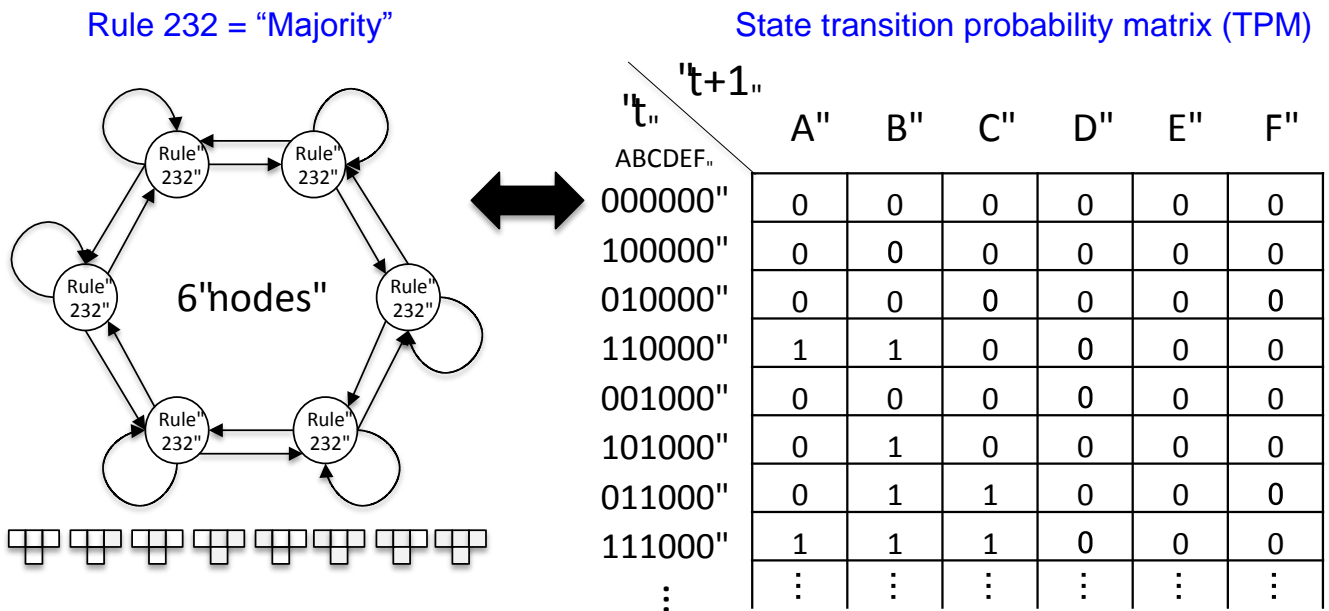


## Supplementary Methods

In the following, we explain how cause and effect repertoires are calculated from the transition probability matrix (TPM). For further information, see Text S2 in [1] and the glossary in [2].

### 1. Transition Probability Matrix (TPM)

The transition probability matrix of a system of  $N$  elements is obtained by perturbing the system  $S$  into all  $2^N$  possible states  $s_t$  and observing the probability distribution of resulting system states  $s_{t+1}$ . It thus describes all possible state transitions of the system and their probabilities assuming each state  $s_t$  with equal probability. Since the ECA considered in this article are deterministic, there is only one possible future state  $s_{t+1}$  for each state  $s_t$ . ECA cells are binary elements and conditionally independent. For these reasons, we can write the TPM in the state  $x$  element format (Figure 1), a compressed version of the typical state  $x$  state format. In the state  $x$  element TPM, each entry specifies the probability of the respective element (A-F, columns) to be in state “1” at time  $t + 1$  following a perturbation into the indicated state (rows) at time  $t$ . While for deterministic ECA all entries in the TPM are either 0 or 1, in binary probabilistic systems any number from 0 to 1 is possible.



**Figure 1.** An  $N = 6$  ECA, implementing rule 232, the majority rule, and its TPM in state  $x$  element format. TPM entries indicate  $p(\text{element}) = 1$ , the probability to be in state “1”.

Conditional independence is a requirement in the IIT formalism, excluding instantaneous causation. Considering the two elements A and B in the system A-F and their respective inputs (Figure 1 and Figure 9 in the main text), for example, conditional independence can be expressed mathematically as:

$$p(AB_{t+1}|ABCF_t) = p(A_{t+1}|ABF_t) \times p(B_{t+1}|ABC_t). \quad (S1)$$

In words, given their inputs at  $t$ , the probability distributions of the states of A and B at time  $t + 1$  can be determined independently.

## 2. Cause Repertoire

The cause repertoire of a mechanism  $M_t$  in its current state  $m_t$  can be obtained from the TPM using Bayes' rule. This is demonstrated below, for the example mechanism  $A_t = 1$ , in the ECA system A-F<sub>t</sub> = 111000 implementing rule 232 (Figure 9 in the main text).  $A_t$  can only possibly constrain its inputs  $ABF_{t-1}$ , but not the other elements in the system. Thus, we consider the cause repertoire  $p_{cause}(ABF_{t-1}|A_t = 1)$ , the distribution of possible past states of  $ABF_{t-1}$  conditioned on  $A_t = 1$ . Using Bayes' rule:

$$p_{cause}(ABF_{t-1}|A_t = 1) = \frac{p(A_t = 1|ABF_{t-1}) \cdot p_{uc}(ABF_{t-1})}{p(A_t = 1)} \quad (S2)$$

Here,  $p(A_t = 1|ABF_{t-1})$  corresponds to A's column in the TPM (Figure 1), averaged across all elements not in the set of elements ABF, with  $p(A_t = 1|ABF_{t-1}) = 0$  for  $ABF_{t-1} = \{000, 100, 010, 001\}$  and  $p(A_t = 1|ABF_{t-1}) = 1$  for  $ABF_{t-1} = \{110, 101, 011, 111\}$ . This distribution is scaled by  $p_{uc}(ABF_{t-1})$ , which here is 1/8 for each past state, the uniform distribution over ABF, since the elements are perturbed into all states with equal probability; and  $p(A_t = 1) = 0.5$ , since A implements the Majority function which results in state "1" for half of its 8 possible input states, again applied with equal probability. Altogether, this results in the cause repertoire  $p_{cause}(ABF_{t-1}|A_t = 1)$  shown in Figure 9B of main text. Note that Equation (S2) is only defined for "possible" states of sets of elements with  $p(M_t = m_t) > 0$ , meaning states that can be reached at  $t + 1$  following a system perturbation at  $t$  (excluding so-called "Garden of Eden" states of the set of elements). By definition, sets of elements in states with  $p(M_t = m_t) = 0$  that cannot be reached from within the system itself also cannot specify cause repertoires. Consequently, cause-effect structures here are only calculated for possible system states.

The cause-repertoire of higher order mechanisms constituted of multiple system elements, such as mechanism  $AB_t = 11$ , is obtained from the product distribution of the individual mechanism elements, for example:

$$p_{cause}(ABCF_{t-1}|AB_t = 1) = \frac{1}{K} \cdot p_{cause}(ABF_{t-1}|A_t = 1) \times p_{cause}(ABC_{t-1}|B_t = 1), \quad (S3)$$

where  $K$  is a normalization factor so that the product probability distribution sums to 1.

The unconstrained cause repertoire is simply the uniform distribution of all possible states of a set of elements.

## 3. Effect Repertoire

The effect repertoire of a mechanism  $M_t$  in its current state  $m_t$  can be obtained from the TPM as demonstrated below for the example mechanism  $A_t = 1$ , in the ECA system A-F<sub>t</sub> = 111000 implementing rule 232 (Figure 9 in the main text).  $A_t$  can only possibly constrain its outputs  $ABF_{t+1}$ , but not the other elements in the system. Thus, we consider the effect repertoire  $p_{effect}(ABF_{t+1}|A_t = 1)$ , which is obtained by fixing the state of element  $A_t$  to "1", while the remaining inputs to  $A_{t+1}$ ,  $B_{t+1}$ , and  $F_{t+1}$  are perturbed independently into all possible states with equal probability. To eliminate effects of correlations through common inputs, the effect repertoire is defined as:

$$\begin{aligned}
 & p_{effect}(ABF_{t+1}|A_t = 1) \\
 &= p_{effect}(A_{t+1}|A_t = 1) \times p_{effect}(B_{t+1}|A_t = 1) \times p_{effect}(F_{t+1}|A_t = 1).
 \end{aligned}
 \tag{S4}$$

The individual effect repertoires can be read out from the TPM columns of the respective elements, averaging over all rows in which  $A_t = 1$  (*i.e.*, conditioning on  $A_t = 1$ ). Since A, B, and F are Majority functions, the fact that one of their inputs ( $A_t$ ) is in state “1” results in  $p(\text{“1” at } t+1) = 0.75$  and  $p(\text{“0” at } t + 1) = 0.25$  for each of them, assuming maximum entropy for the other two inputs. The resulting product distribution  $p_{effect}(ABF_{t+1}|A_t = 1)$  is shown in Figure 9B in the main text.

For higher order mechanisms such as  $AB_t = 11$ , the effect repertoire is calculated in the same way, only now averaging over all rows in the TPM where  $AB_t = 11$ .

The unconstrained effect repertoire is the product distribution of all elements under no constraints, *i.e.*, averaging all rows of the TPM for the individual elements without conditioning and then taking the product distribution. Since all elements are Majority functions, their individual unconstrained probability distribution at  $t + 1$  is uniform  $p(\text{“1”}) = p(\text{“0”}) = 0.5$ .

## References

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2. Tononi, G. Integrated information theory. *Scholarpedia* **2015**, *10*, 4164.

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