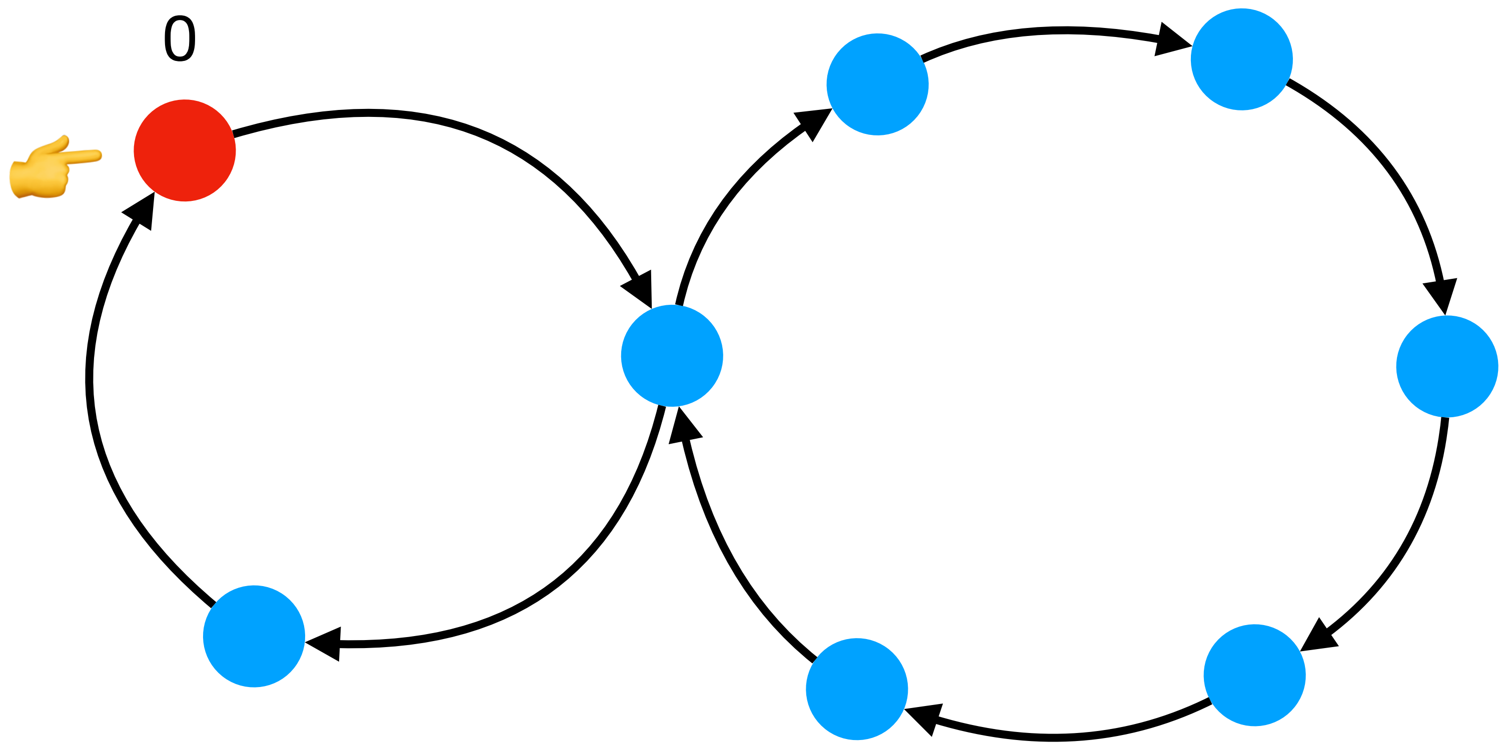
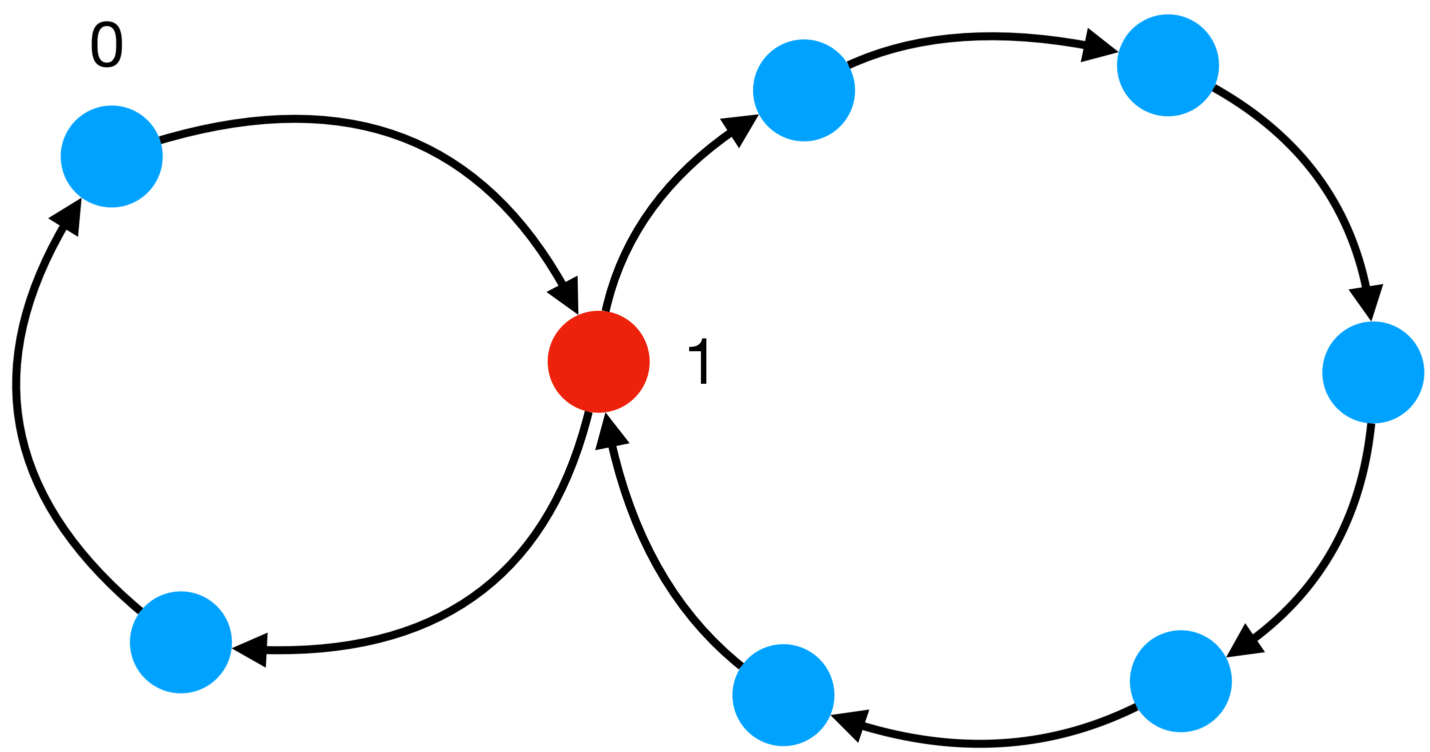


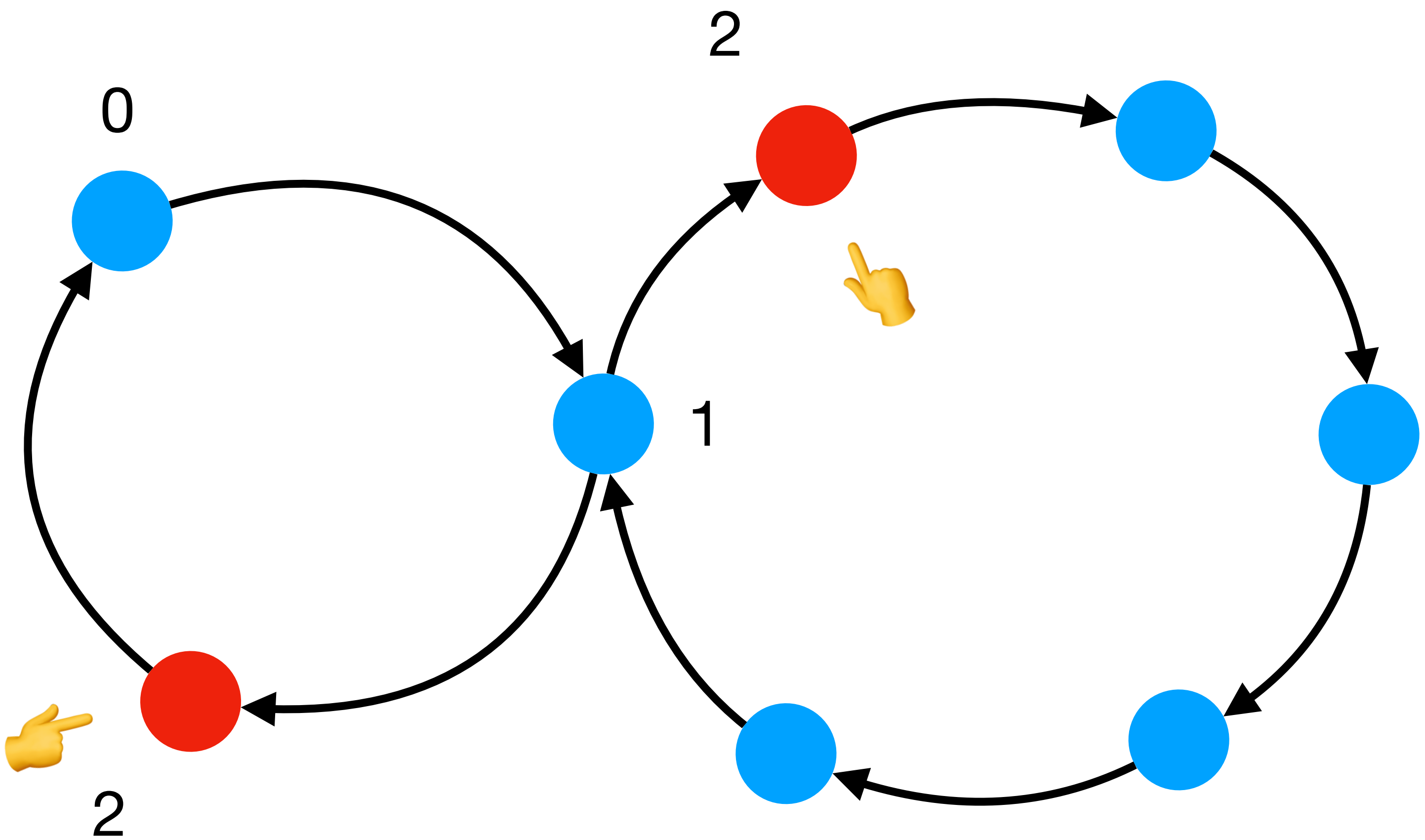
⏰ = 0

🗝 Lemma in action



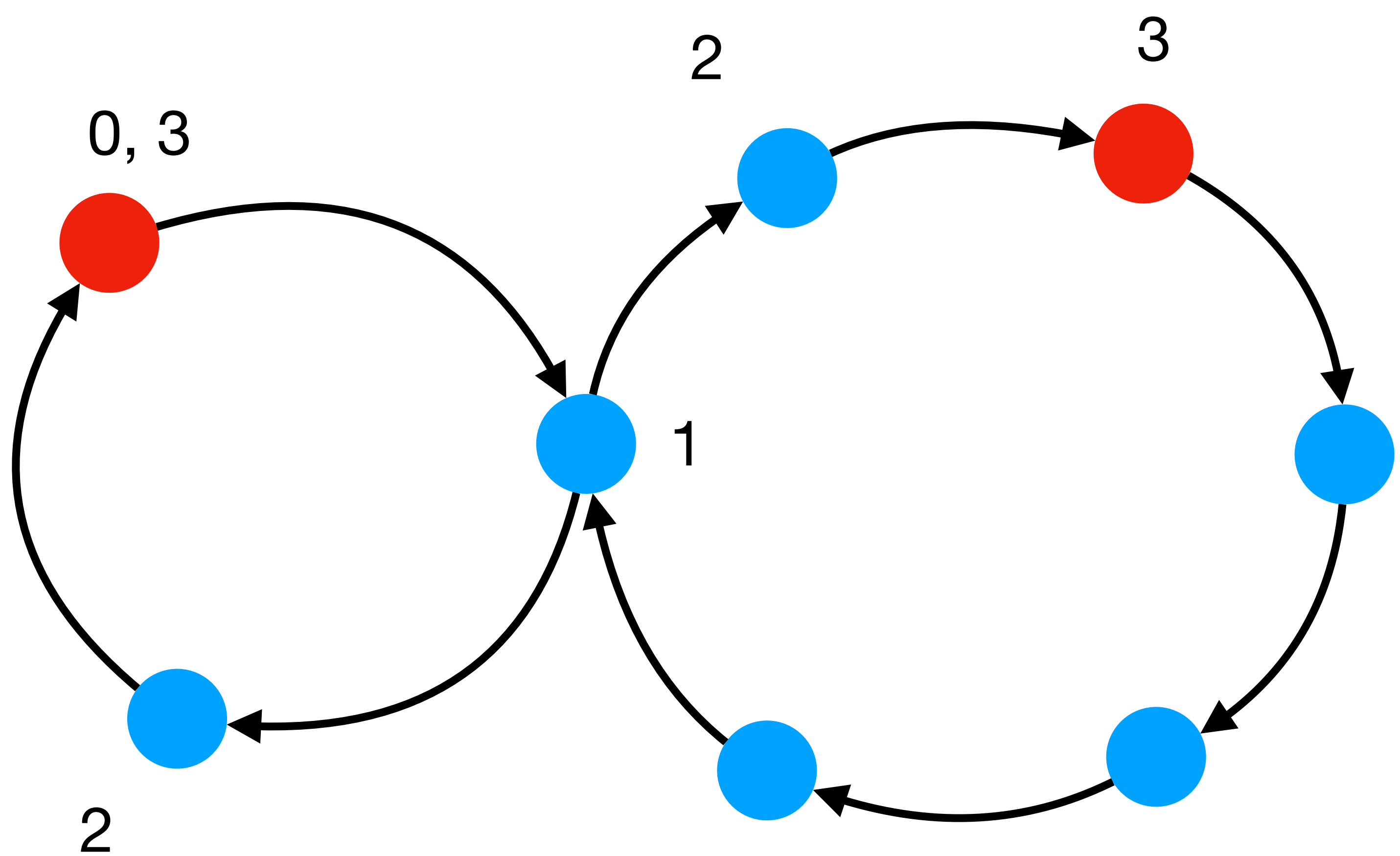
⏰ = 1

🗝 Lemma in action



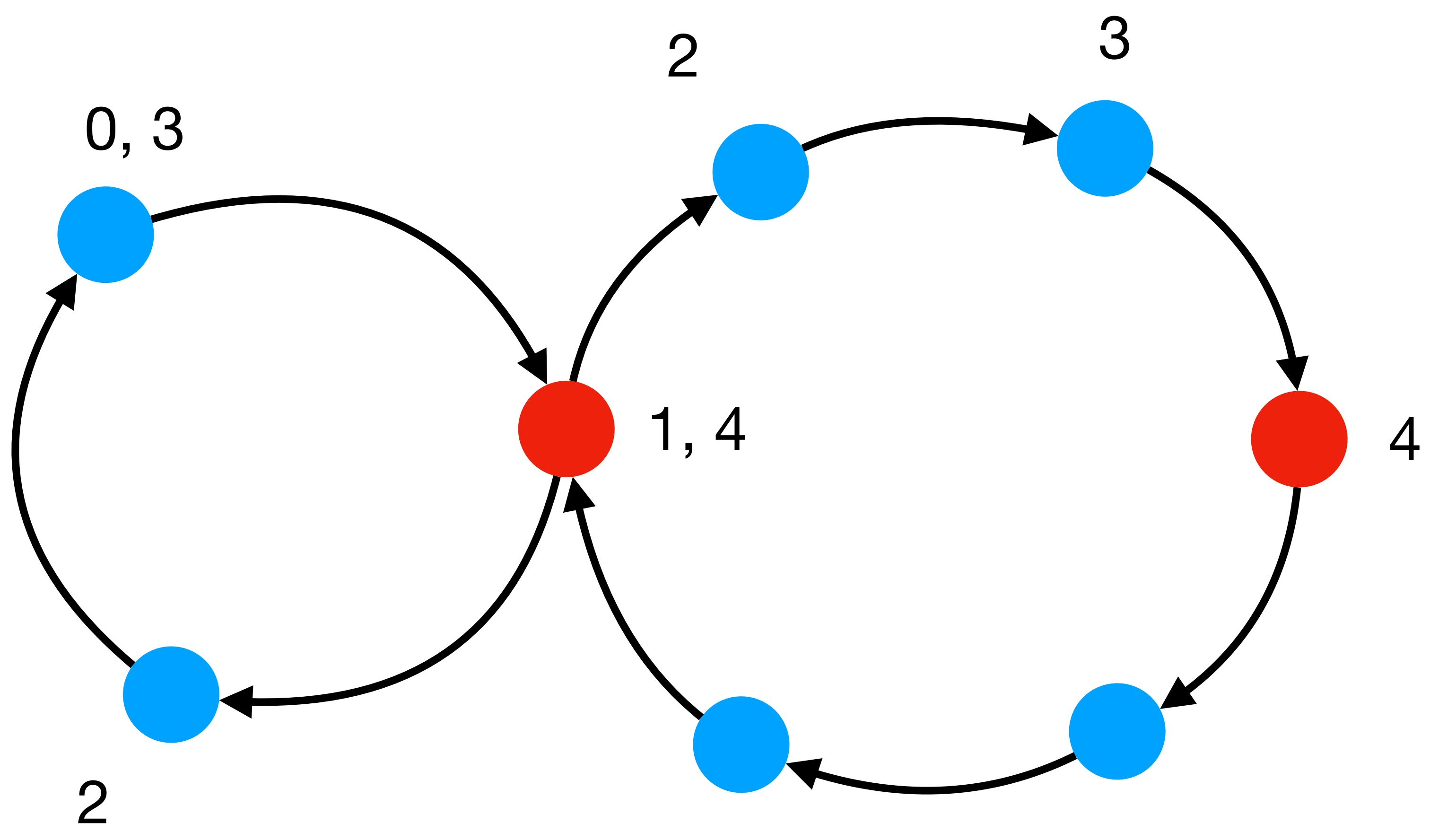
⏰ = 2

🗝️ Lemma in action



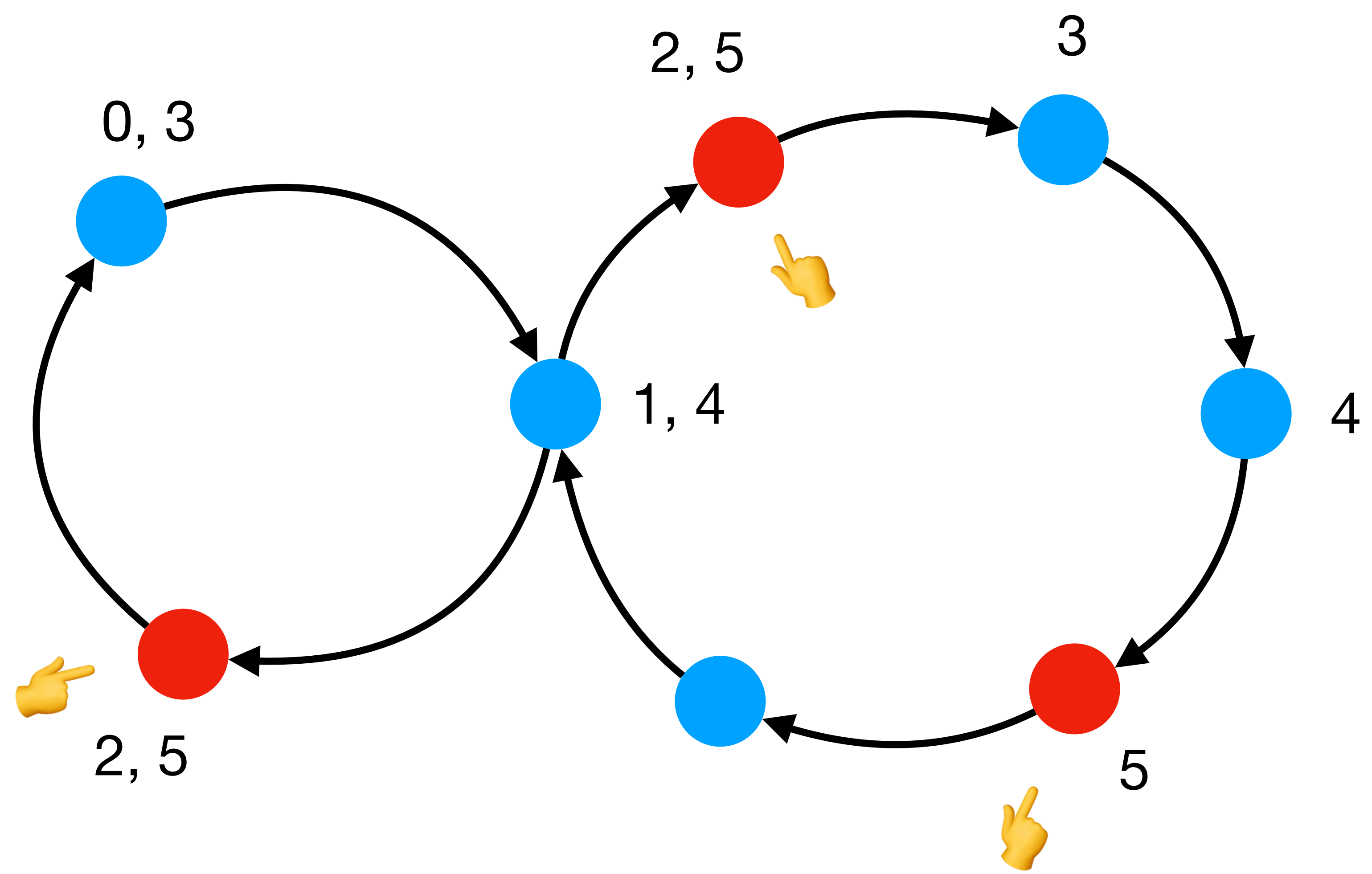
⏰ = 3

🗝 Lemma in action



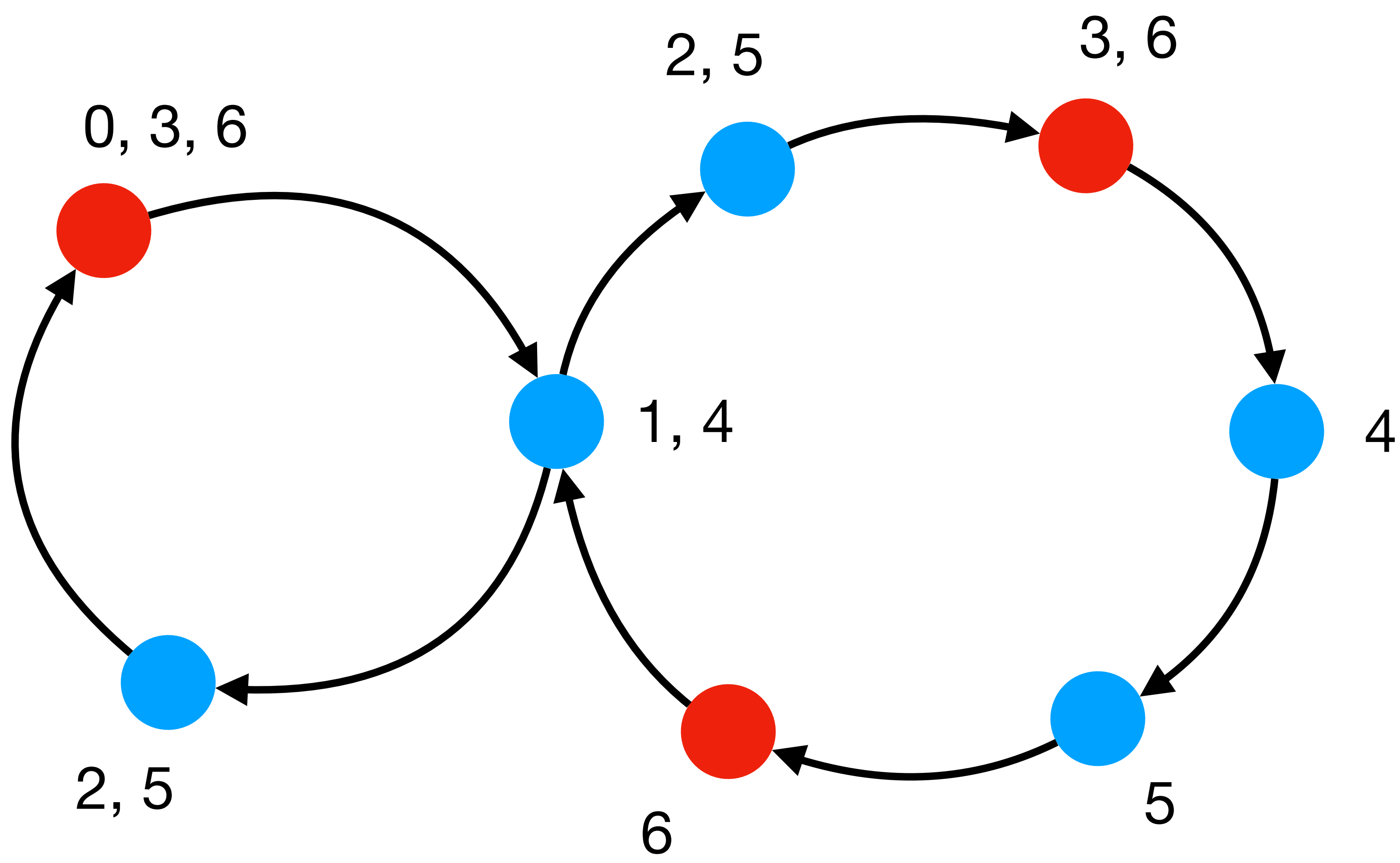
⏰ = 4

🗝 Lemma in action



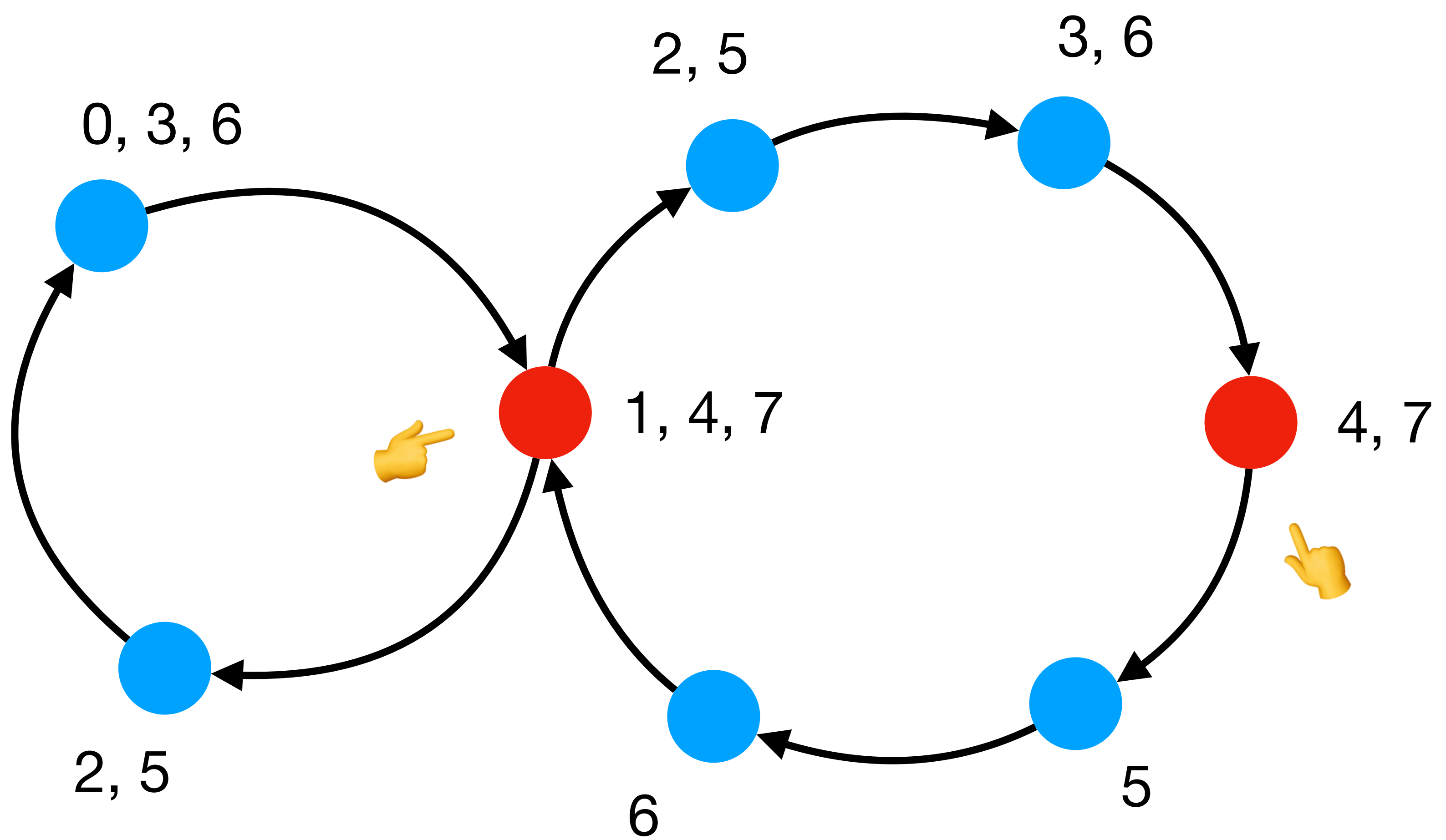
⏰ = 5

🗝 Lemma in action



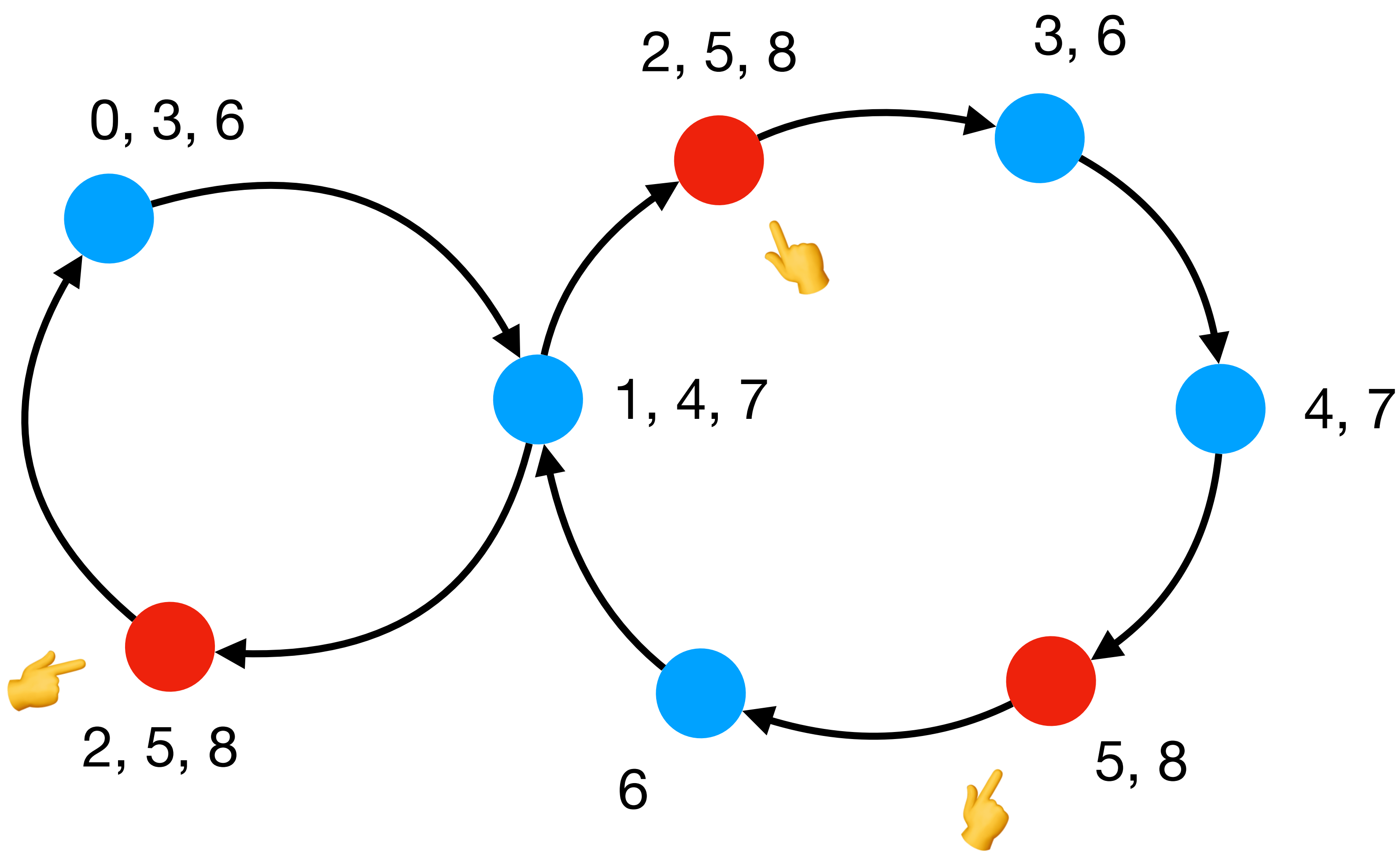
⏰ = 6

🗝 Lemma in action



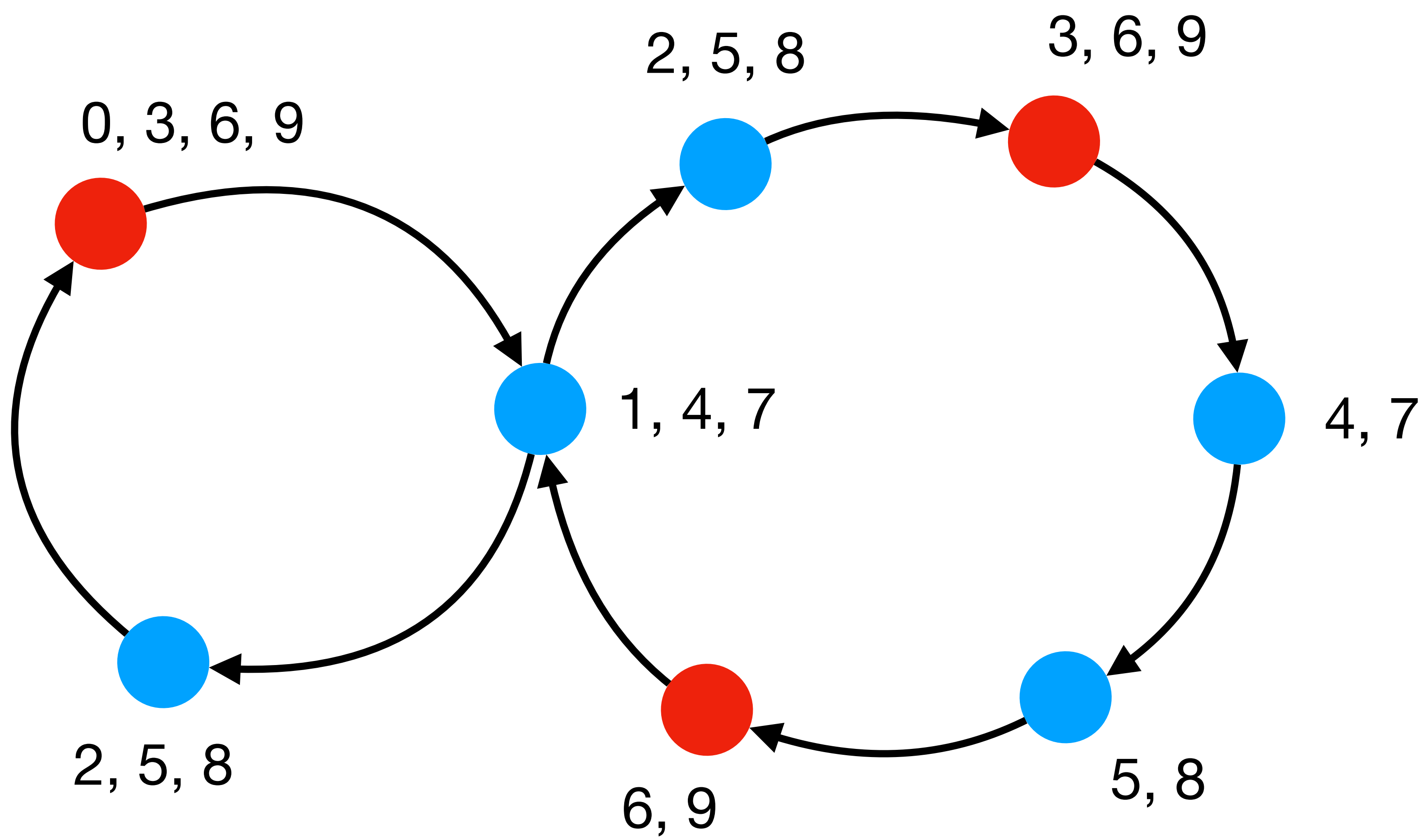
⏰ = 7

🗝 Lemma in action



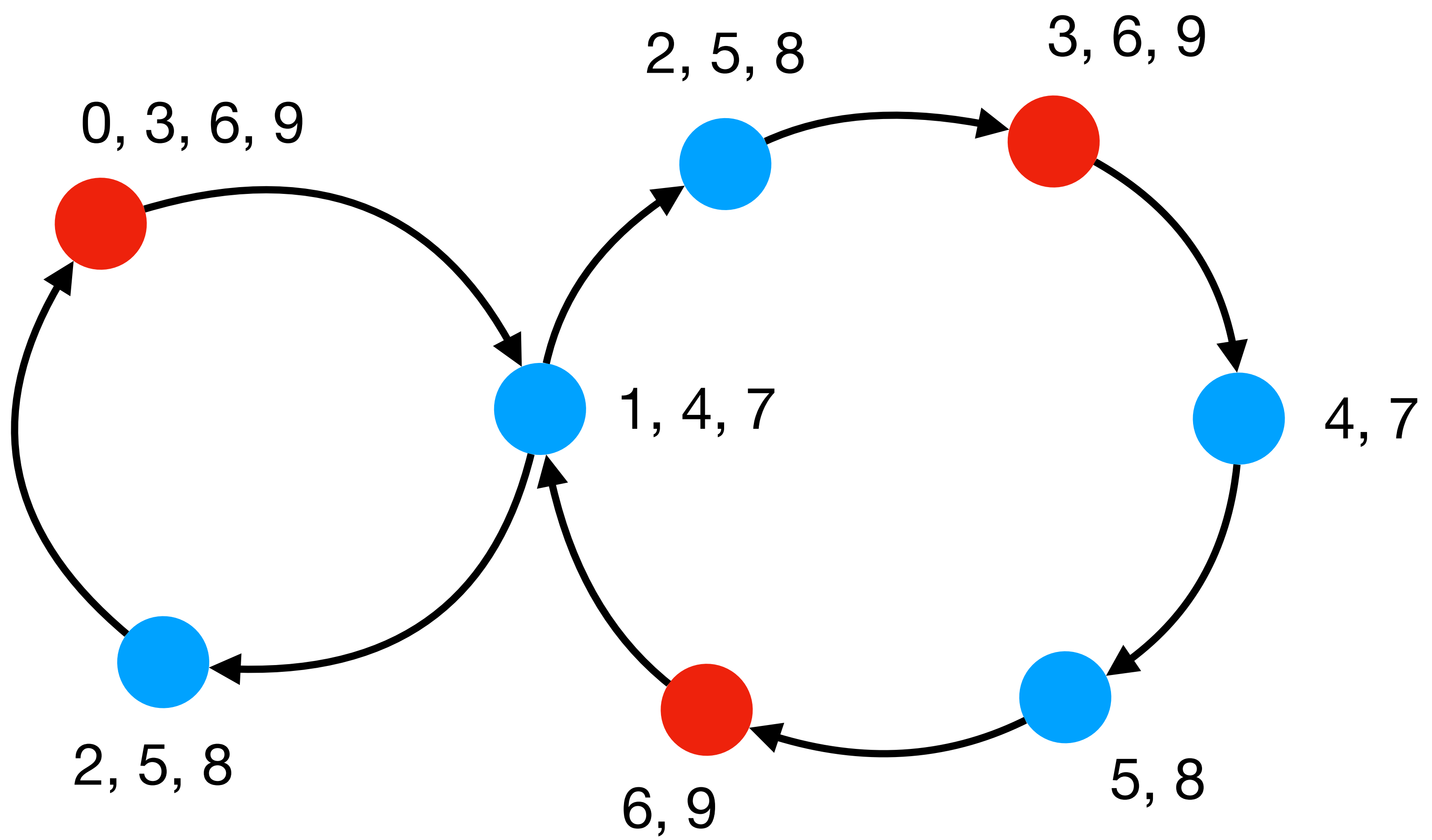
⏰ = 8

🗝 Lemma in action



⏰ = 9

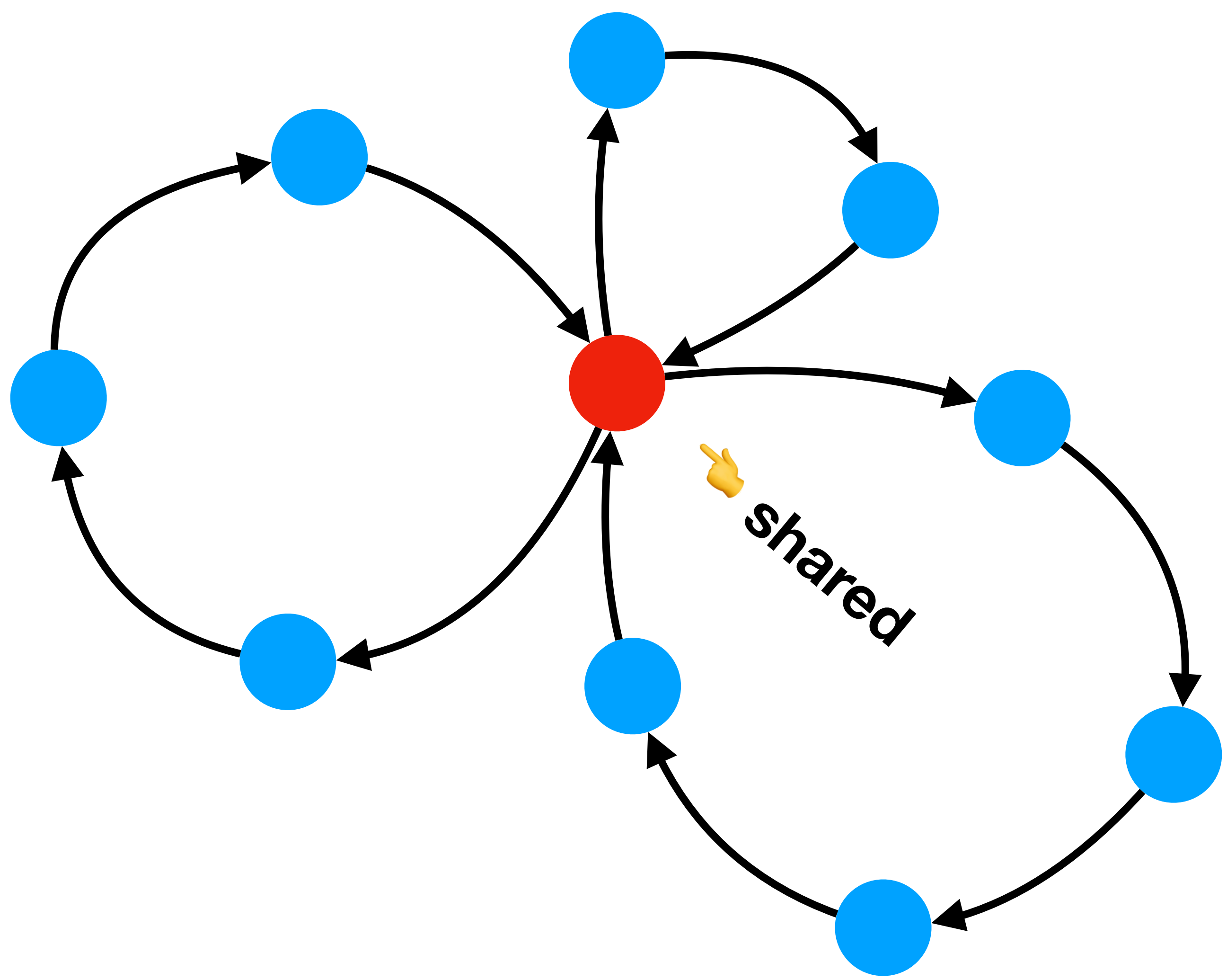
🗝️ Lemma in action



All reactions are enabled every 3 = gcd(3, 6) steps

Flower-shaped dependencies

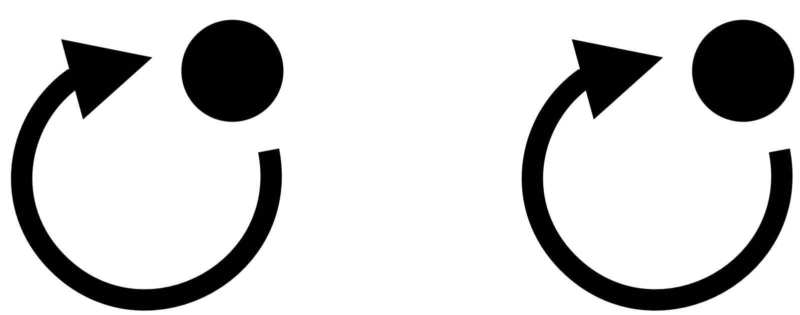
Flowers 🌼



🌼 Theorem

IF the dependency graph of a RS consists only of a flower of self-sustaining, non-self-inhibiting cycles (petals) with at lest of them of coprime lengths

THEN the RS has exactly two fixed points.



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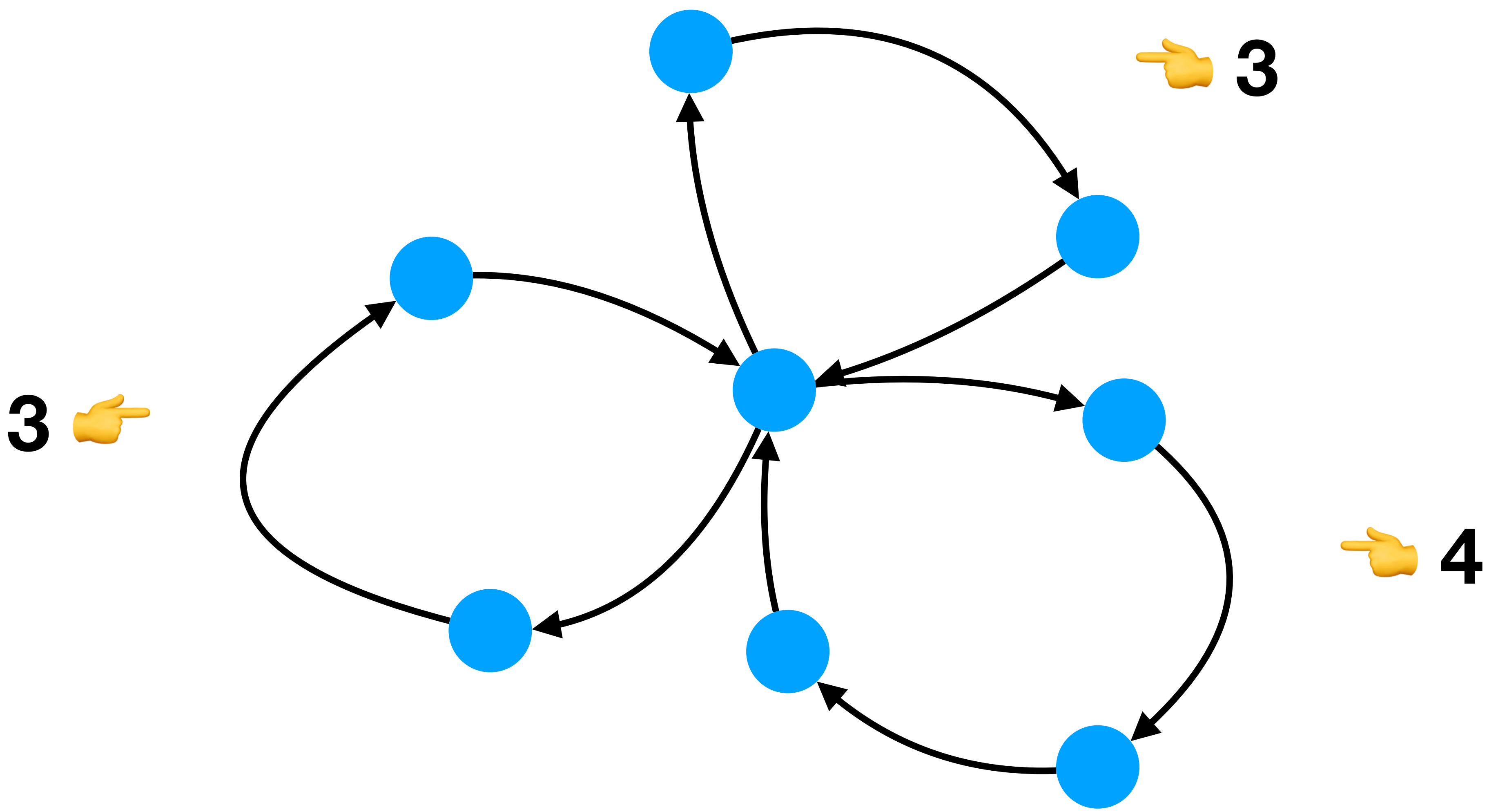

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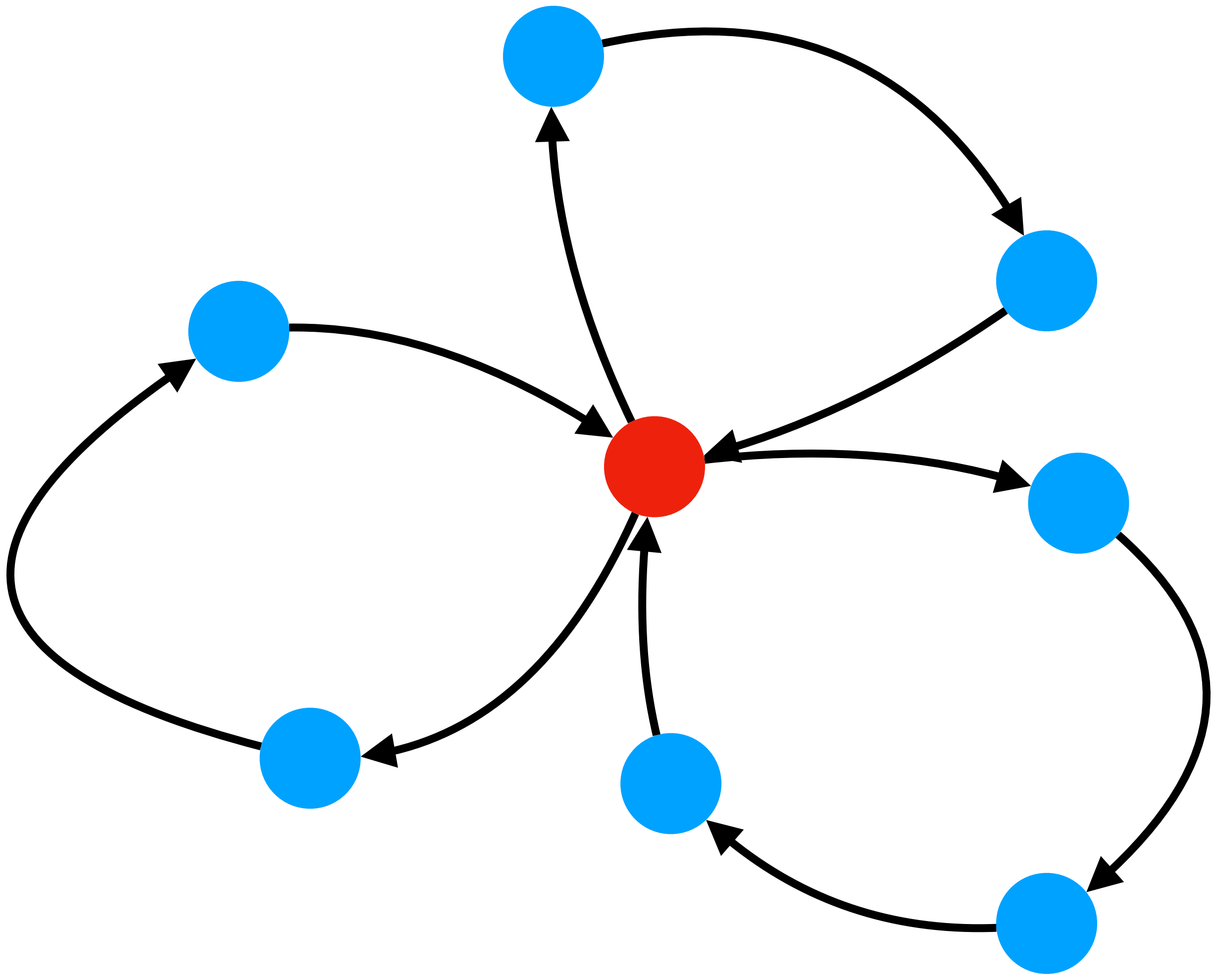

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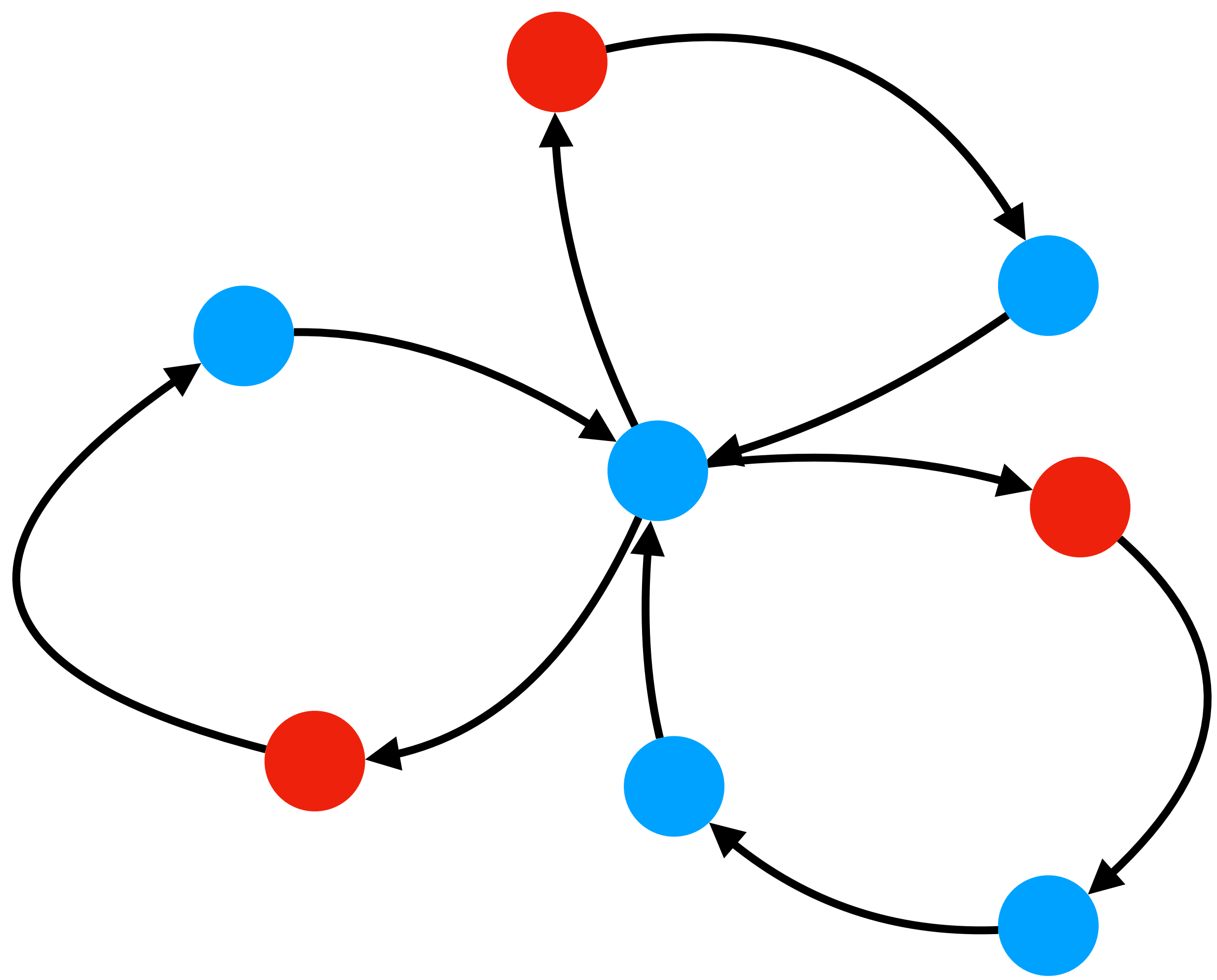

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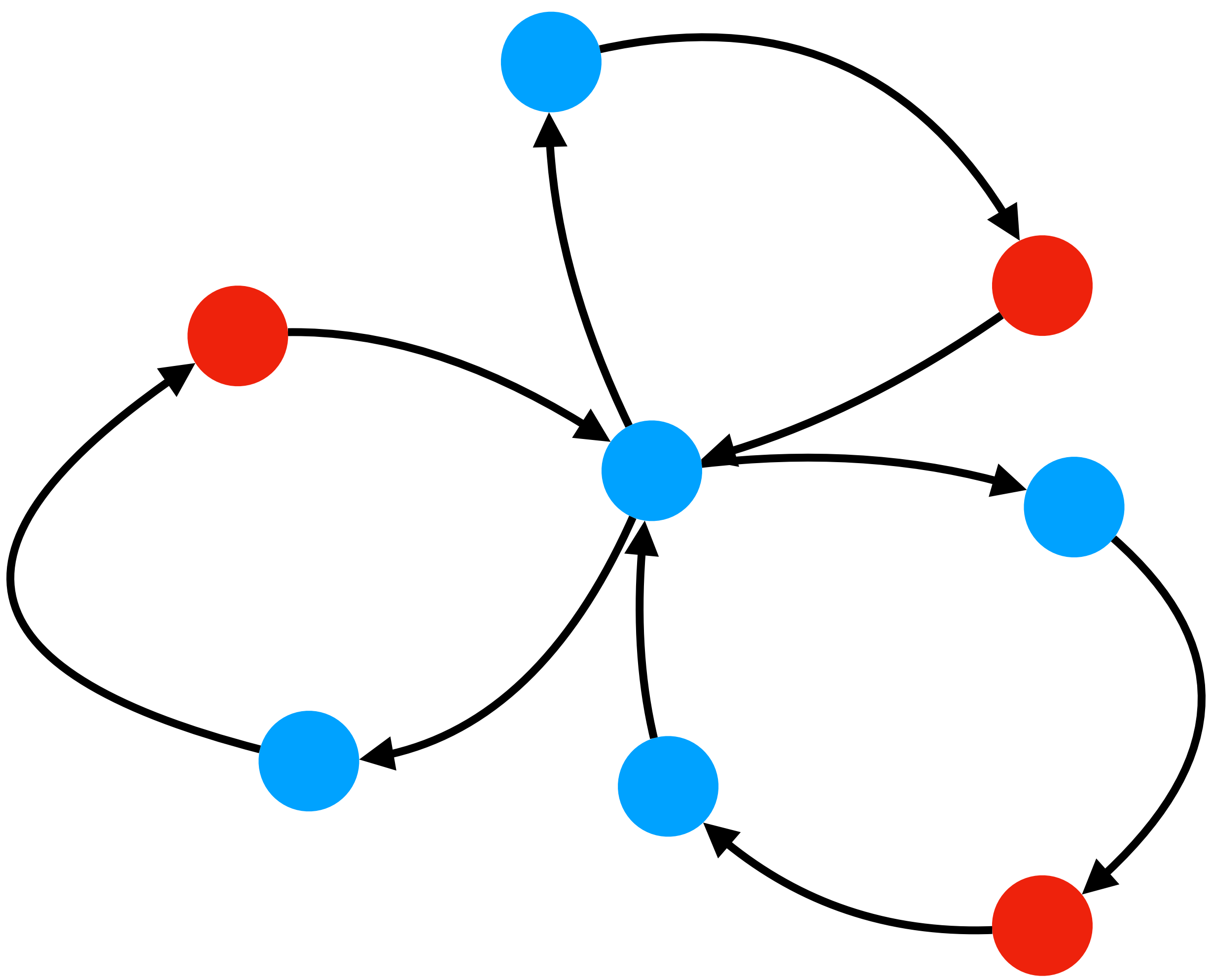

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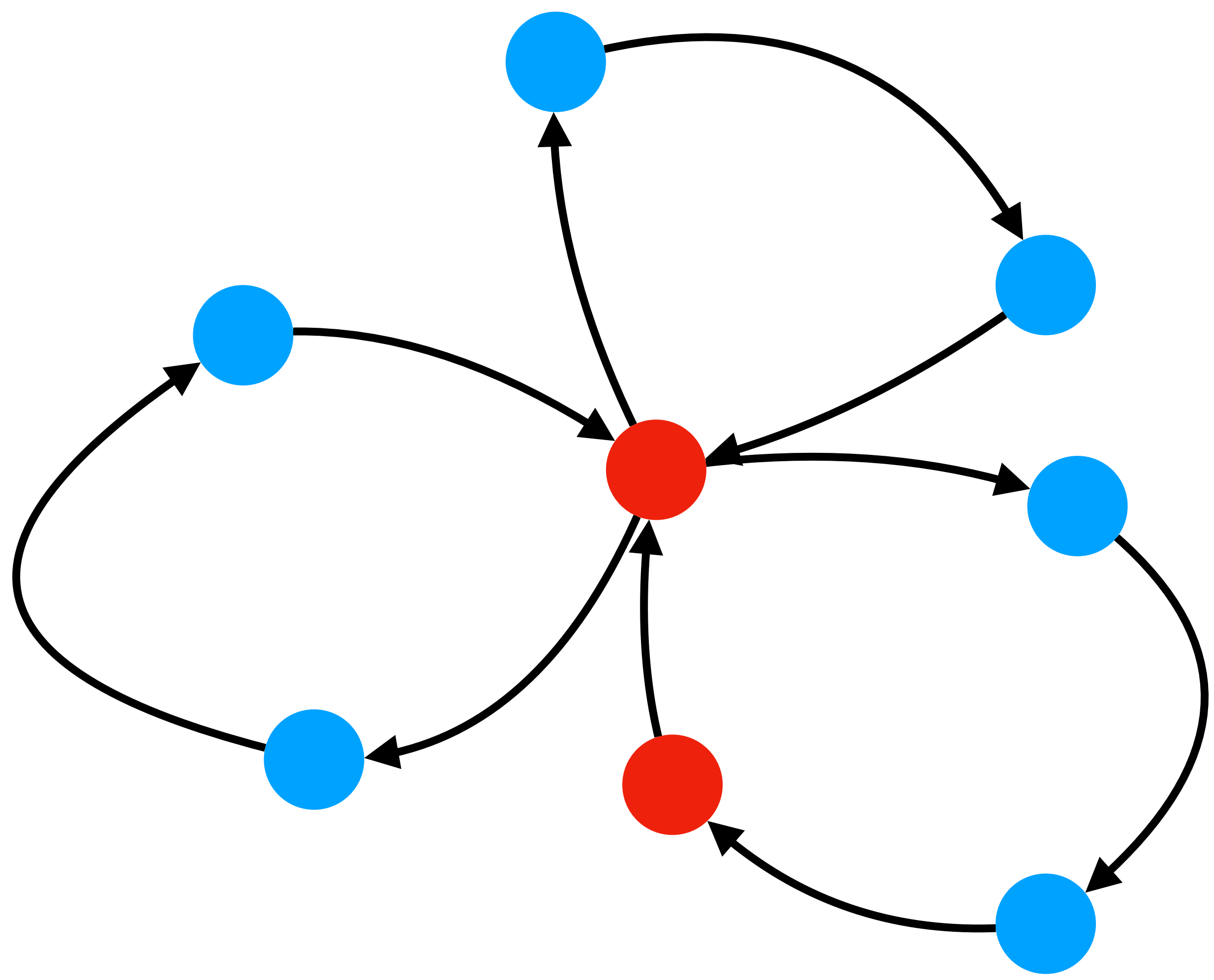

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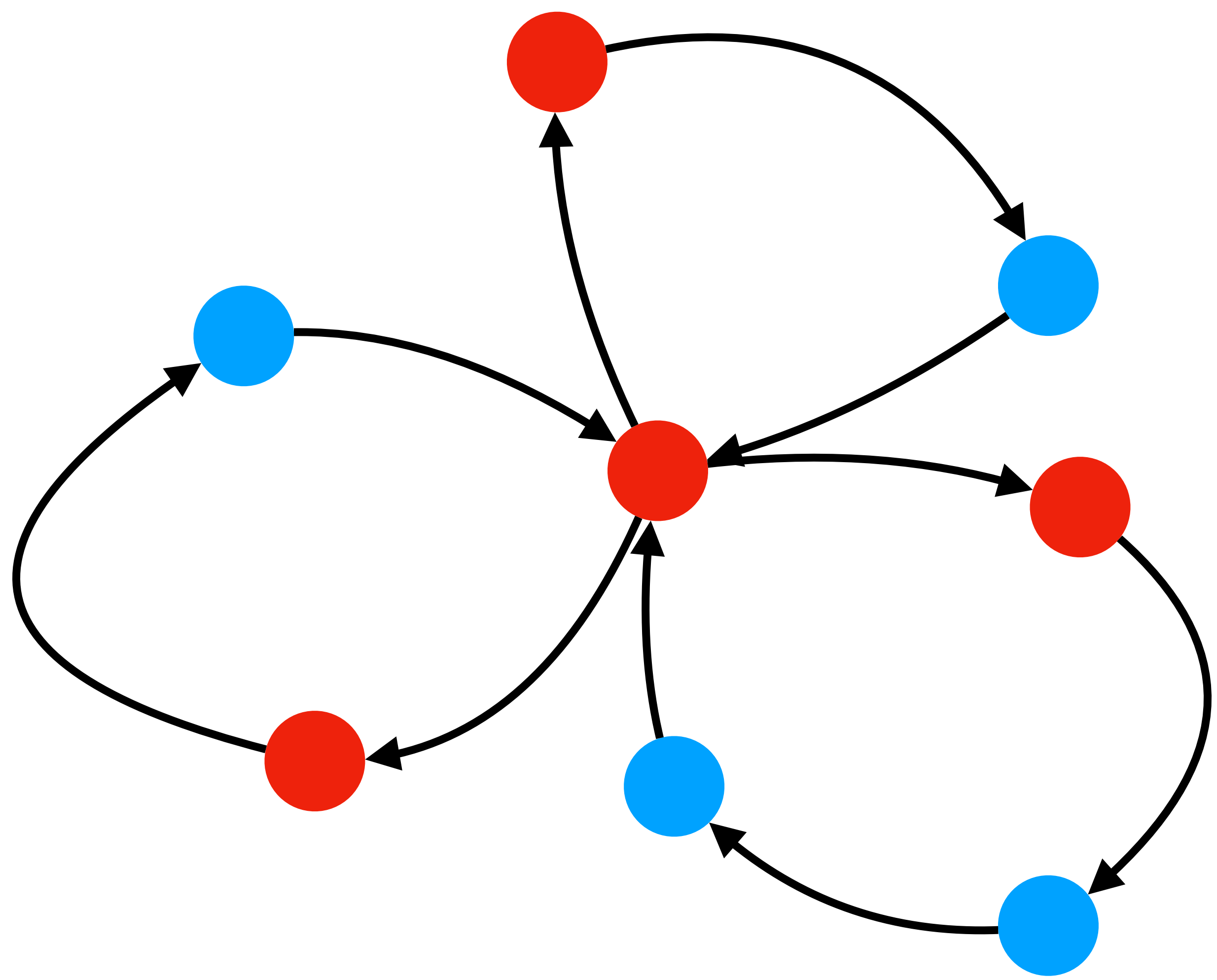

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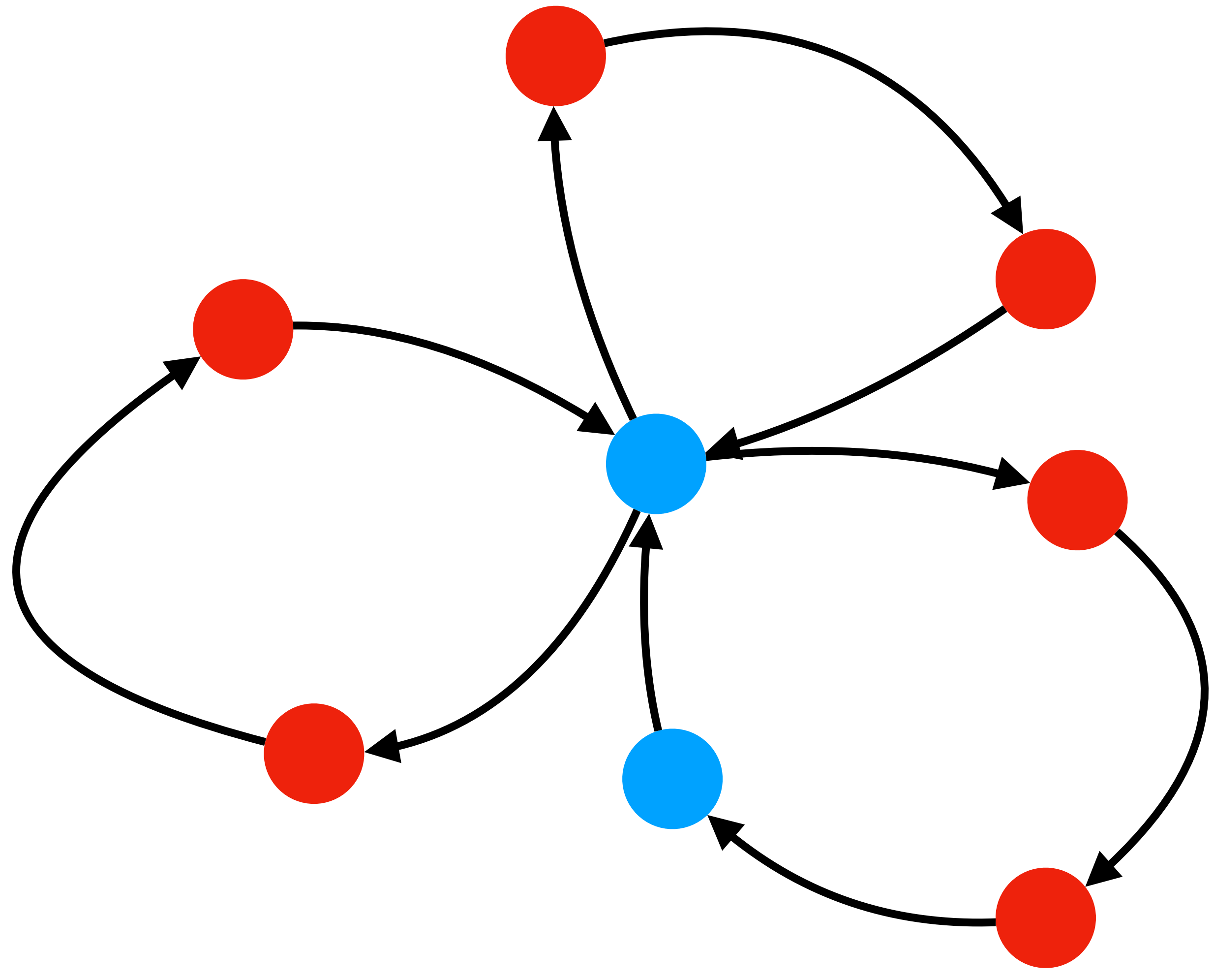

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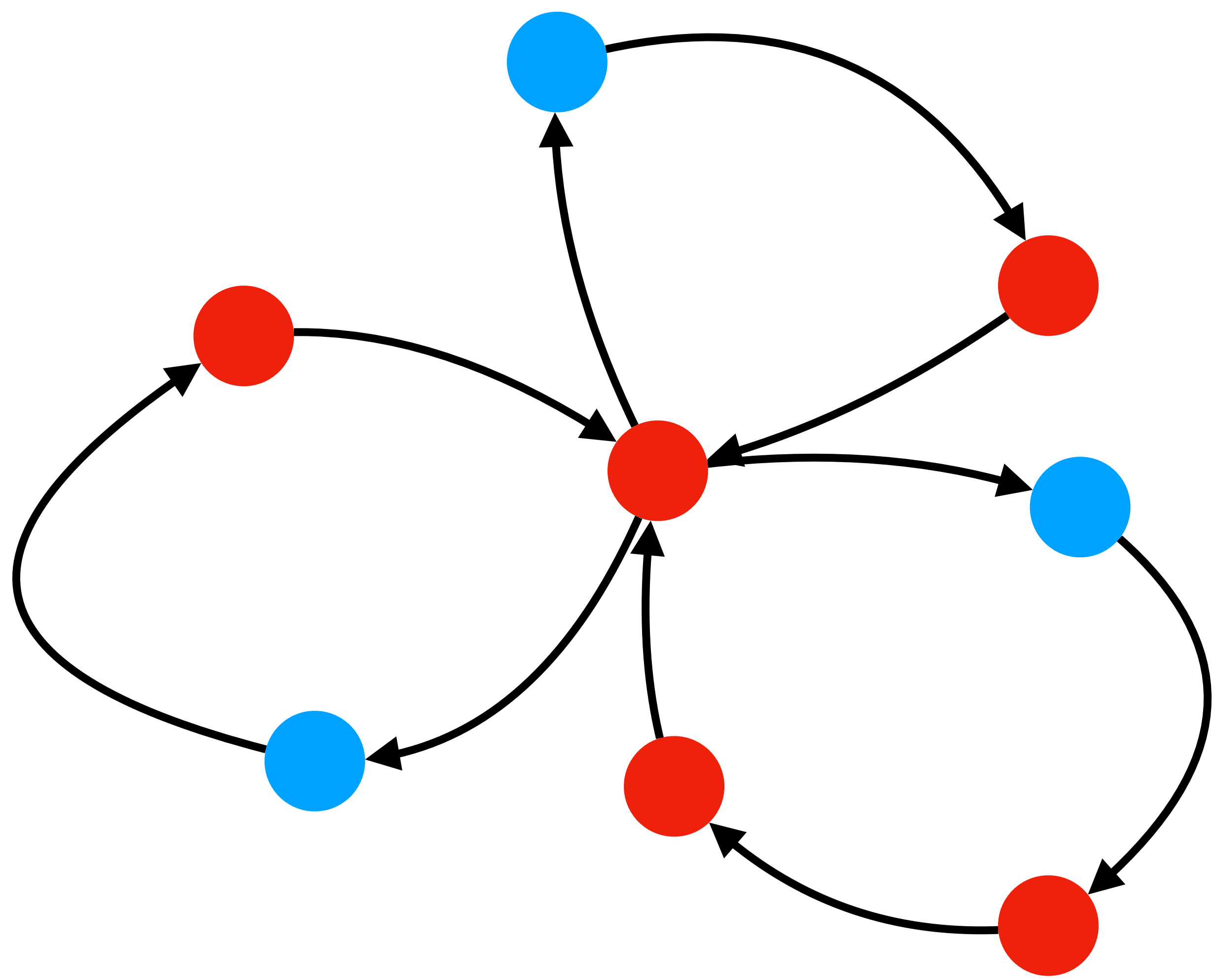

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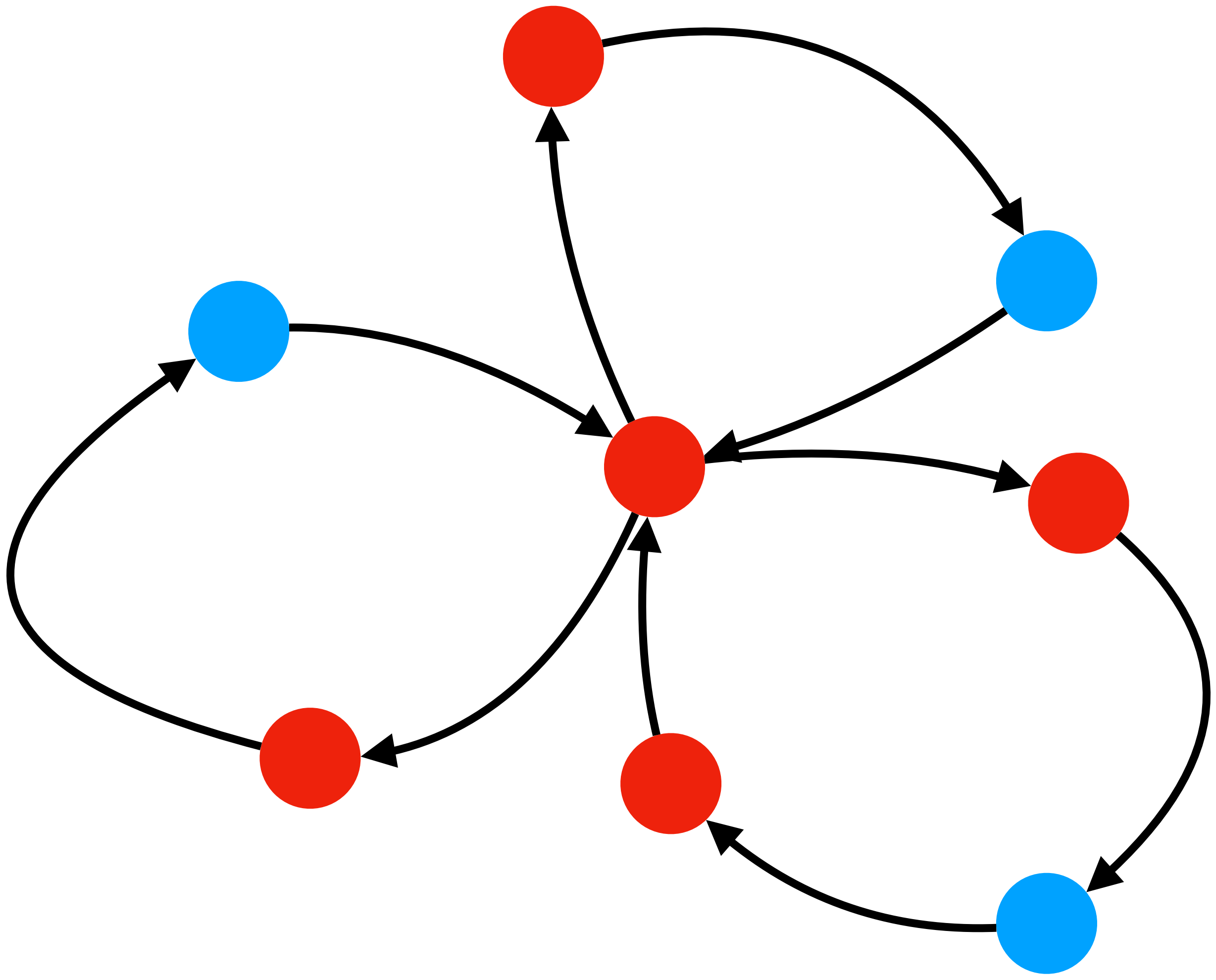

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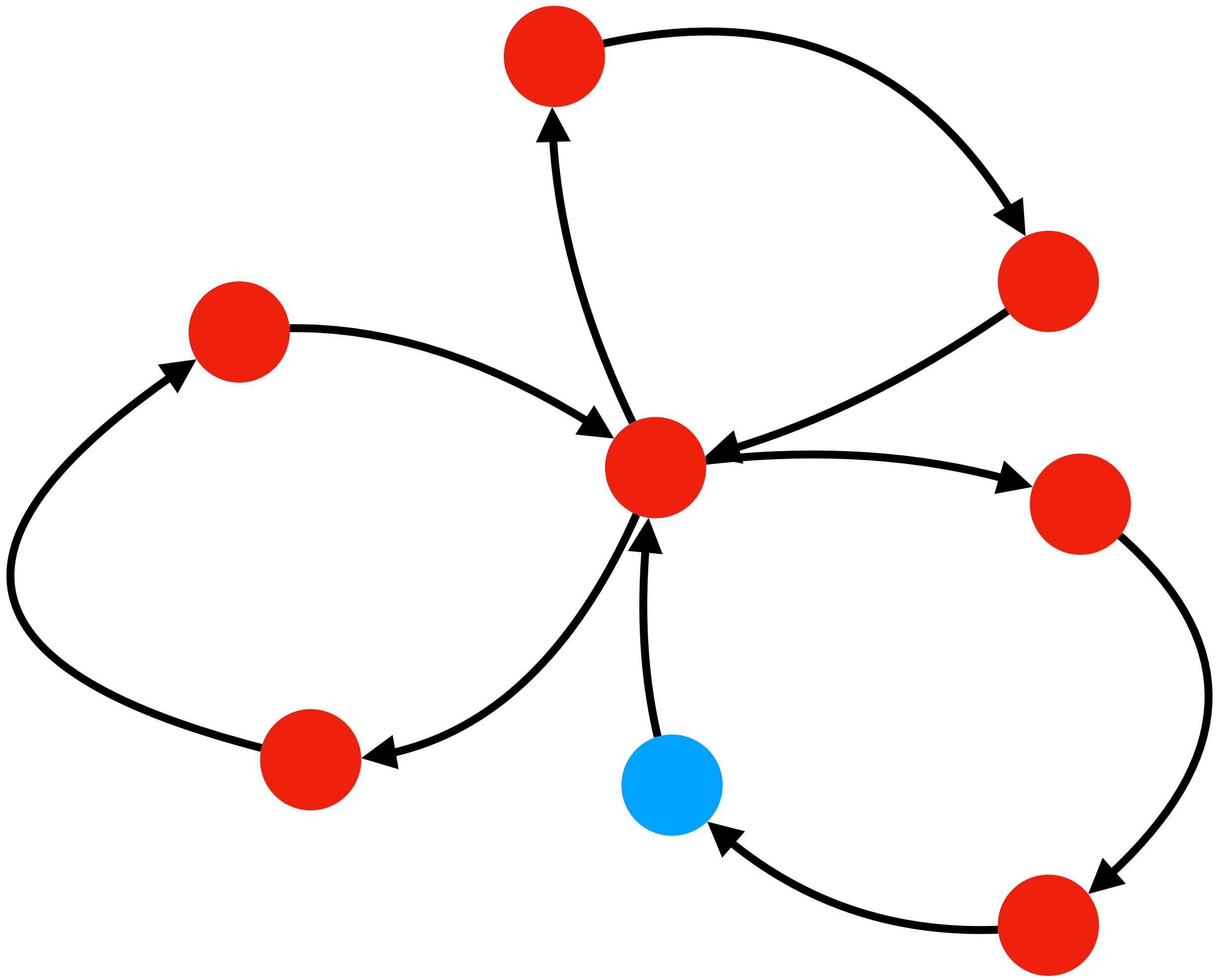

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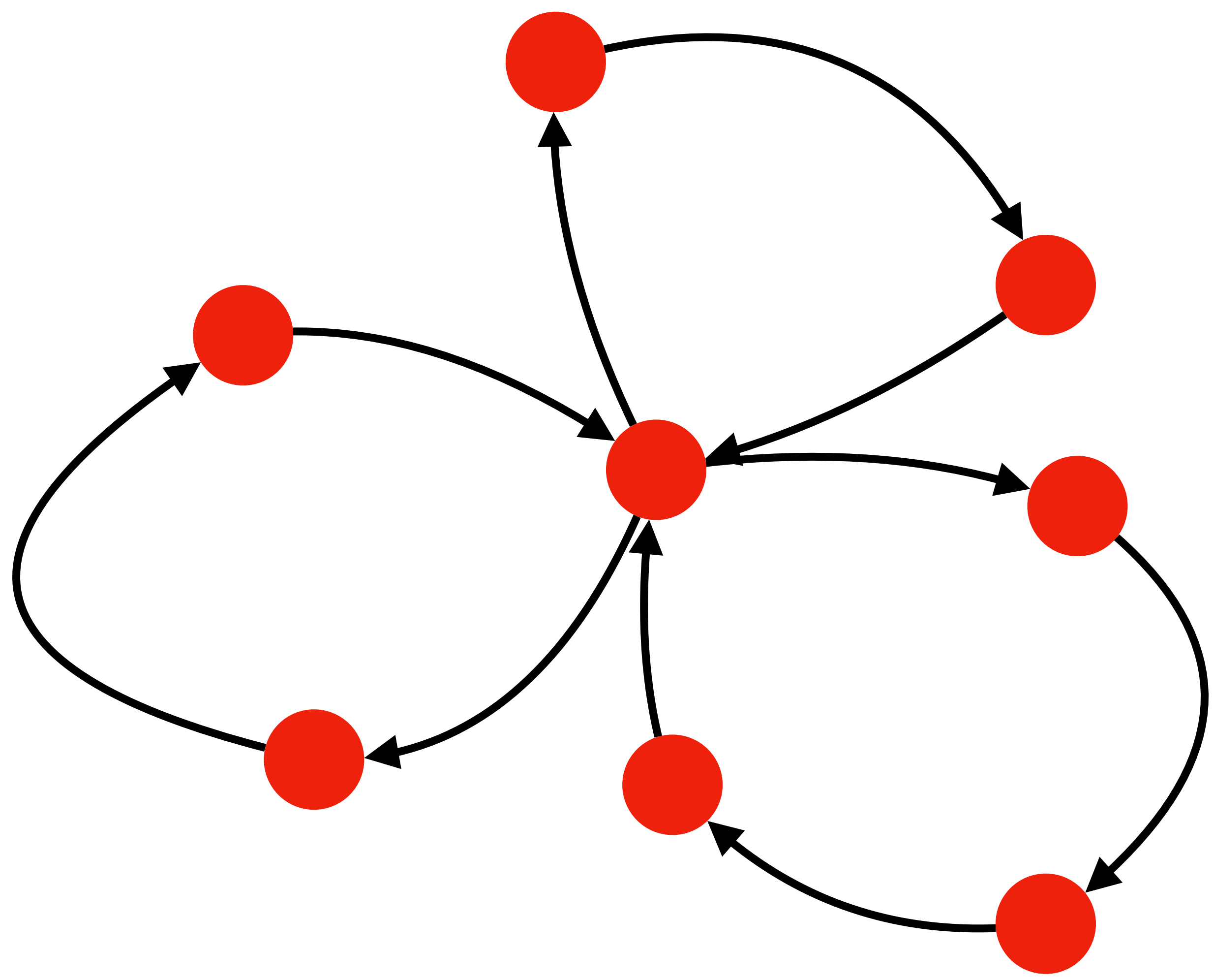
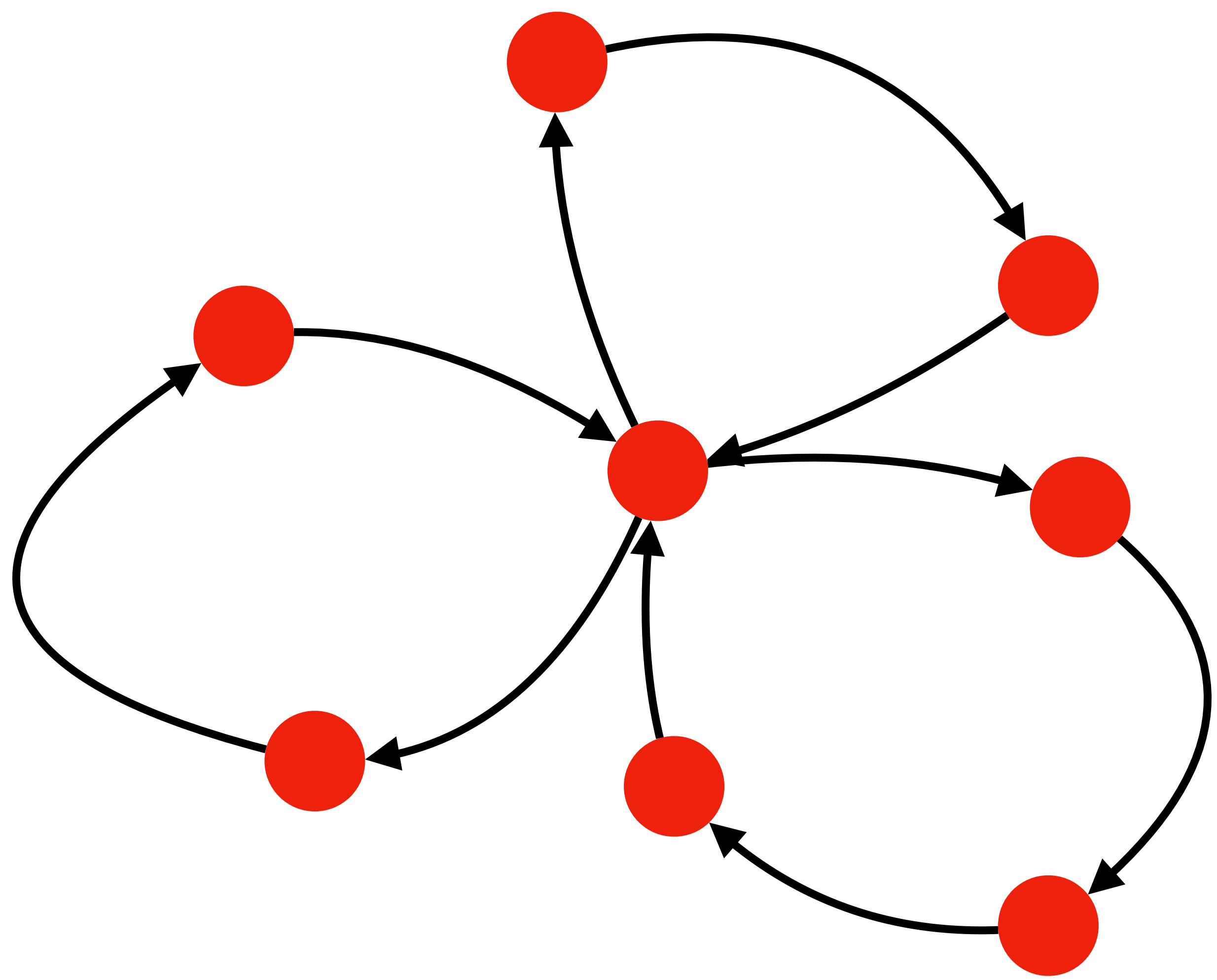


Theorem in action



All reactions enabled every 1 = gcd(3, 4) step! Saturation!

🌼 Theorem in action

- When all reactions are always enabled
  the products are always the same: $T = \bigcup\{P_a : a \in A\}$

- Thus the RS enters a nonempty fixed point: $res_{\mathcal{A}}(T) = T$

- The second fixed point is by definition the empty state $\varnothing$

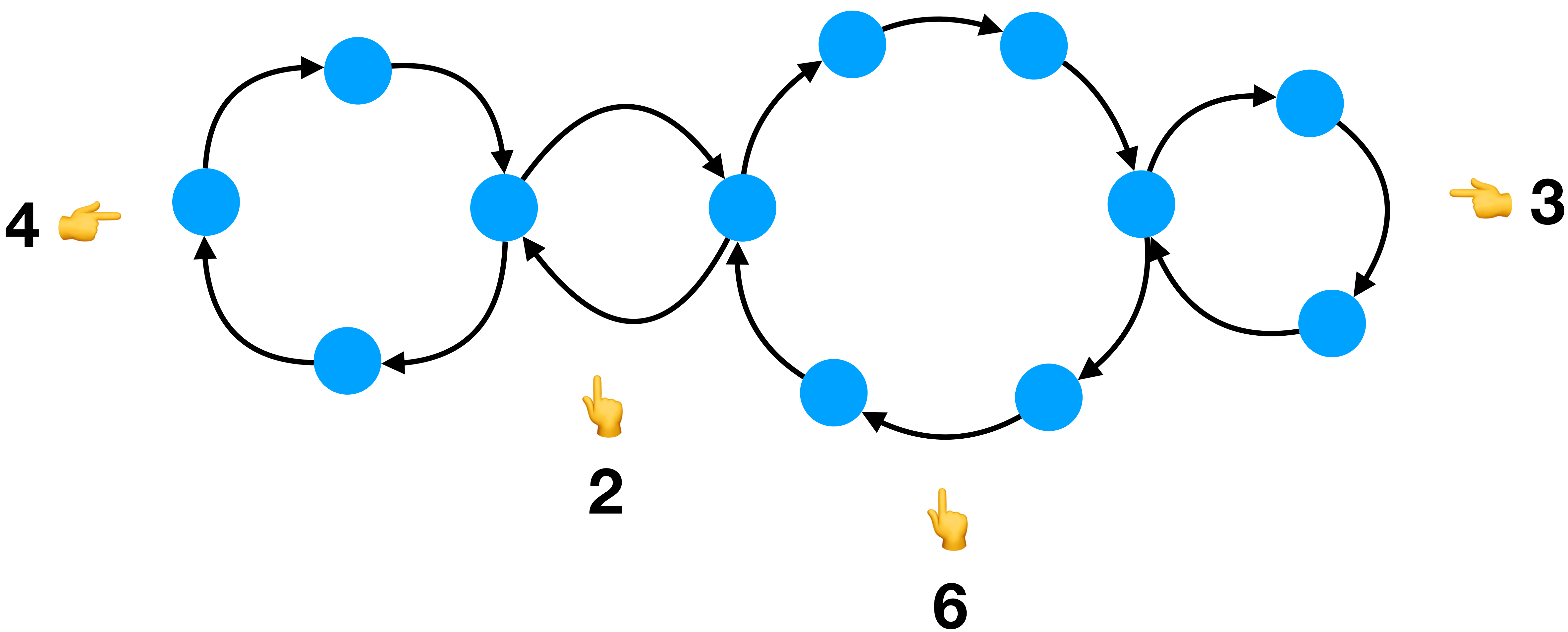
Chain-shaped dependencies

⛓️ Theorem

IF the dependency graph of a RS consists only of a chain of self-sustaining, non-self-inhibiting cycles containing two cycles of coprime lengths,

THEN the RS has exactly two fixed points

⛓️ Theorem in action



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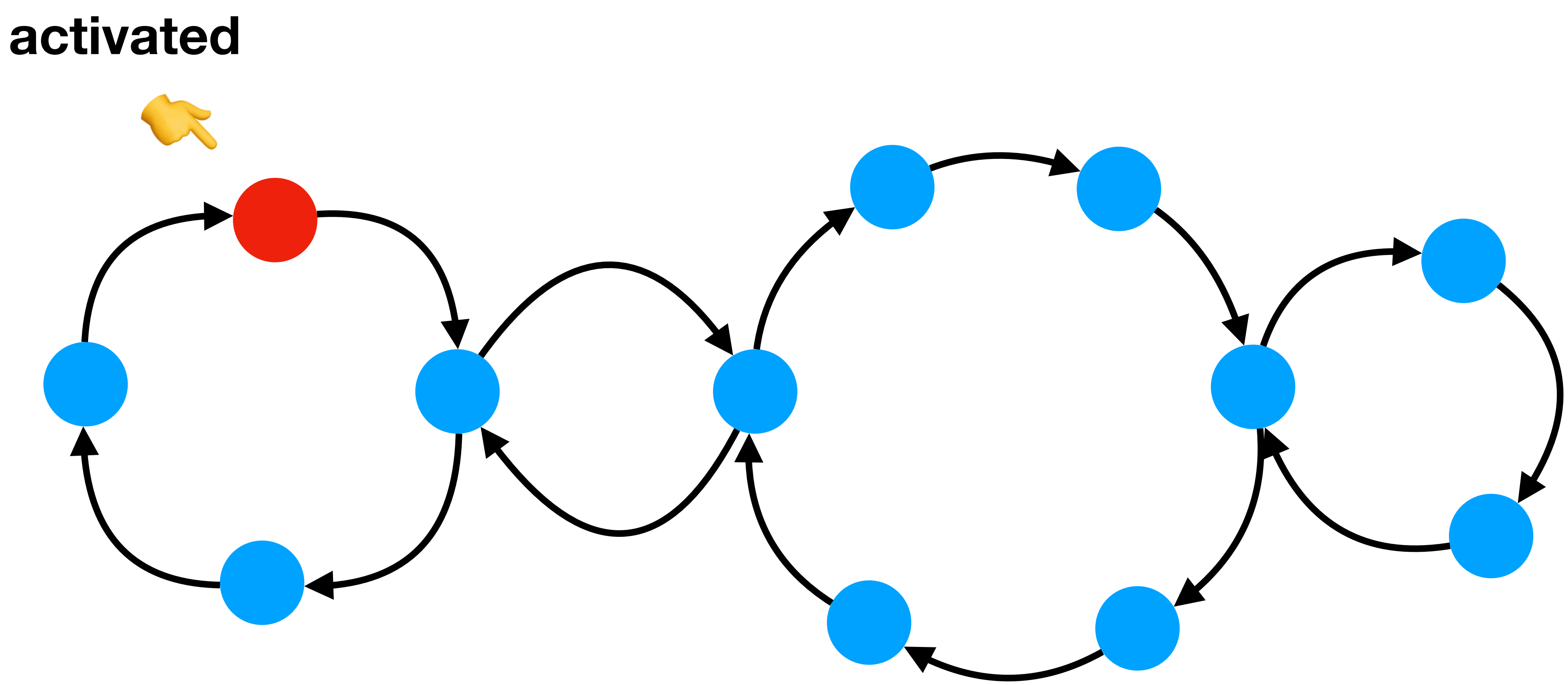

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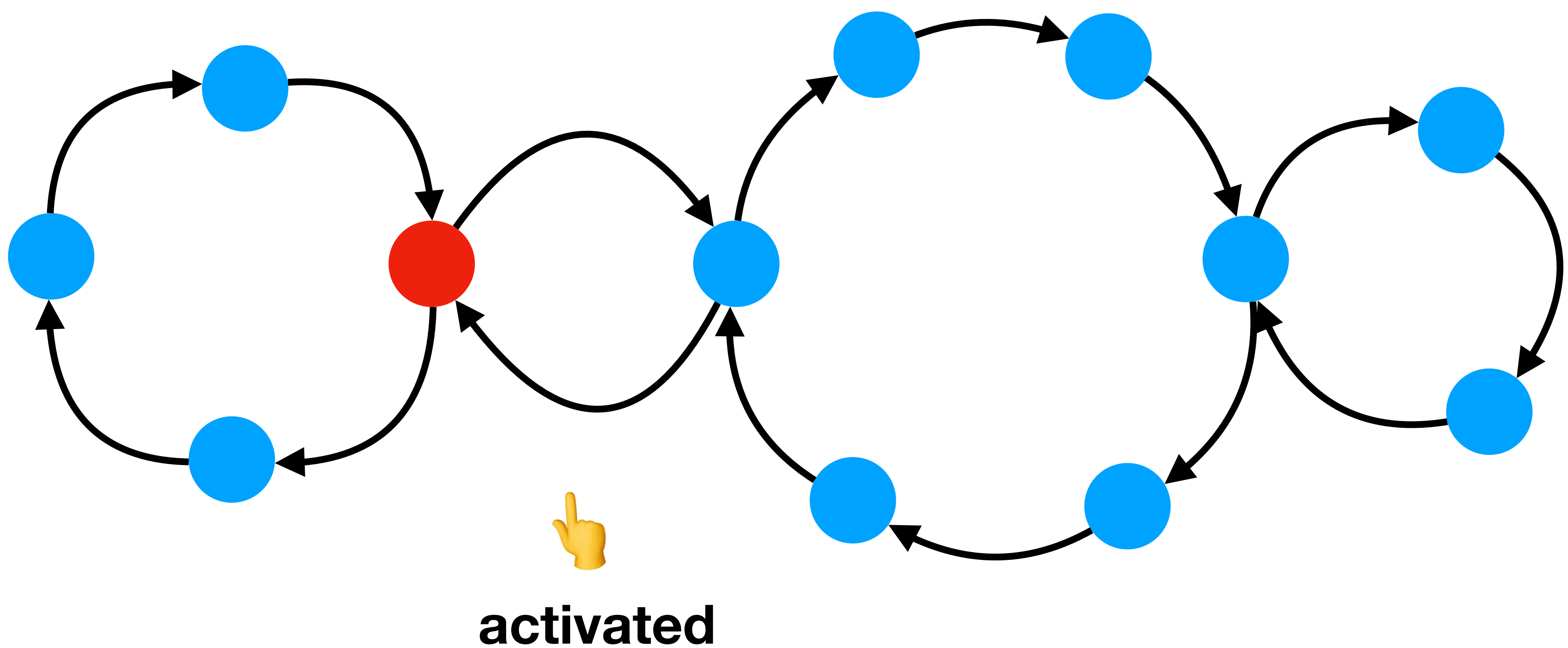

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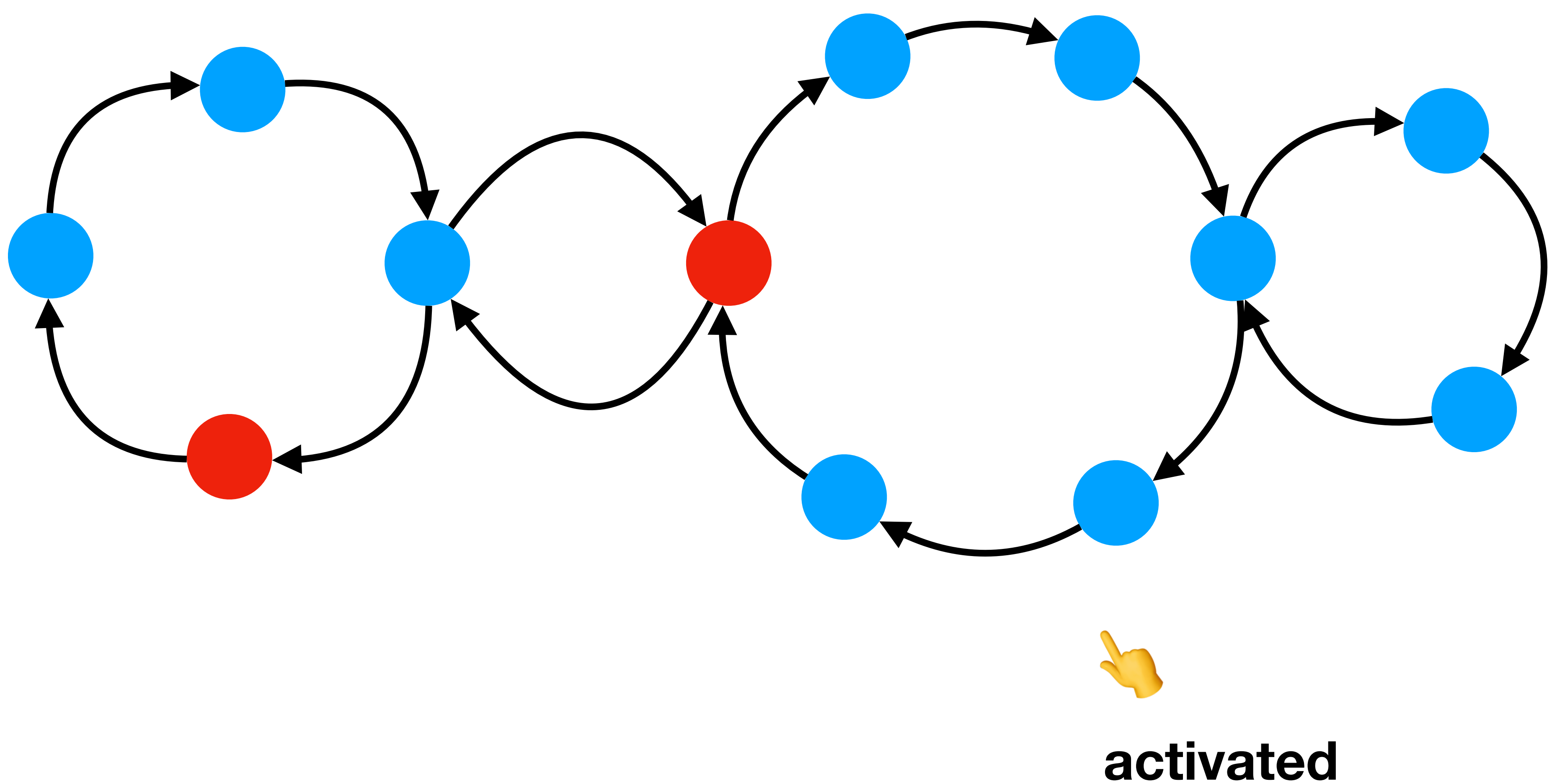

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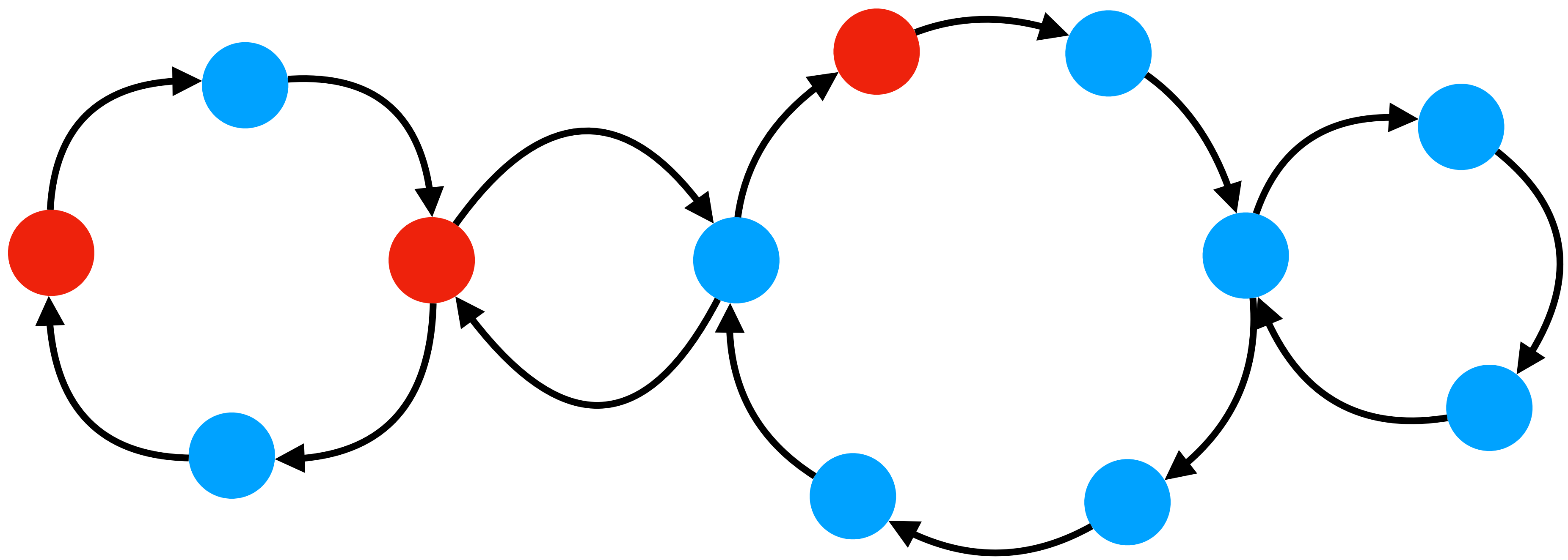

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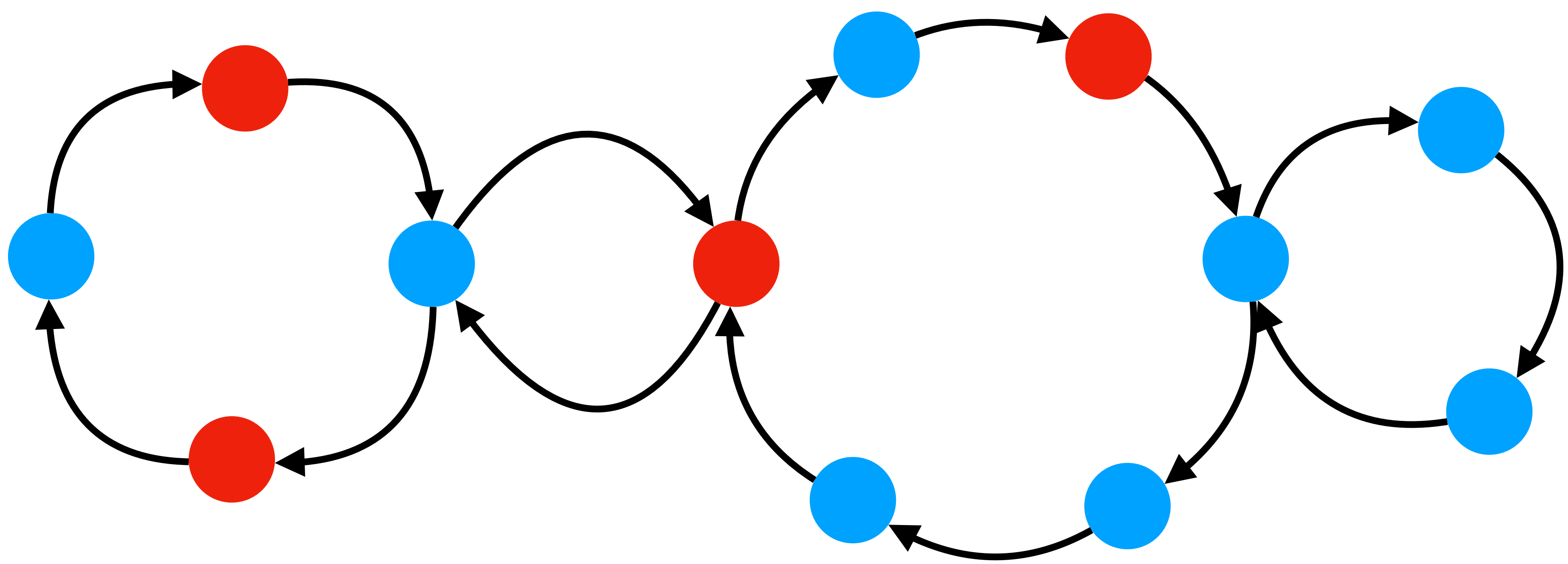

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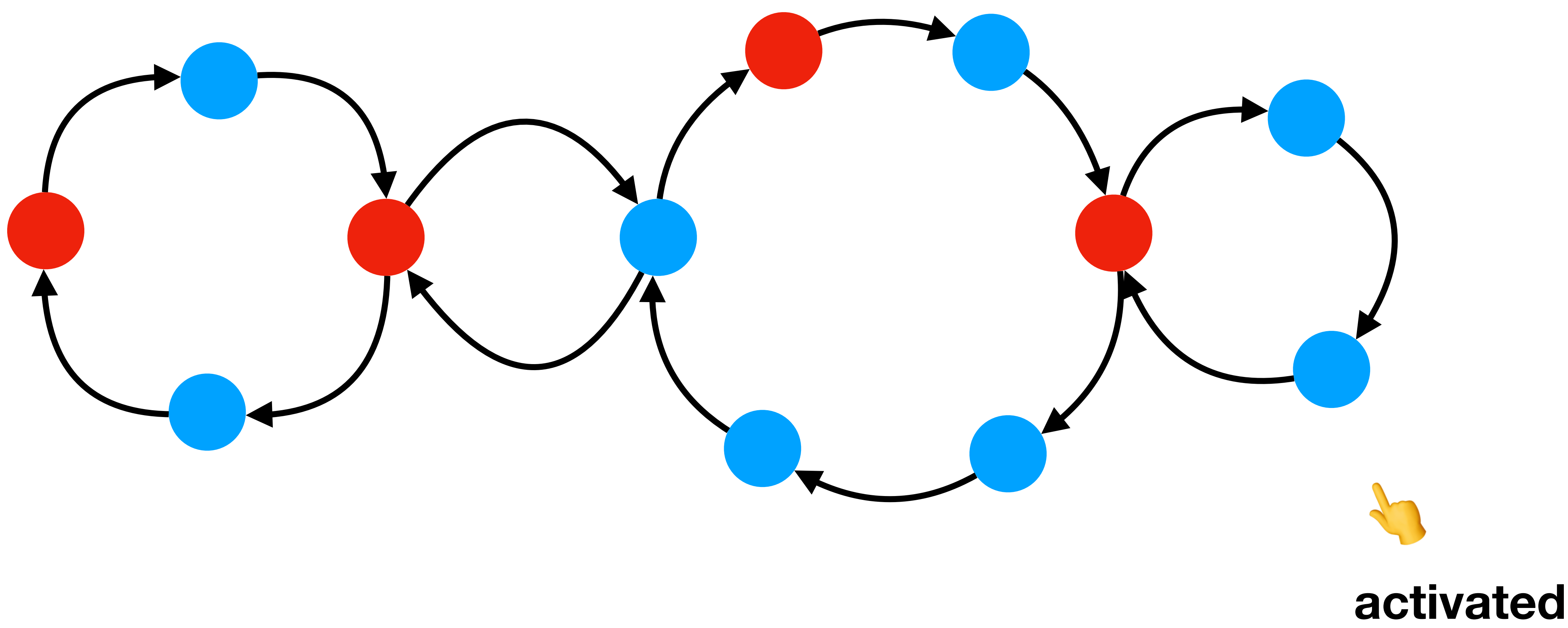

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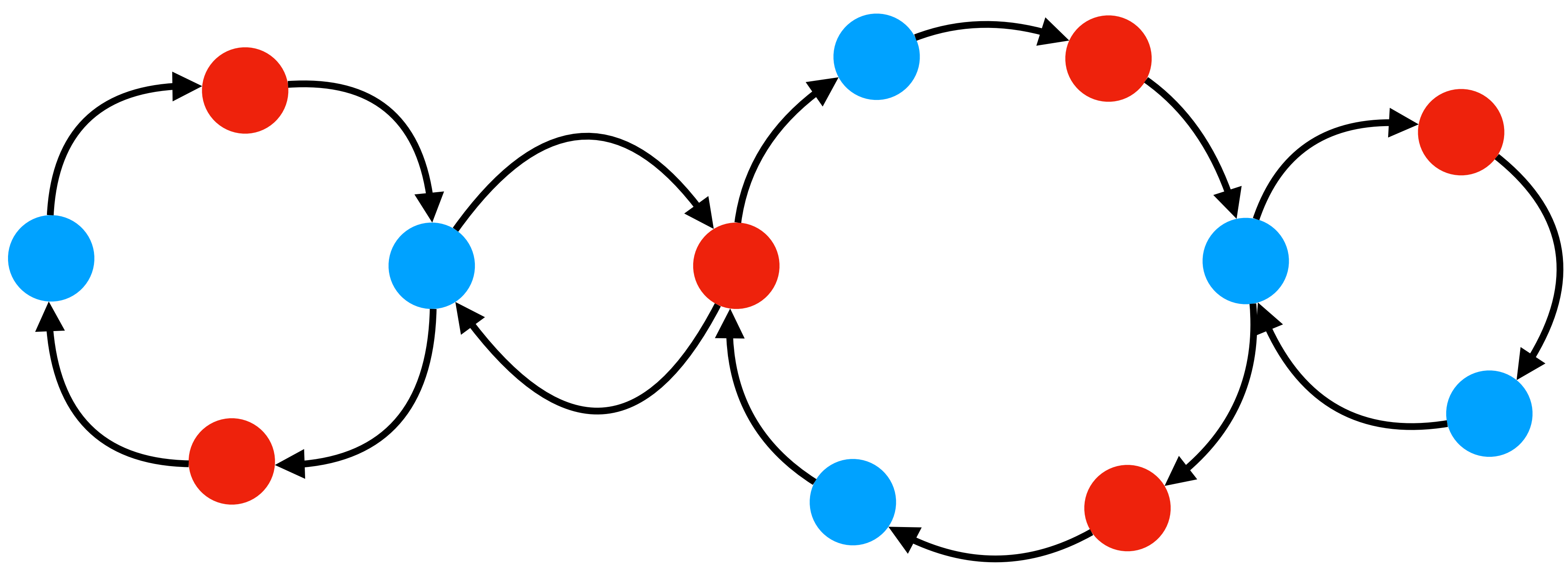

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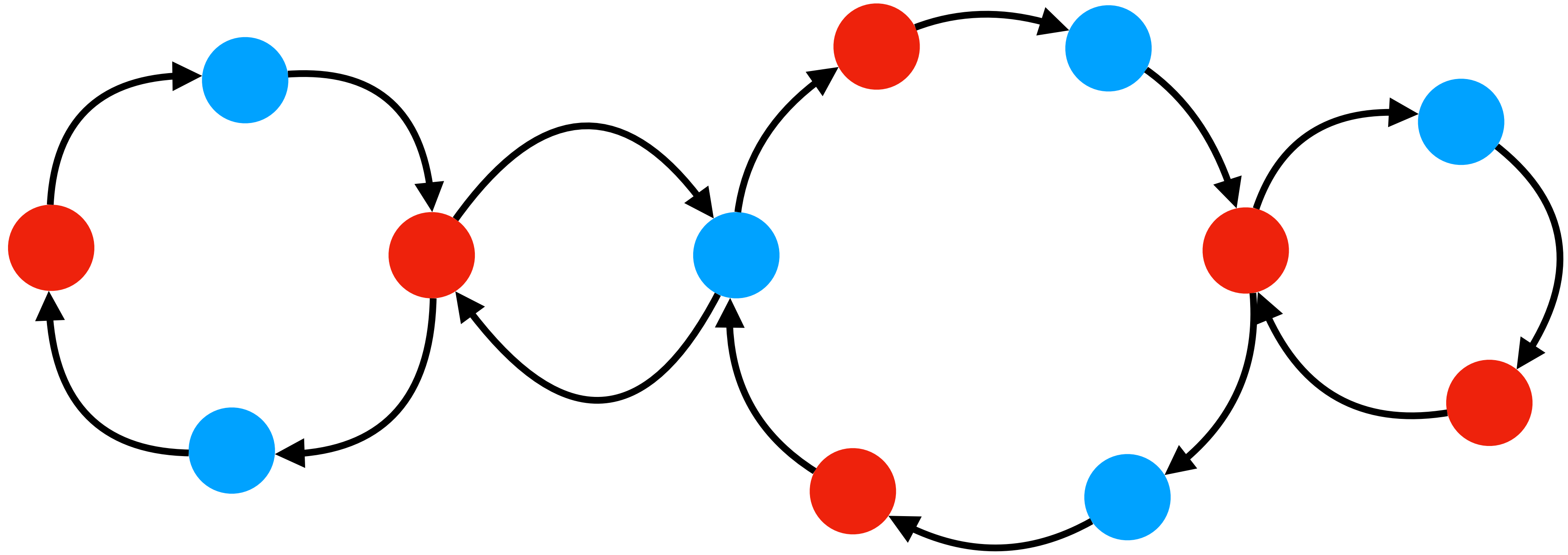

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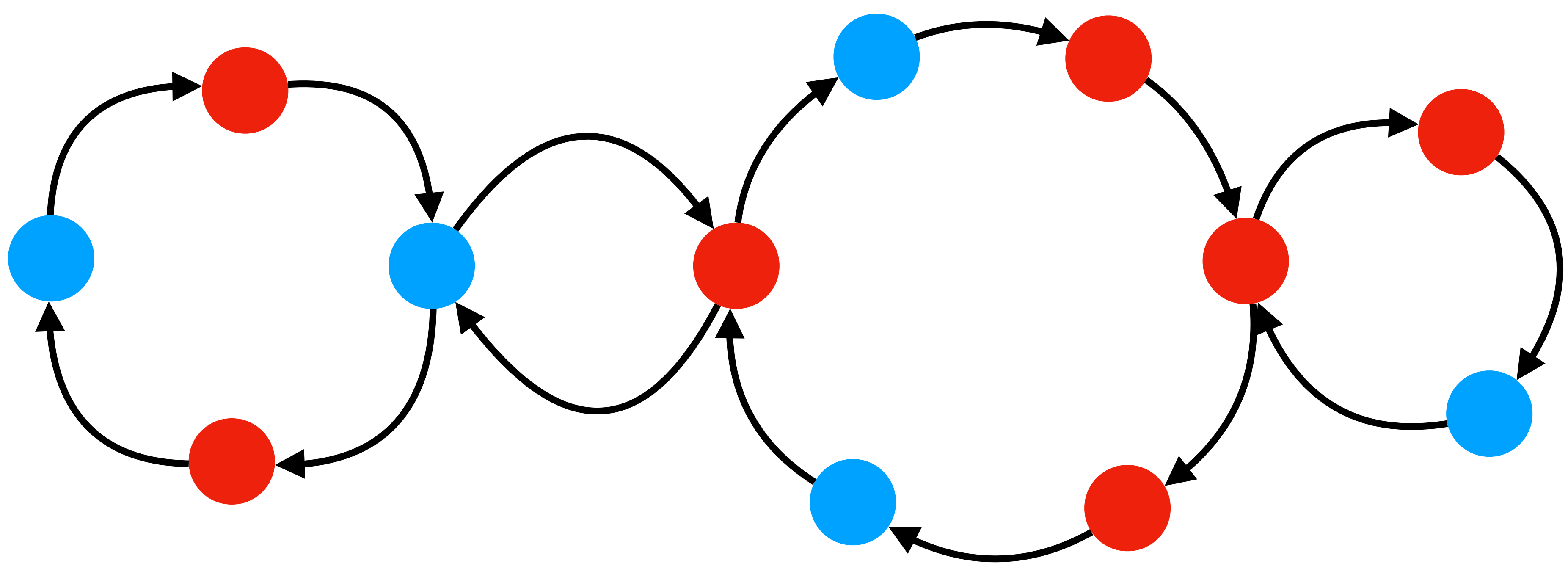

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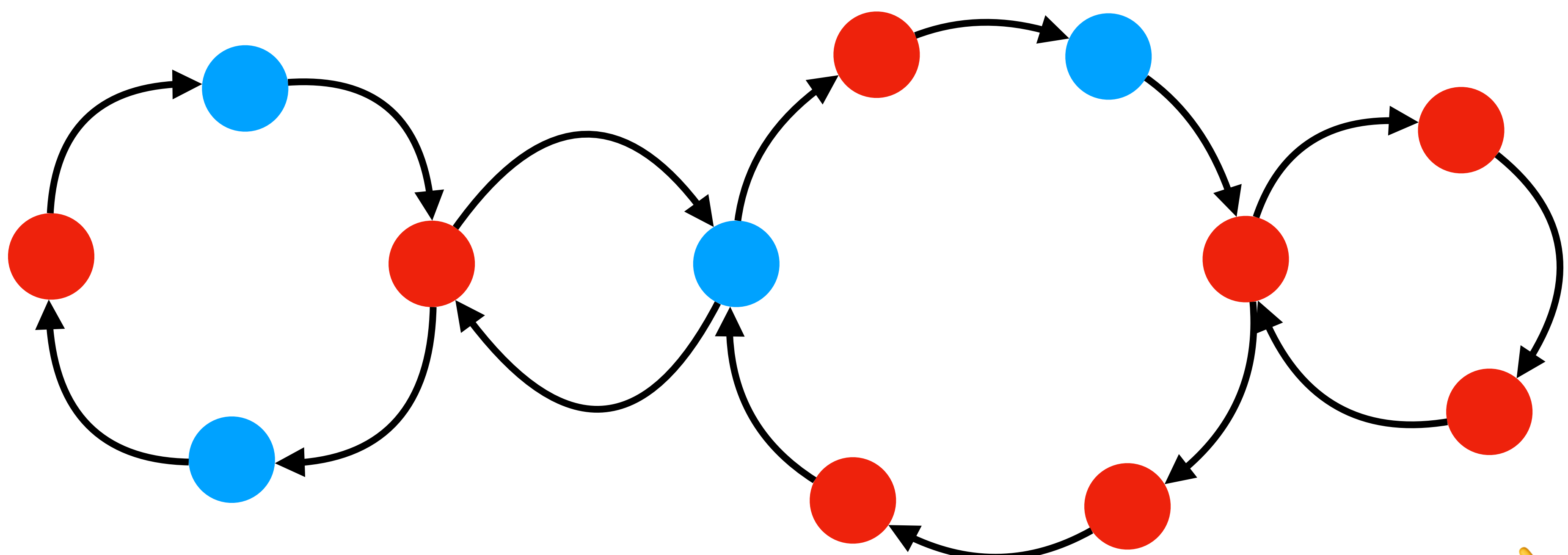

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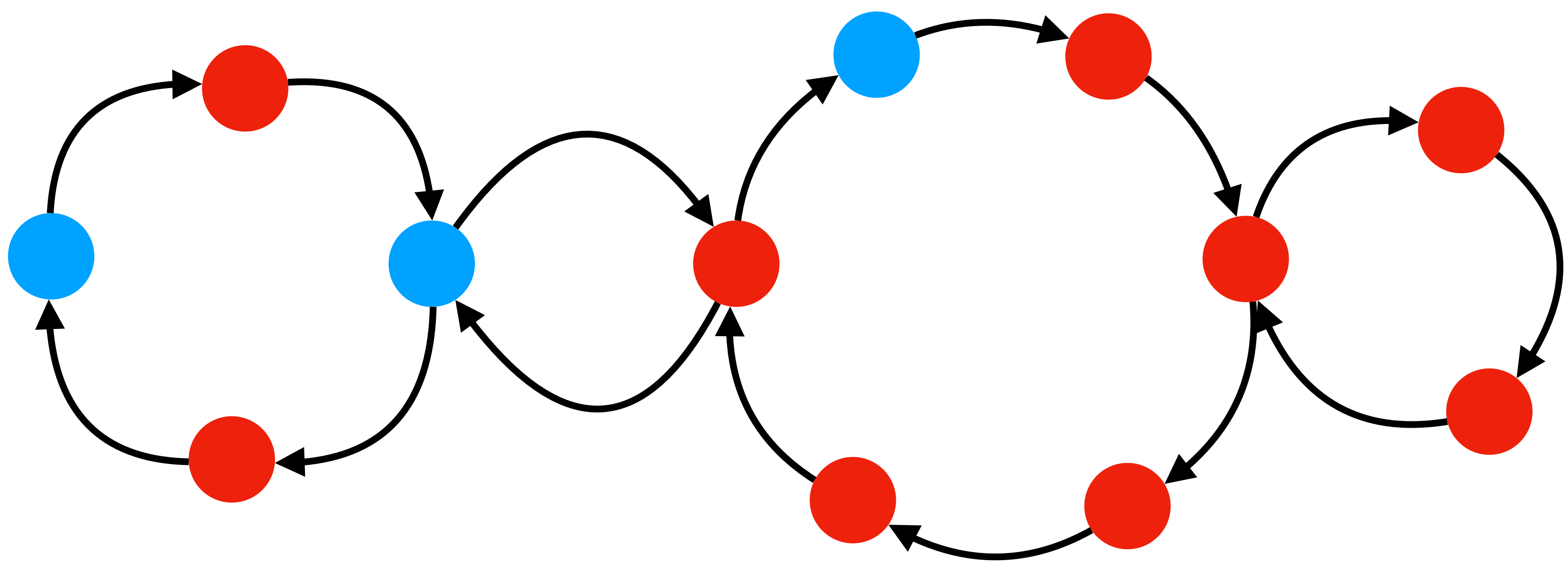
saturated

⛓ Theorem in action



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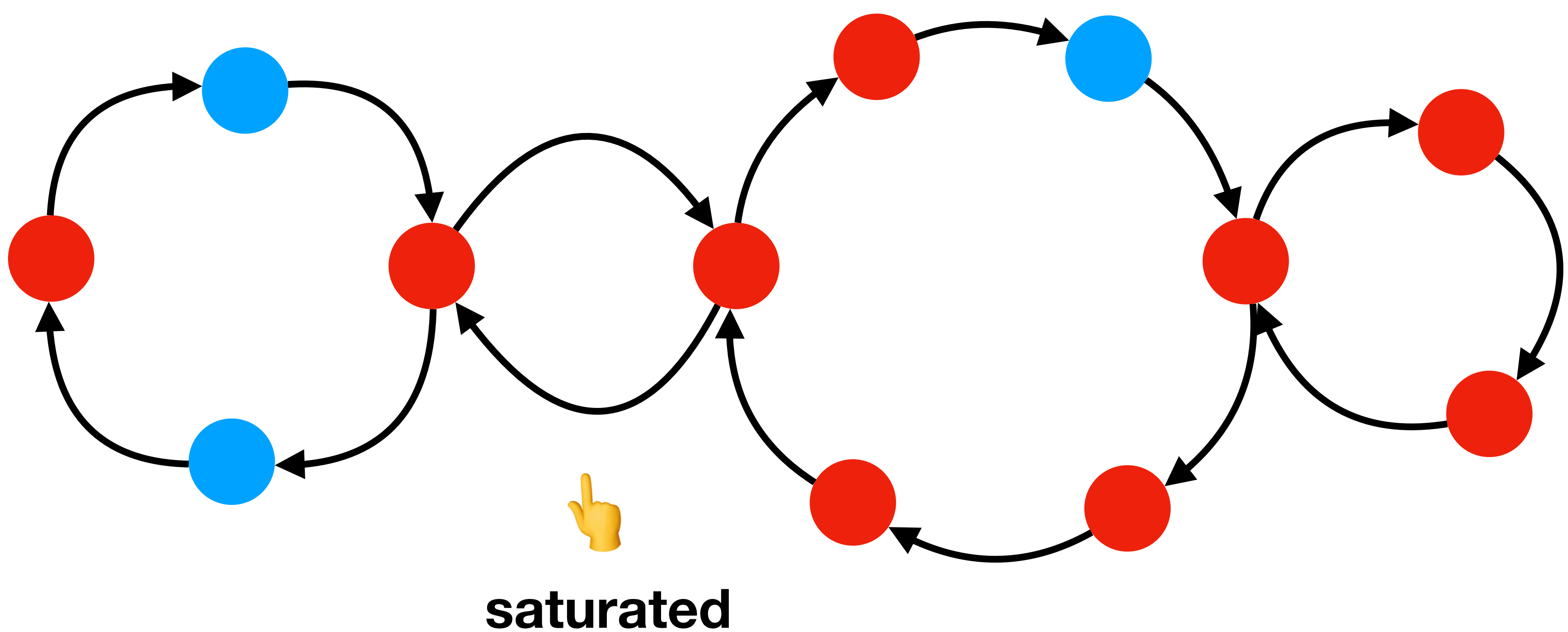
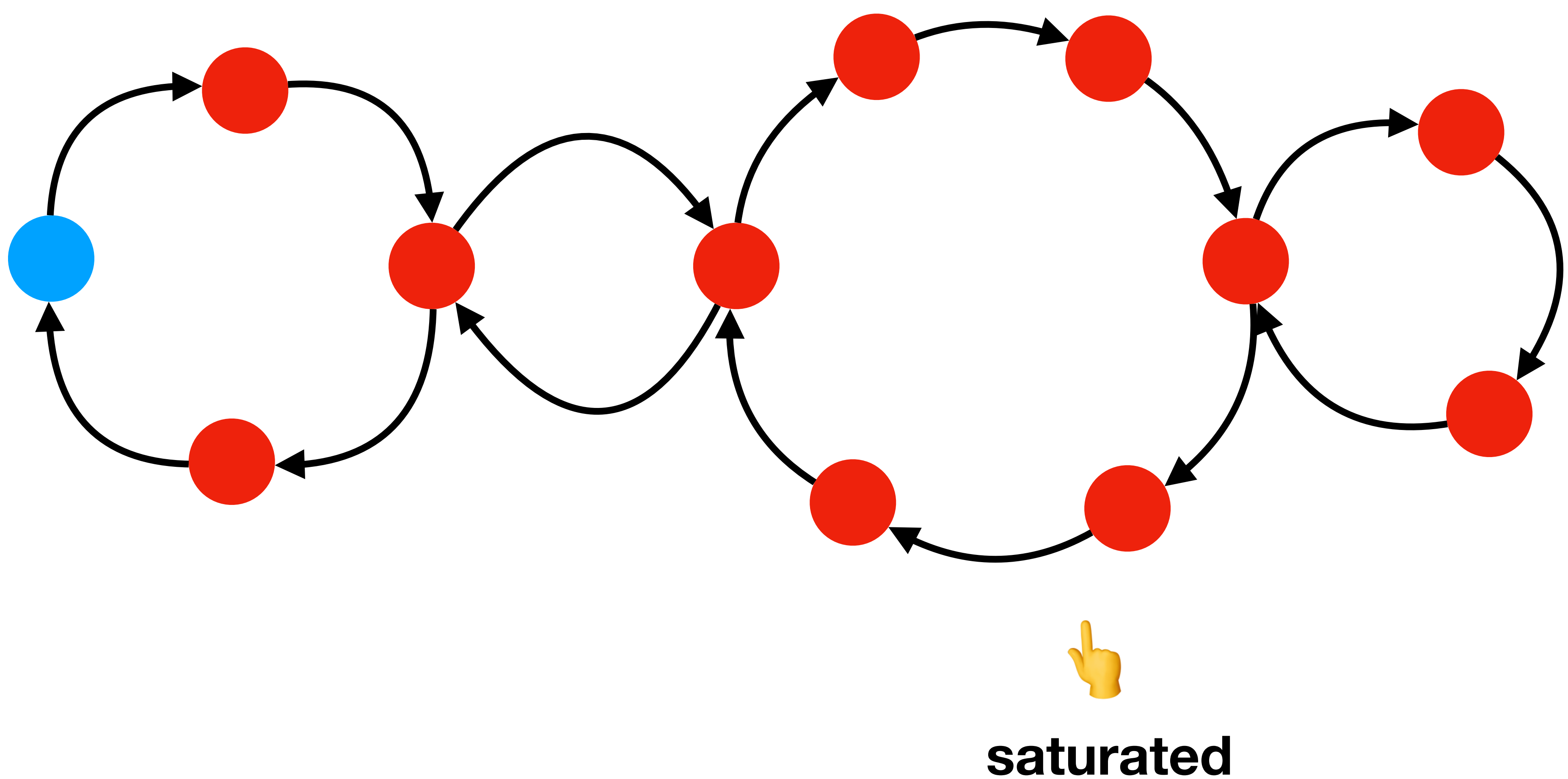


Theorem in action



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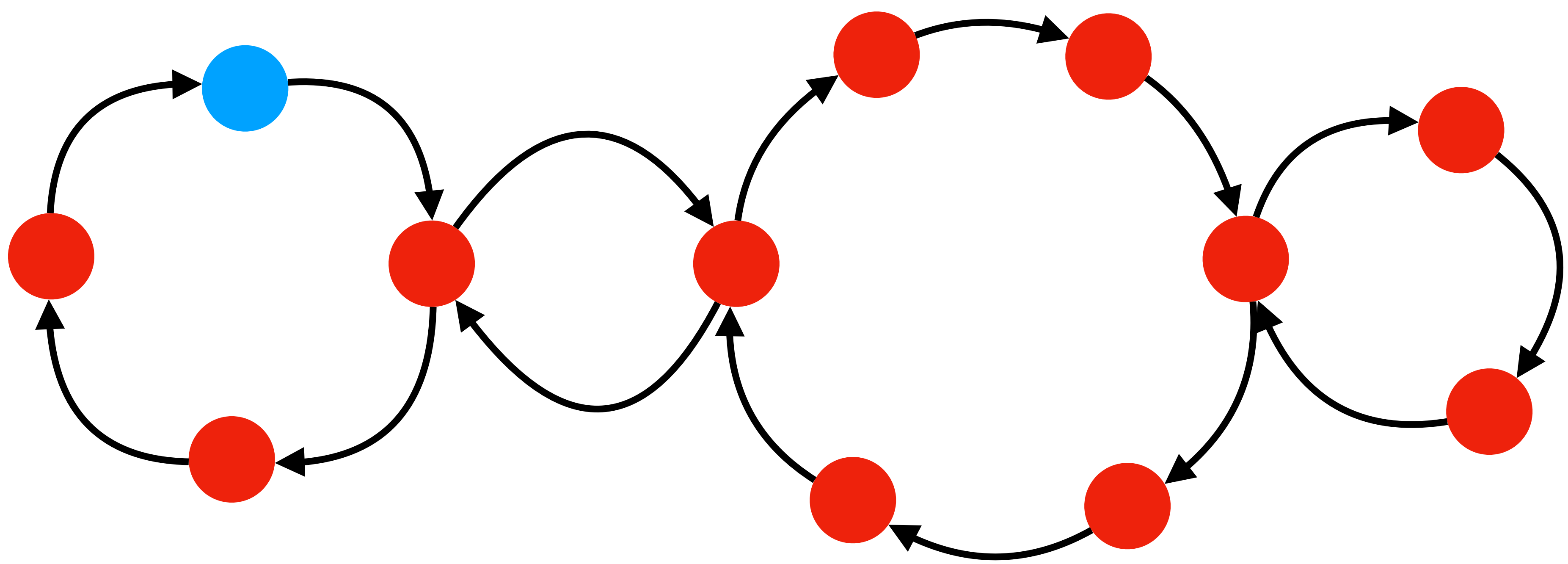

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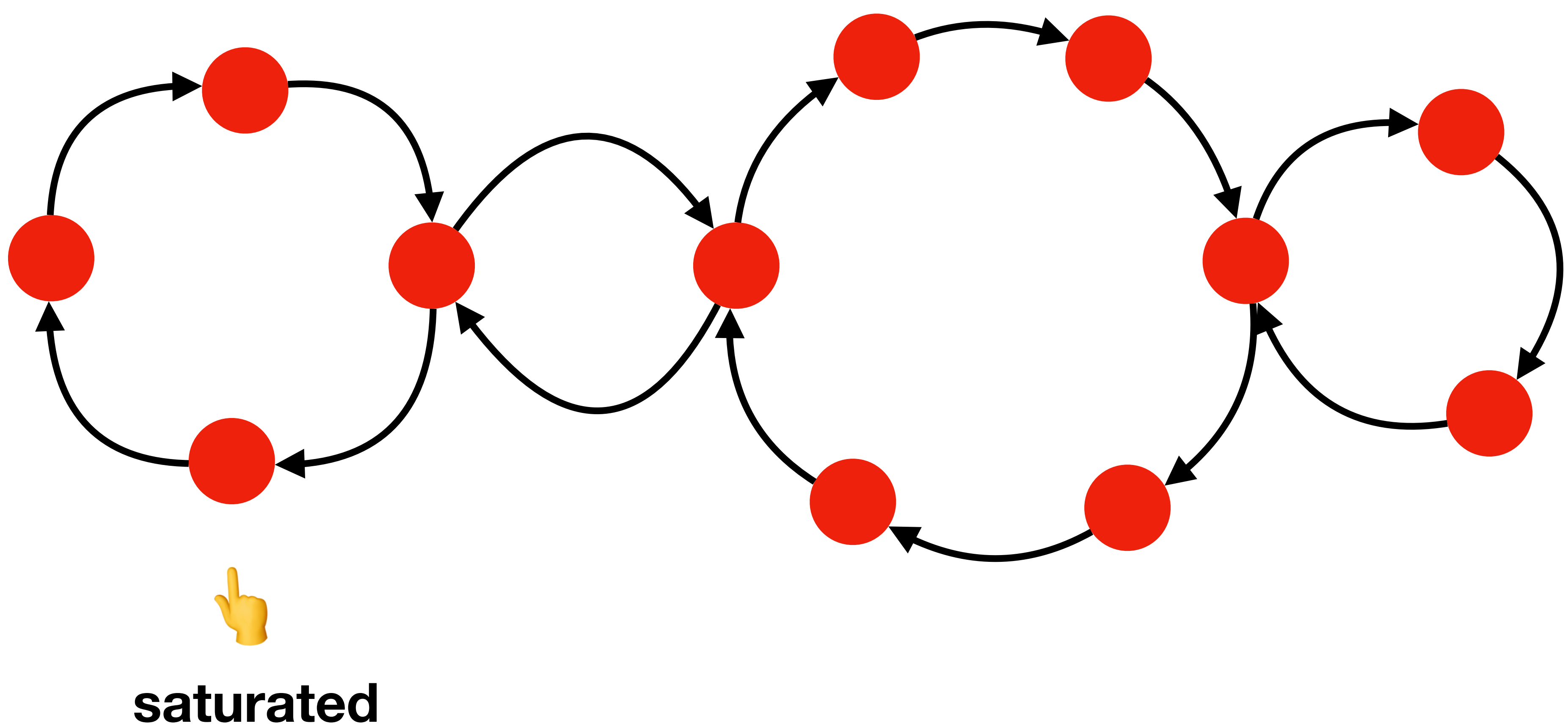

Conclusions

Summary

Behaviour of RS having a dependency graph consisting of self-sustaining, non-self-inhibiting cycles:

- With a single cycle of length n,
  the dynamics of the RS contains only cycles
  of length dividing n

- With a chain or flower with two cycles of coprime length,
  the RS has exactly two fixed points

Future work

- Does restricting the dependency graphs to cycles, chains and flowers reduce the complexity of decision problems related to the dynamics? (e.g., fixed points, reachability)
- Investigate the relationship with Boolean automata networks and their interaction graphs
- Investigate more sophisticated dependency graphs (e.g., pre-periods, multiple intersections between cycles)

Dziękuje za uwagę! 😊

Thanks for your attention!