An Introduction to Artificial Chemistries:

Algebra

applied to Informatics

applied to Biology

Algebra (Informatics (Chemistry ∩ Biology))

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Dublin City University
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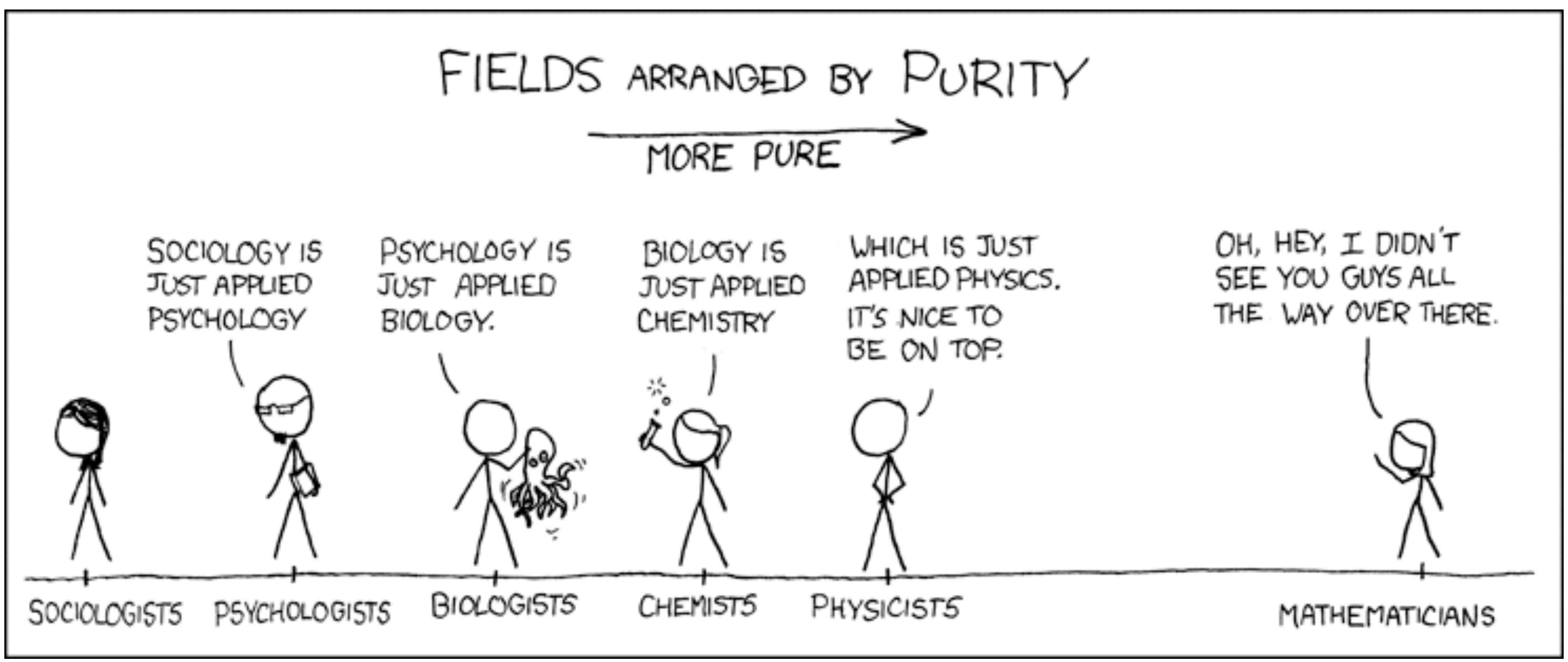
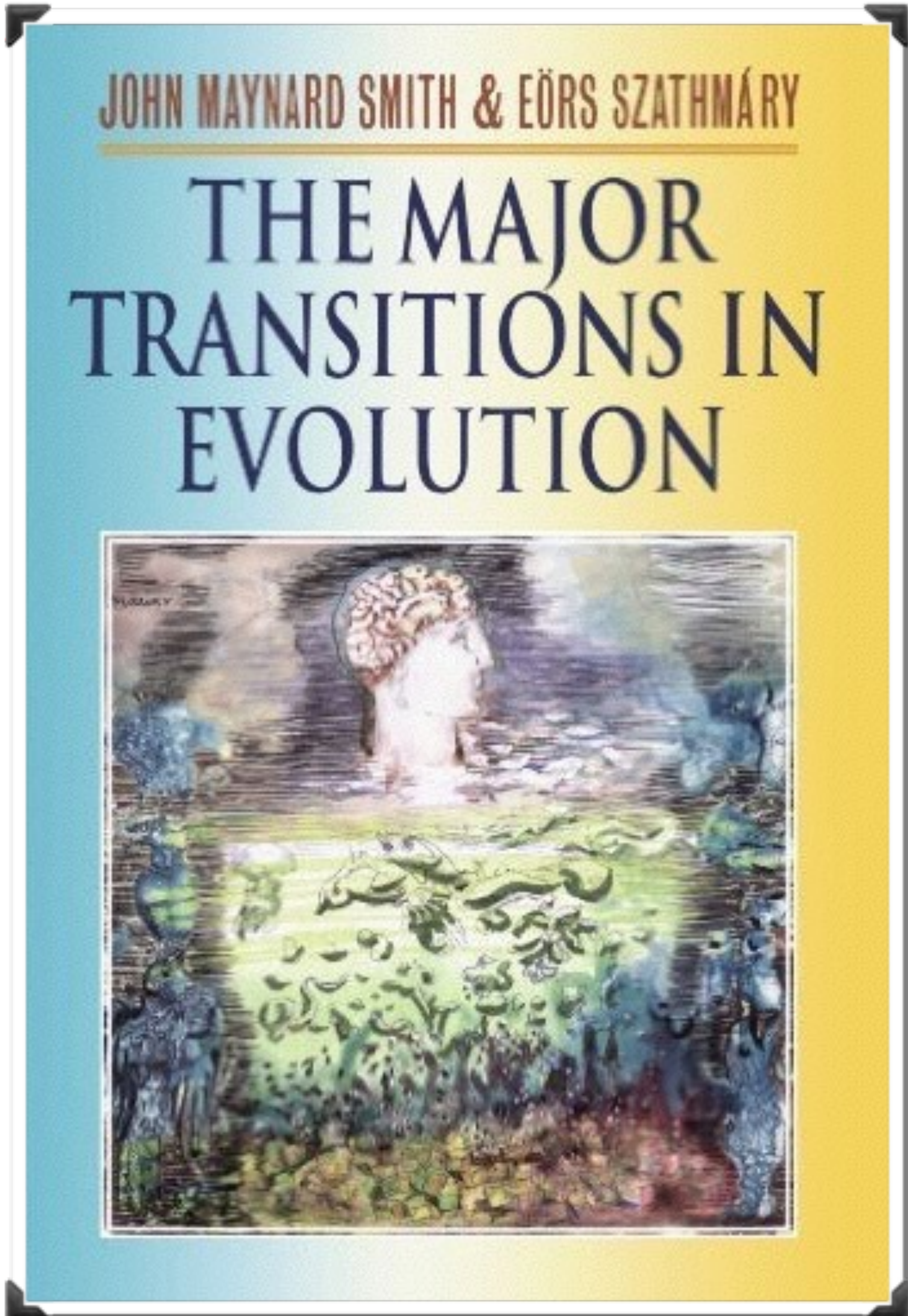
Jena Center of Bioinformatics

Geometry and Computer Science, Pescara, 8 May 2017

- 1843 Emergence (1843 - John Stuart Mill - A System of Logic)
- 1921 Emergent Evolution (1923 - Lloyd Morgan - Emergent Evolution)
- 1940s Cybernetics (1952 - Ashby - Design for a Brain)
- 1995 Book: Major Transitions in Evolution



The Major Transition in Evolution



Maynard Smith and Szathmáry identified several properties common to the transitions:

- **<u>Smaller entities have often come about together to form larger entities.</u>** e.g. Chromosomes, eukaryotes, sex multicellular colonies.
- Smaller entities often become differentiated as part of a larger entity. e.g. DNA & protein, organelles, anisogamy, tissues, castes
- The smaller entities are often unable to replicate in the absence of the larger entity. e.g. DNA, chromosomes, Organelles, tissues, castes
- The smaller entities can sometimes disrupt the development of the larger entity, e.g. Meiotic drive (selfish non-Mendelian genes), parthenogenesis, cancers, coup d'état
- New ways of transmitting information have arisen.e.g. DNA-protein, cell heredity, epigenesis, universal grammar.

https://en.wikipedia.org/wiki/The_Major_Transitions_in_Evolution

The Major Evolutionary Transitions

REVIEW ARTICLE

The major evolutionary transitions

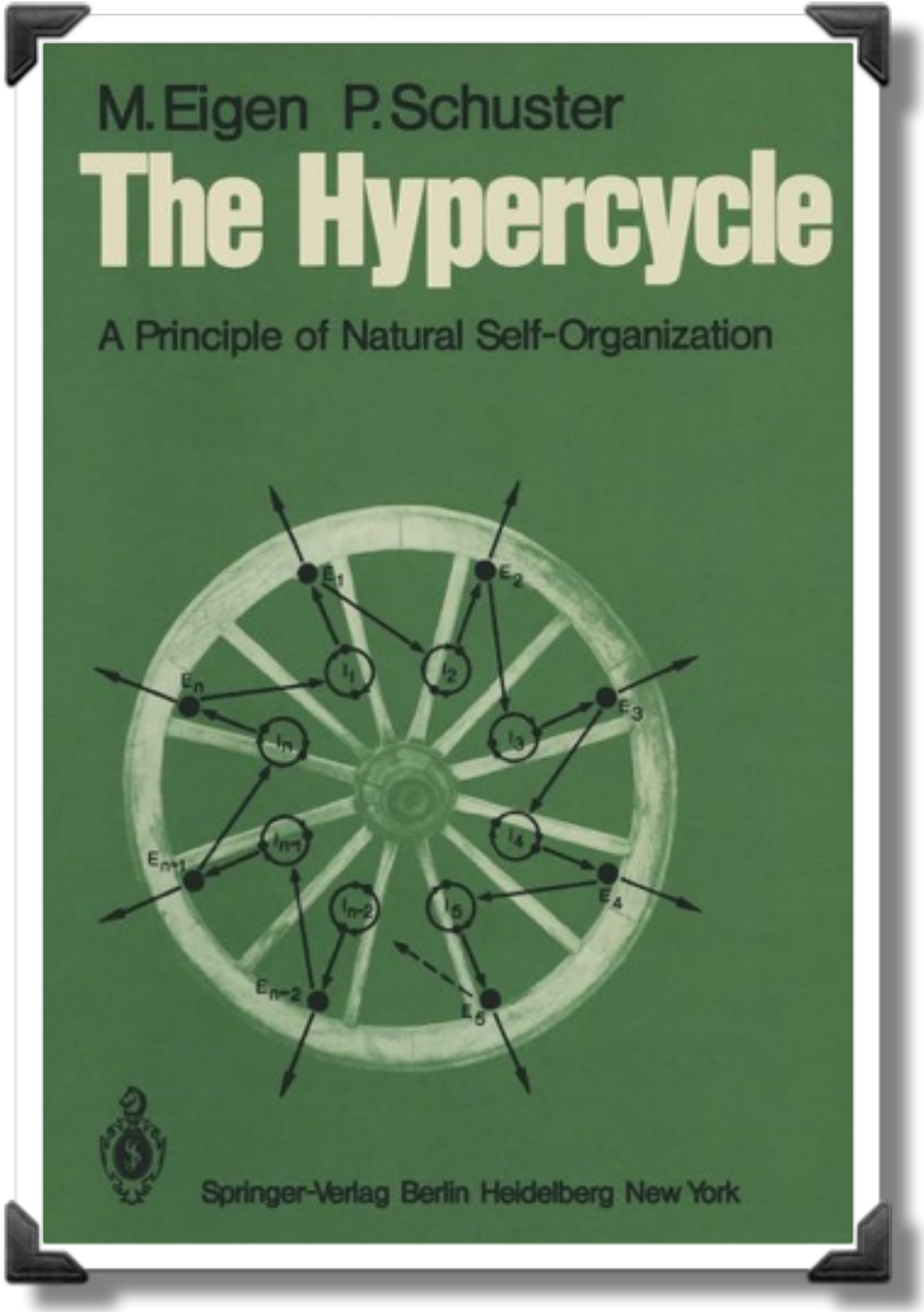
Eörs Szathmáry & John Maynard Smith

There is no theoretical reason to expect evolutionary lineages to increase in complexity with time, and no empirical evidence that they do so. Nevertheless, eukaryotic cells are more complex than prokaryotic ones, animals and plants are more complex than protists, and so on. This increase in complexity may have been achieved as a result of a series of major evolutionary transitions. These involved changes in the way information is stored and transmitted.

NATURE · VOL 374 · 16 MARCH 1995 227

TABLE 1 The major transitions[1]
Replicating molecules to populations of molecules in compartments
Unlinked replicators to chromosomes
RNA as gene and enzyme to DNA and protein (genetic code)
Prokaryotes to eukaryotes
Asexual clones to sexual populations
Protists to animals, plants and fungi (cell differentiation)
Solitary individuals to colonies (non-reproductive castes)
Primate societies to human societies (language)

- 1843 Emergence (1843 - John Stuart Mill - A System of Logic)
- 1921 Emergent Evolution (1923 - Lloyd Morgan - Emergent Evolution)
- Control Theory
- 1940s Cybernetics (1952 - Ashby - Design for a Brain)
- 1956 Artificial Intelligence
- Self Organised Criticality
- 1963 Chaotic Theory (1987 James Gleick - Chaos: The Making of a new Science)
- - Robotics (1984 - Braitenberg Vehicles)
- 1984 Complex Systems (1995 - M Gell Mann - What is Complexity)
- 1986 Artificial Life (1991 - Thomas Ray - Tierra)
- 1977 Artificial Chemistries (1996 - Walter Fontana - The Barrier of Objects)
- 2001 Chemical Organisation Theory (2007 - Dittrich, Speroni - Chemical Organisation Theory)



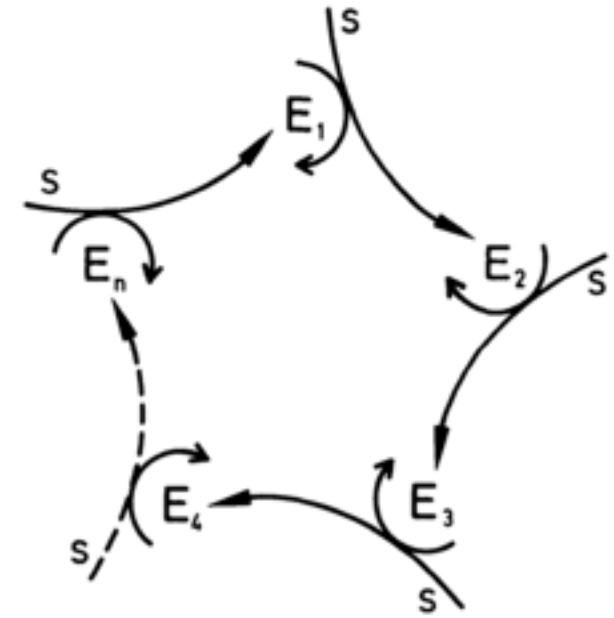


Fig. 4. *The catalytic cycle* represents a higher level of organization in the hierarchy of catalytic schemes. The constituents of the cycle $E_1 \rightarrow E_n$ are themselves catalysts which are formed from some energy-rich substrates (S), whereby each intermediate E_i is a catalyst for the formation of E_{i+1}. The catalytic cycle seen as an entity is equivalent to an autocatalyst, which instructs its own reproduction. To be a catalytic cycle it is sufficient, that only one of the intermediates formed is a catalyst for one of the subsequent reaction steps.

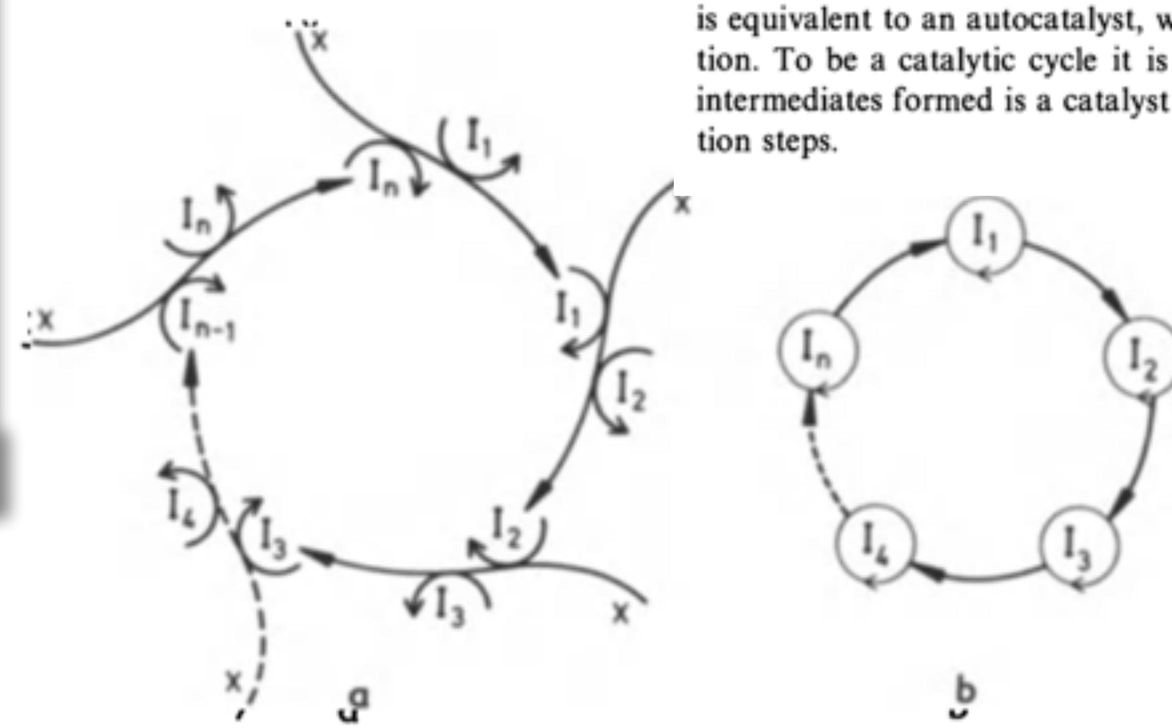
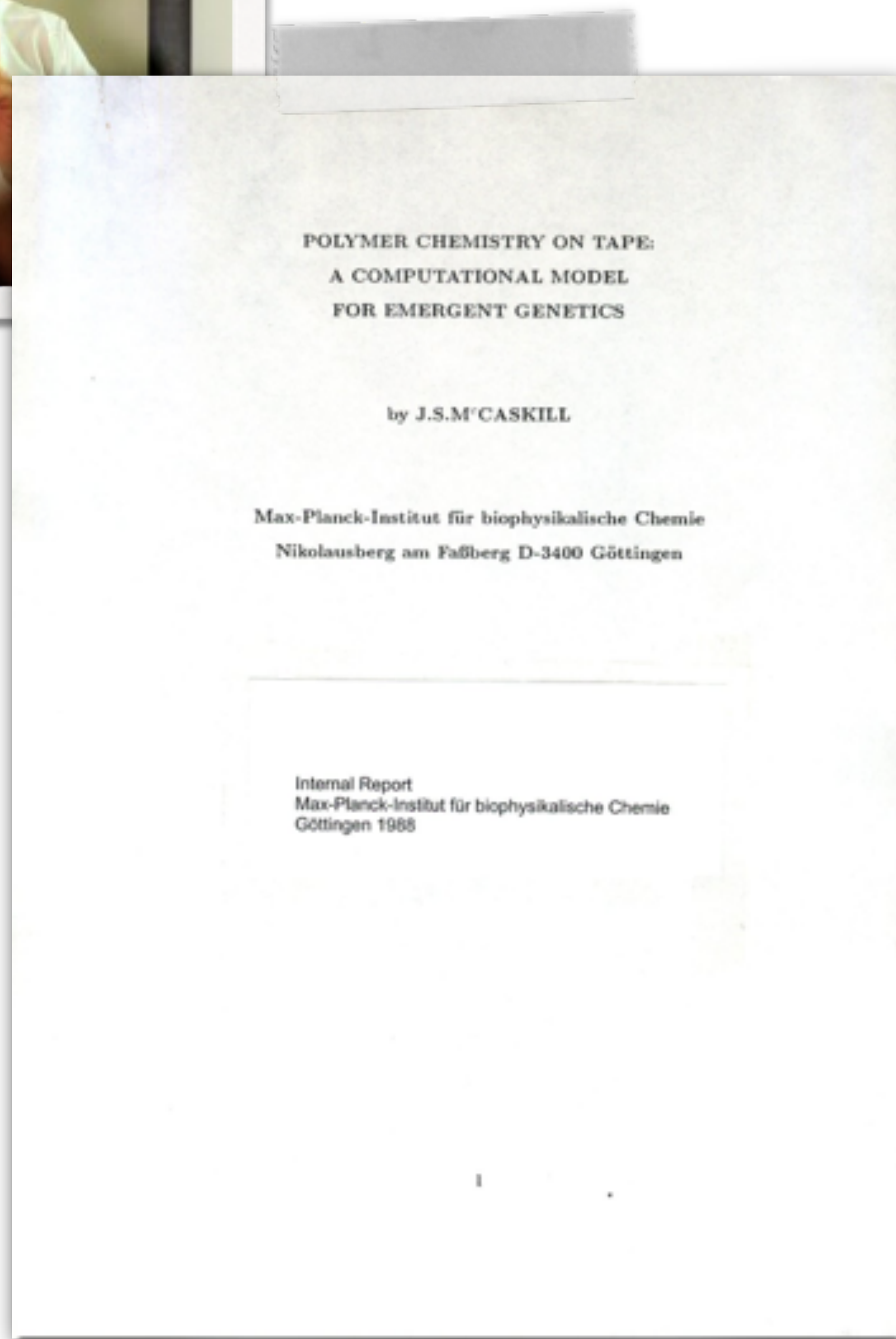


Fig. 7. *A catalytic hypercycle* consists of self-instructive units I_i with two-fold catalytic functions. As autocatalysts or – more generally – as catalytic cycles the intermediates I_i are able to instruct their own reproduction and, in addition, provide catalytic support for the reproduction of the subsequent intermediate (using the energy-rich building material X). The simplified graph (b) indicates the cyclic hierarchy

Polymer Chemistry on Tape



POLYMER CHEMISTRY ON TAPE:
A COMPUTATIONAL MODEL
FOR EMERGENT GENETICS

by J.S.M^cCASKILL

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Nikolausberg am Faßberg D-3400 Göttingen

Internal Report
Max-Planck-Institut für biophysikalische Chemie
Göttingen 1988

1

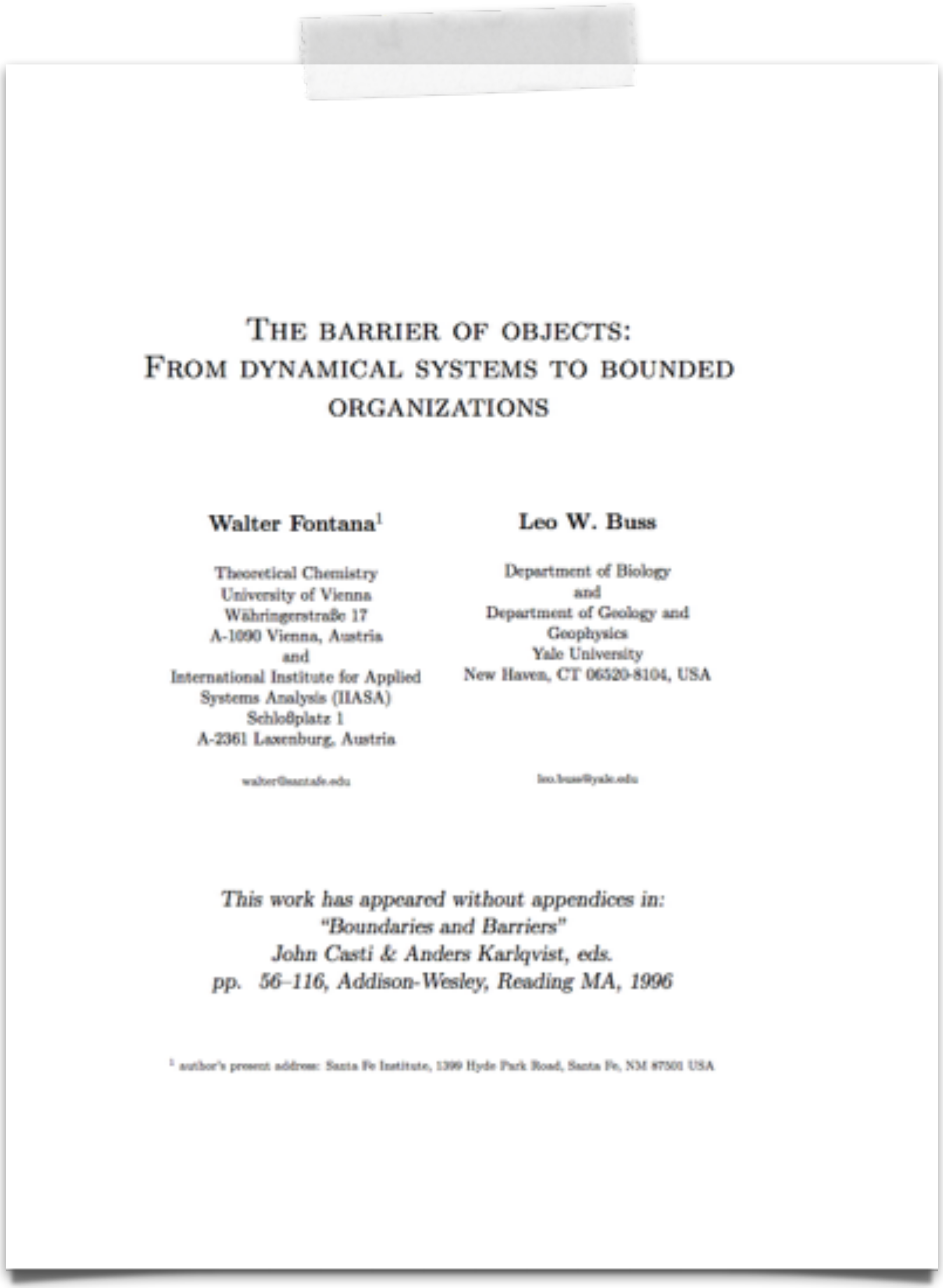
from RNA model

↓

Abstraction

Artificial Chemistry

Constructive Dynamical Systems



THE BARRIER OF OBJECTS:
FROM DYNAMICAL SYSTEMS TO BOUNDED ORGANIZATIONS

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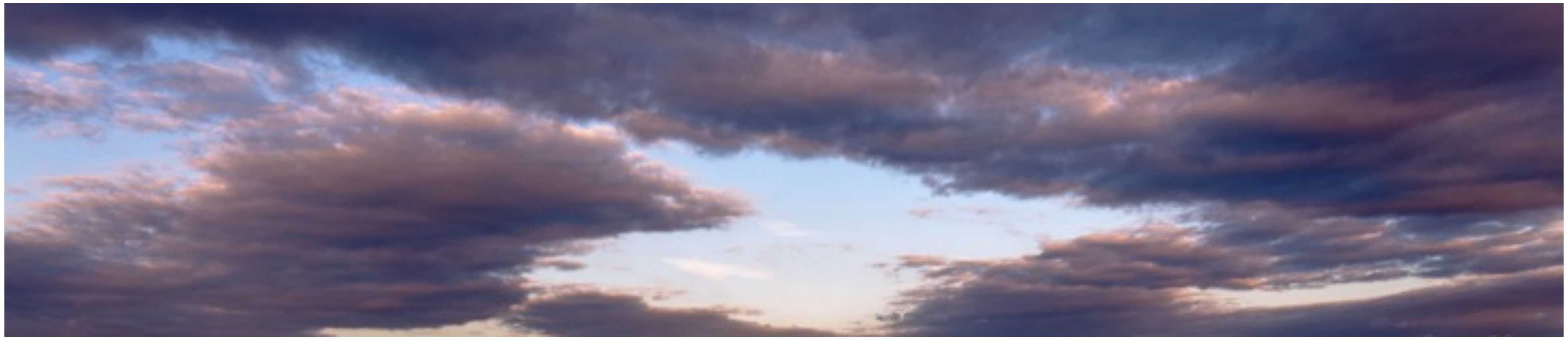
This work has appeared without appendices in:
"Boundaries and Barriers"
John Casti & Anders Karlqvist, eds.
pp. 56–116, Addison-Wesley, Reading MA, 1996

[1] author's present address: Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501 USA

Constructing the Molecules

Constructing the "Objects"

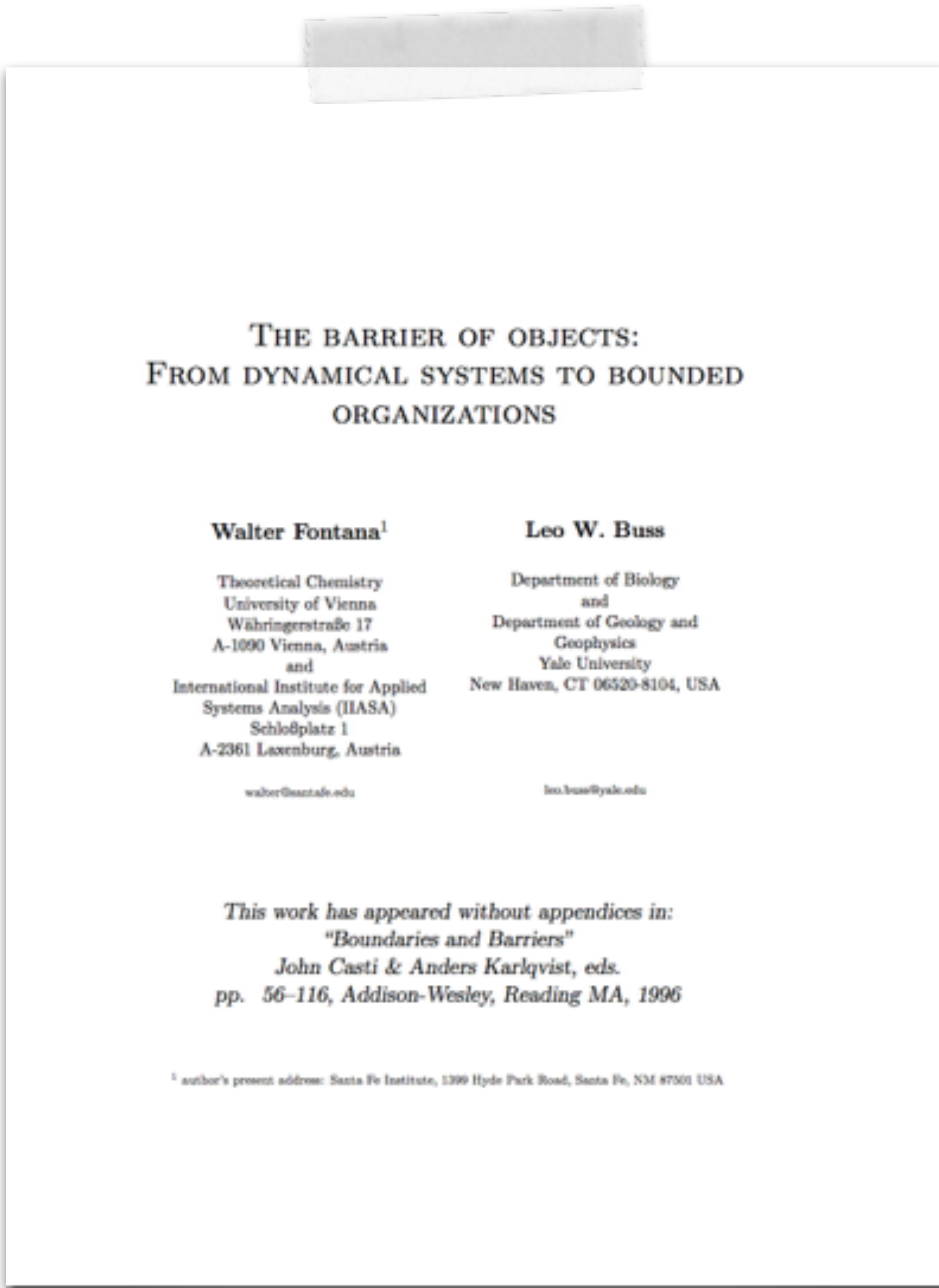


Historical Problems:

We use Ordinary Differential Equations to model the world

In an ODE there is no novelty

Artificial Chemistry as a crude abstraction of a Constructive Dynamical System



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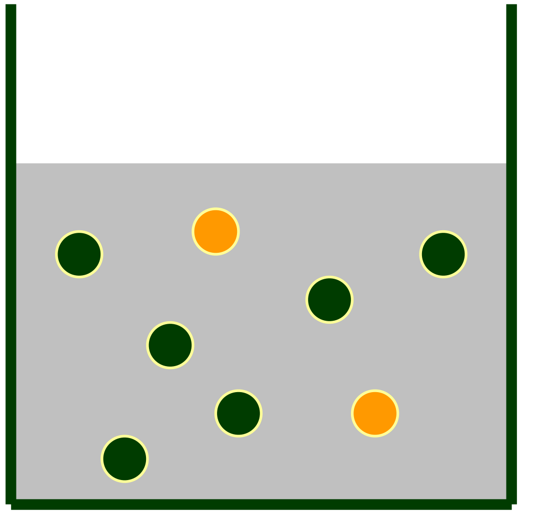
Infinite Molecular Types

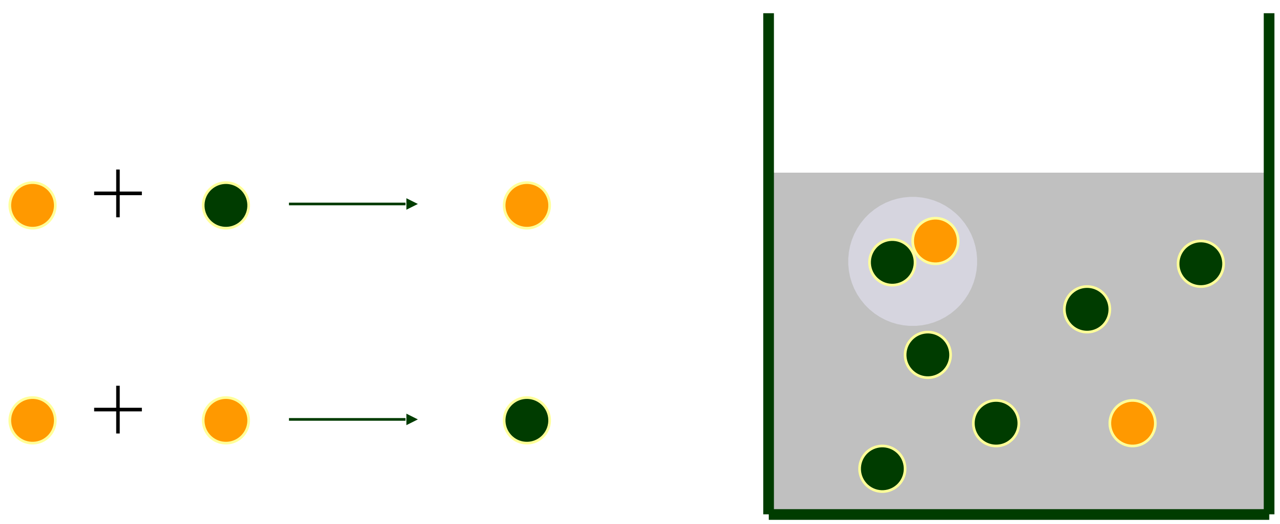
All Reaction Catalytic

No Conservation of Mass

Out-flux from each Molecule

Well Stirred





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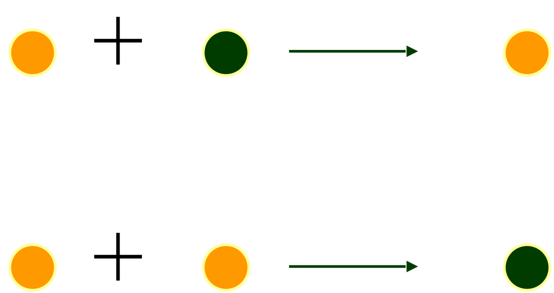

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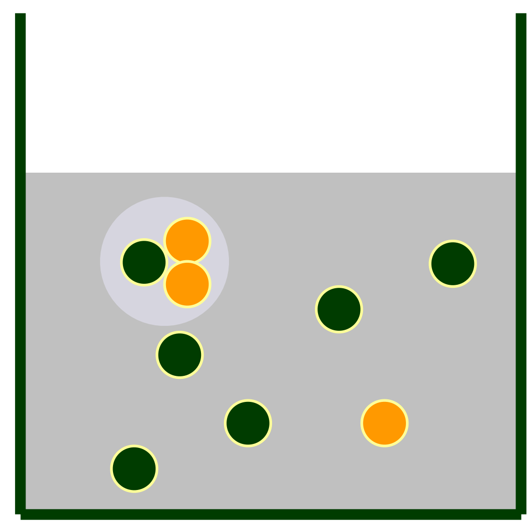

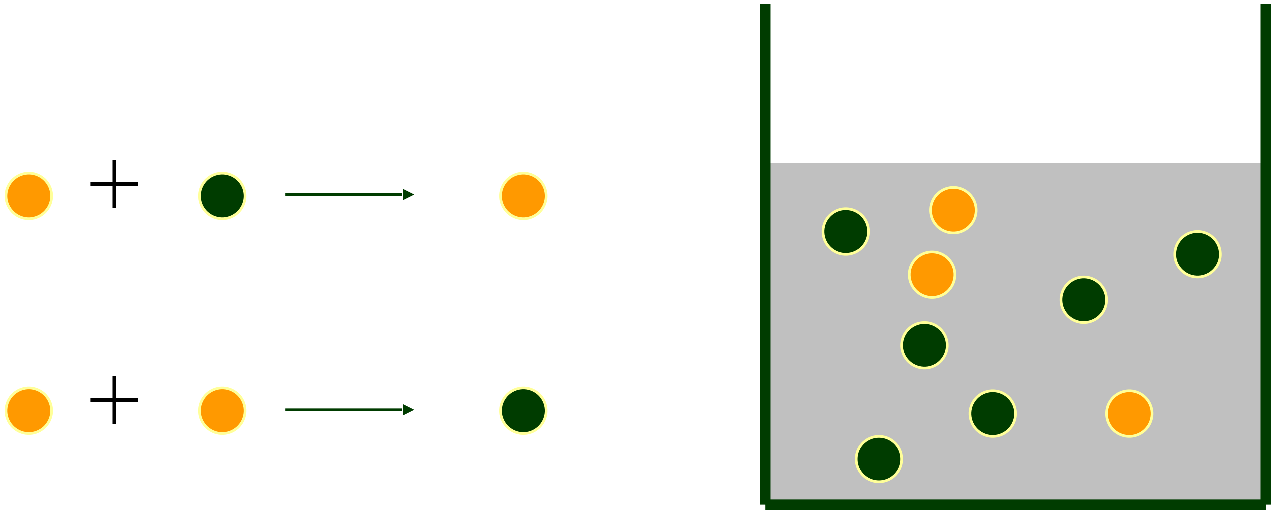

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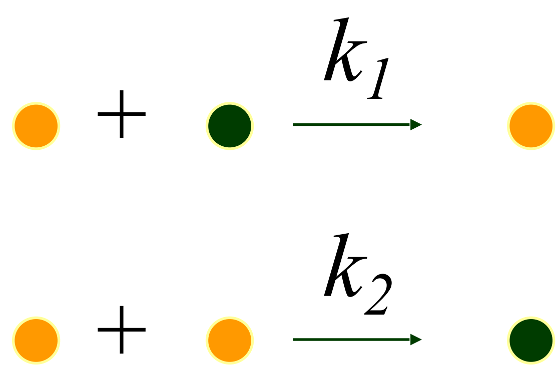

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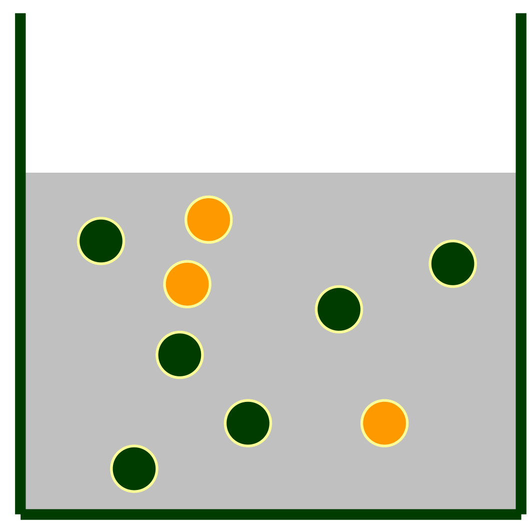

$$dx_1/dt = k_2\, x_2\, x_2$$

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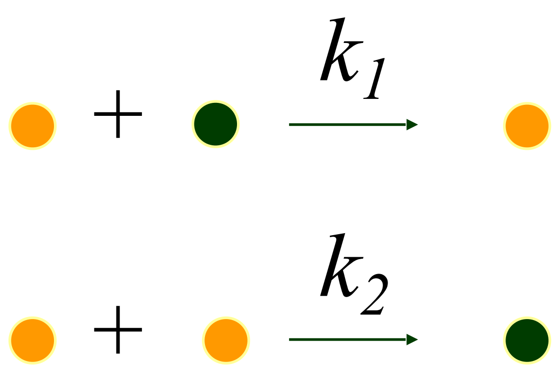

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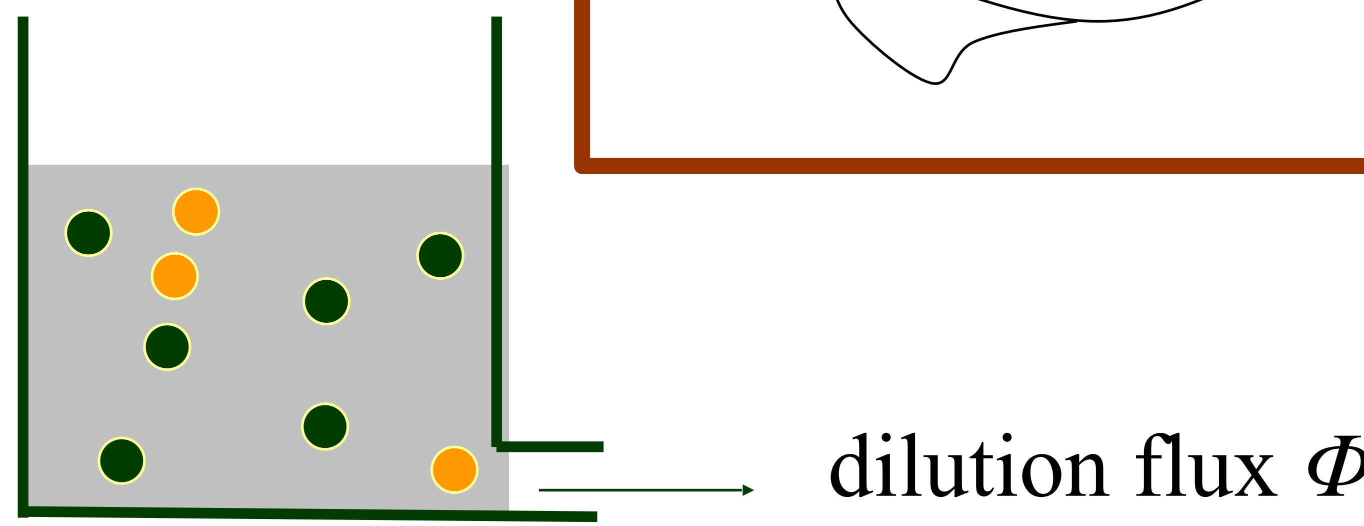

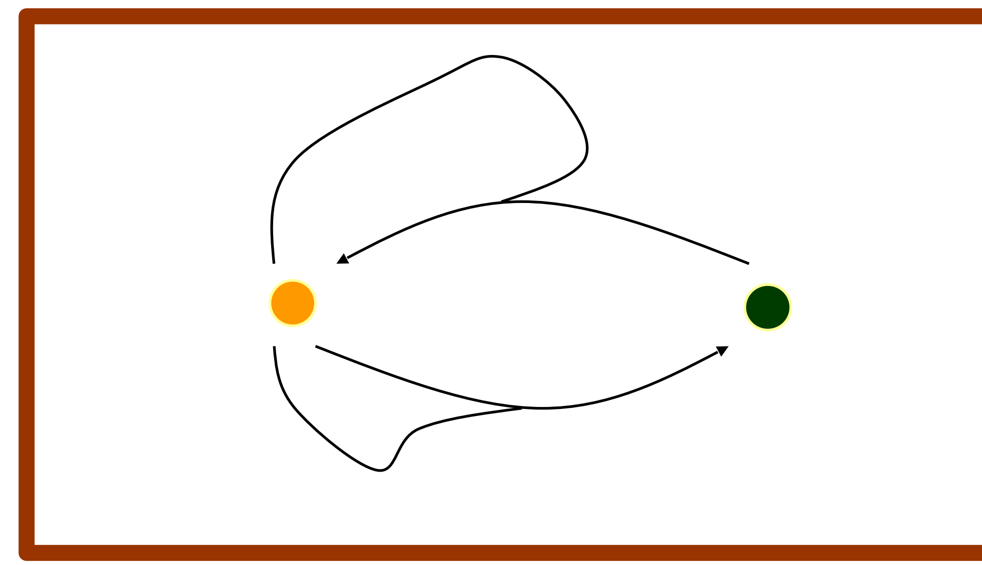

$$dx_1/dt = k_2\, x_2\, x_2 - x_1\, \Phi$$

$$dx_2/dt = k_1\, x_1\, x_2 - x_2\, \Phi$$

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s_1 s_2	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
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7	6	11	6	11	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	15	14	15
8	5	9	5	9	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	13	12	13
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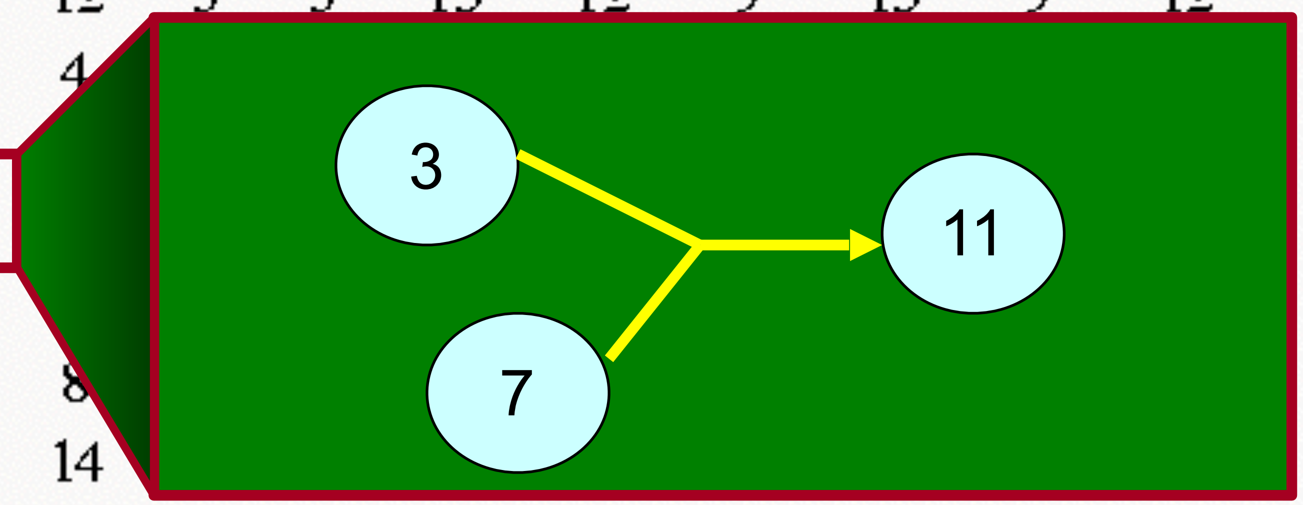

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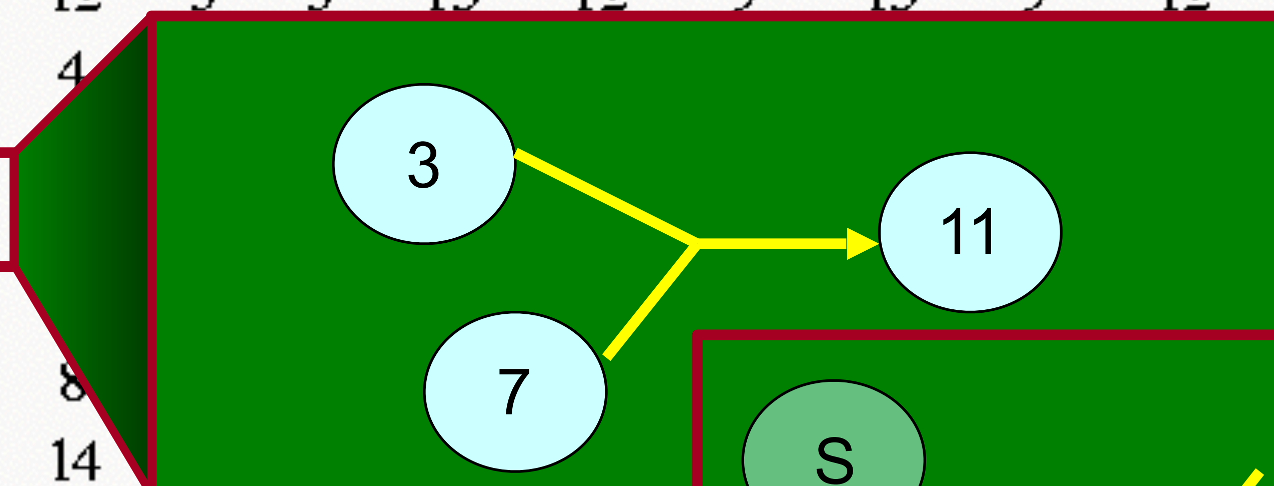
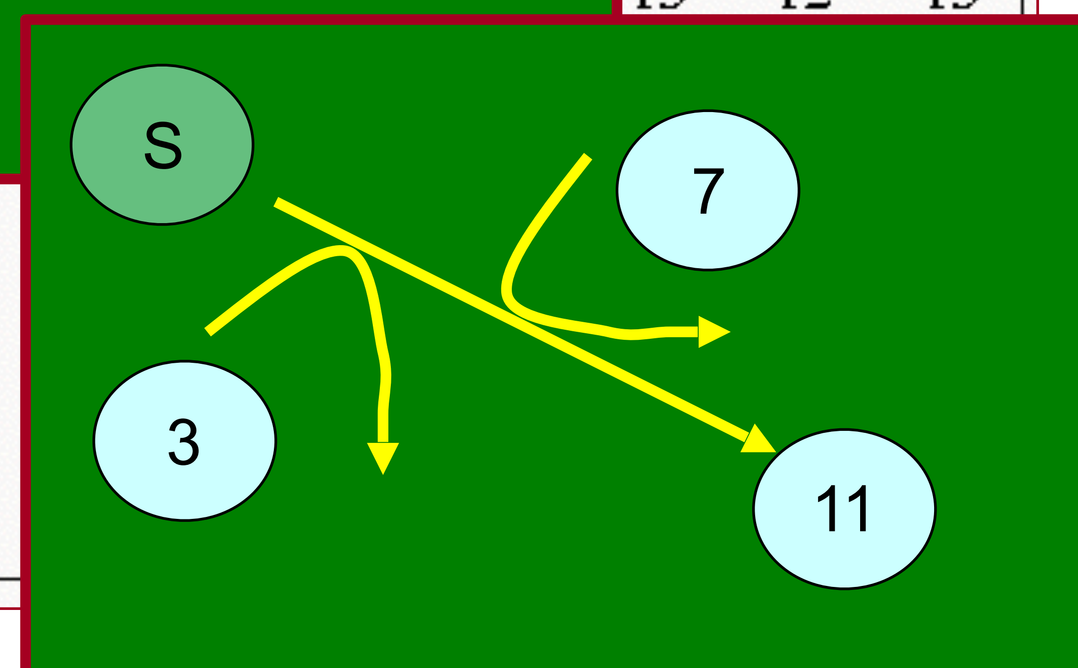
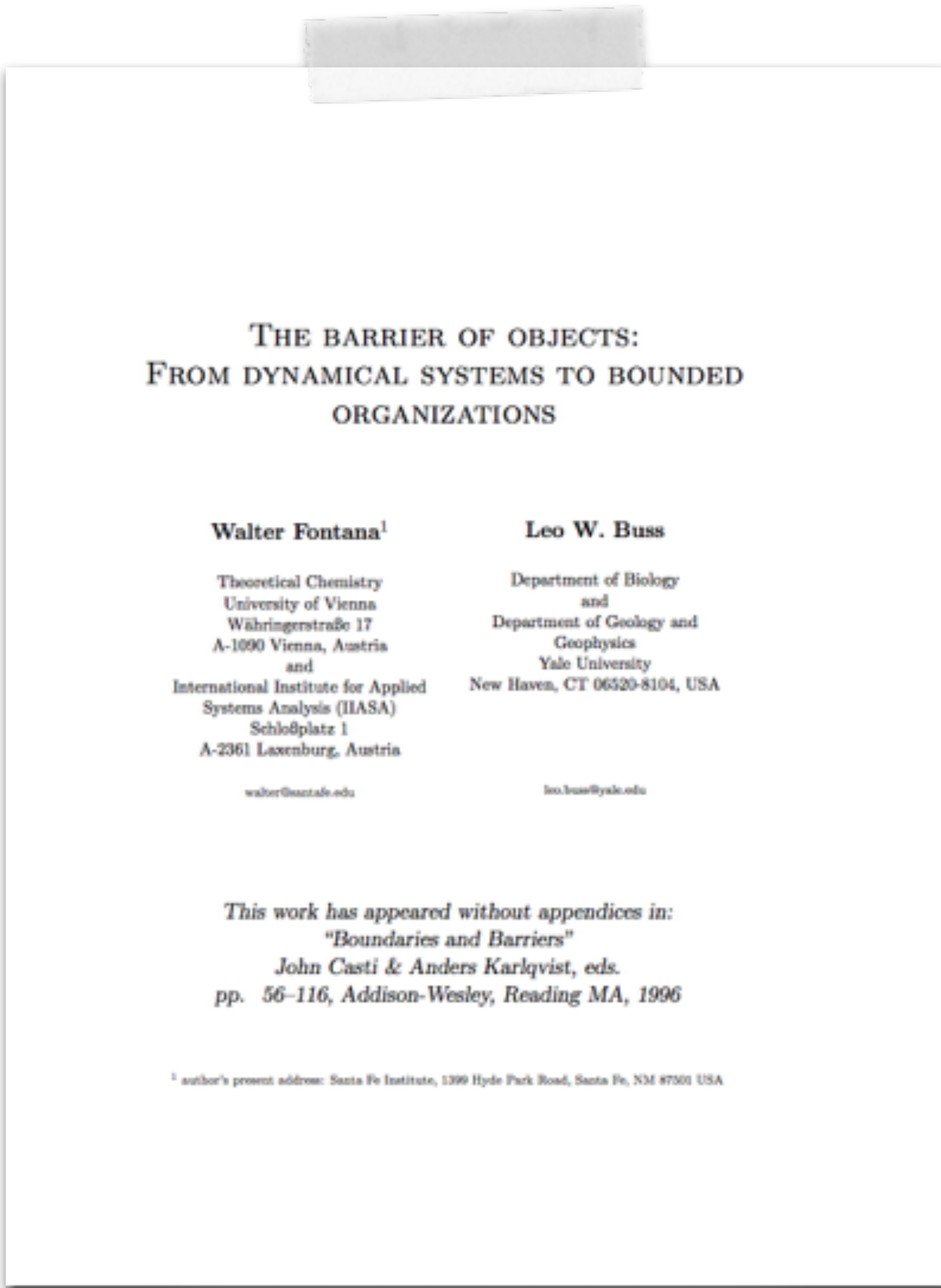




Artificial Chemistry as a crude abstraction of a Constructive Dynamical System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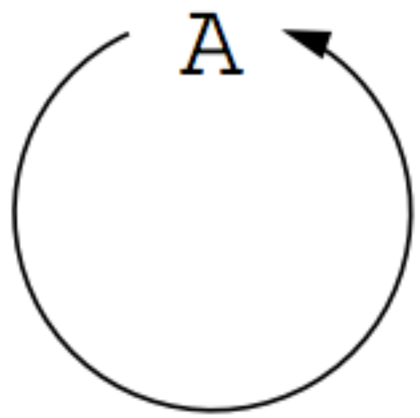
Infinite Molecular Types

All Reaction Catalytic

No Conservation of Mass

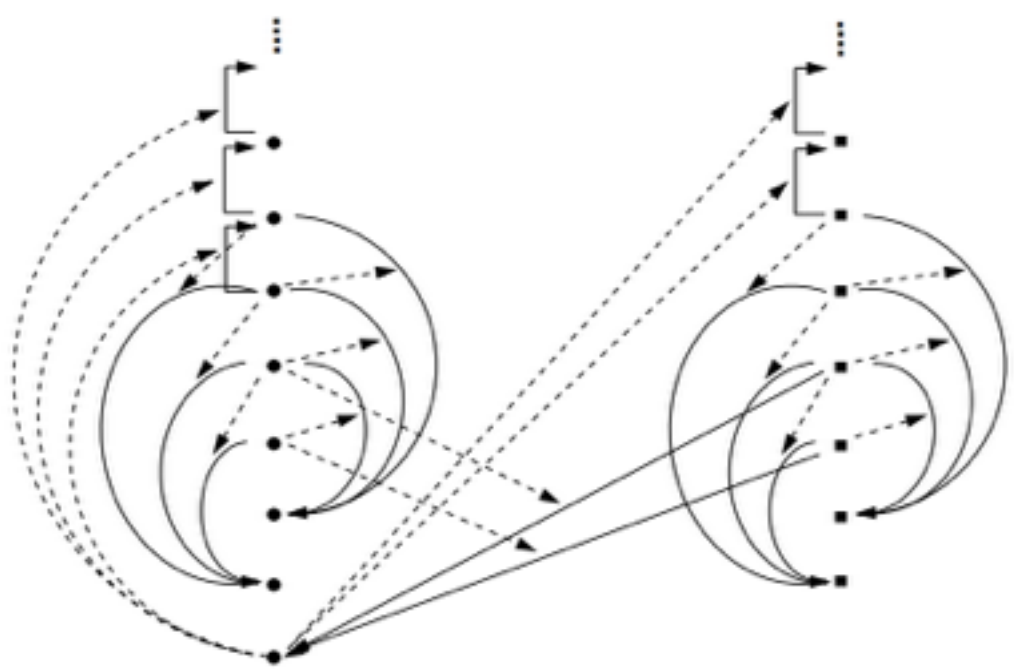
Out-flux from each Molecule

Well Stirred



Organisations as Emerging Objects

An Organisation is defined as a Closed and Self Maintaining set



Closed: all the reactions recreate elements inside

Self Maintaining: There is an internal reaction that recreate each Molecule

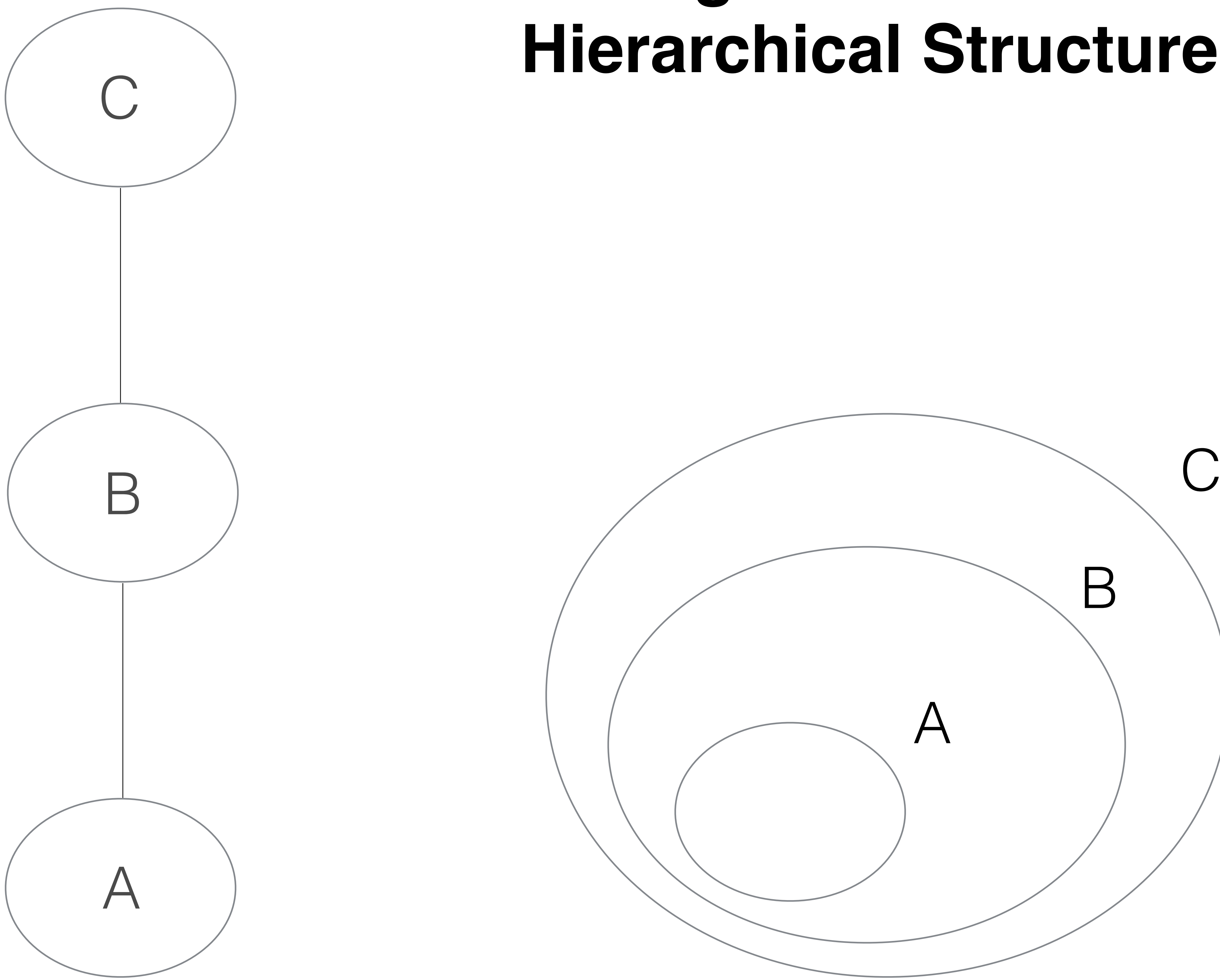
What would be conserved if the "tape were played twice"

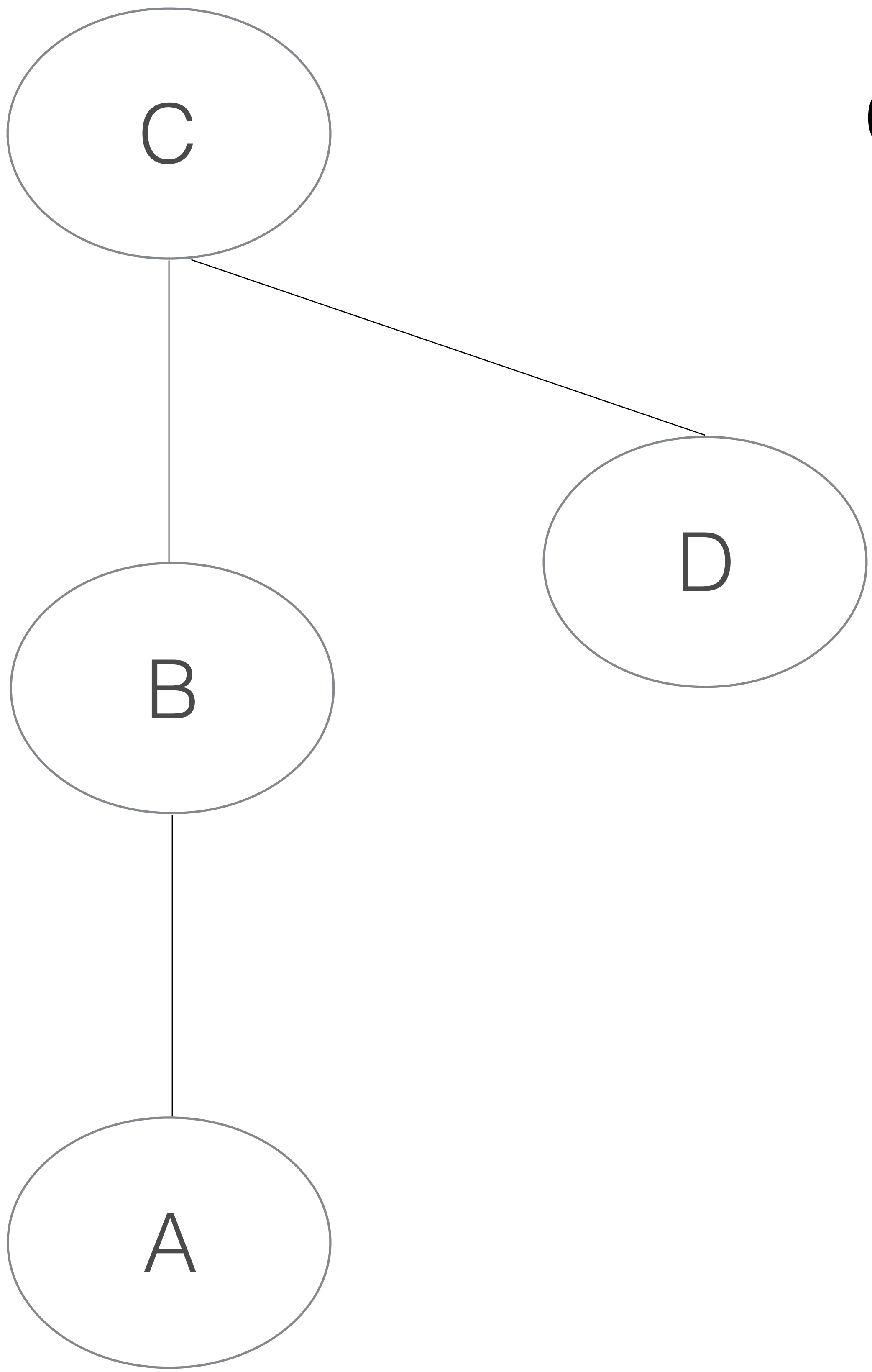

What would be conserved if "the tape were played twice"?

We develop an abstract chemistry
[…]
the following features are generic to this particular abstraction of chemistry;
hence, they would be expected to reappear if "the tape were run twice":

- hypercycles of self-reproducing objects arise;
- if self-replication is inhibited, self-maintaining organisations arise;
- self maintaining organisations, once established, can combine into higher-order self-maintaining organisations.

Organisations as Hierarchical Structures





Organisations as Partially Ordered Structures

Not all Organisations are comparable

Closure and Self Maintenance in Catalytic Flow Systems

Closed Sets

If given a set of element S,

each interaction will just create elements of that set we say that the set is closed:

$\forall$ x,y $\in$ S x(y) $\Rightarrow$ S

then S is closed

Self Maintaining Sets

If given a set of element S,

each element (x) is created by a reaction pathway inside the set (y,z),

then the set is self maintaining:

$\forall\ x \in S \quad \exists\ y, z \in S$ such that $x = y(z)$

Organisations

A set who is both closed and self maintaining is an Organisation

organisations

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organisations

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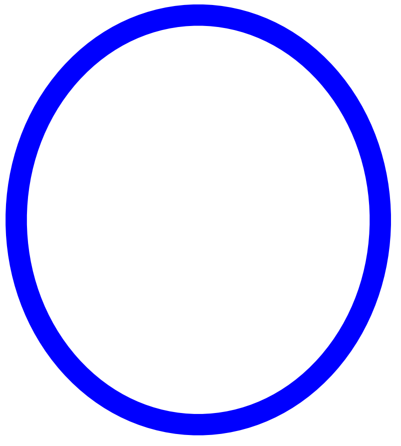

organisations

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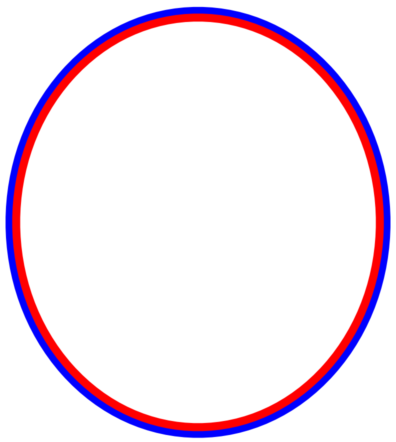
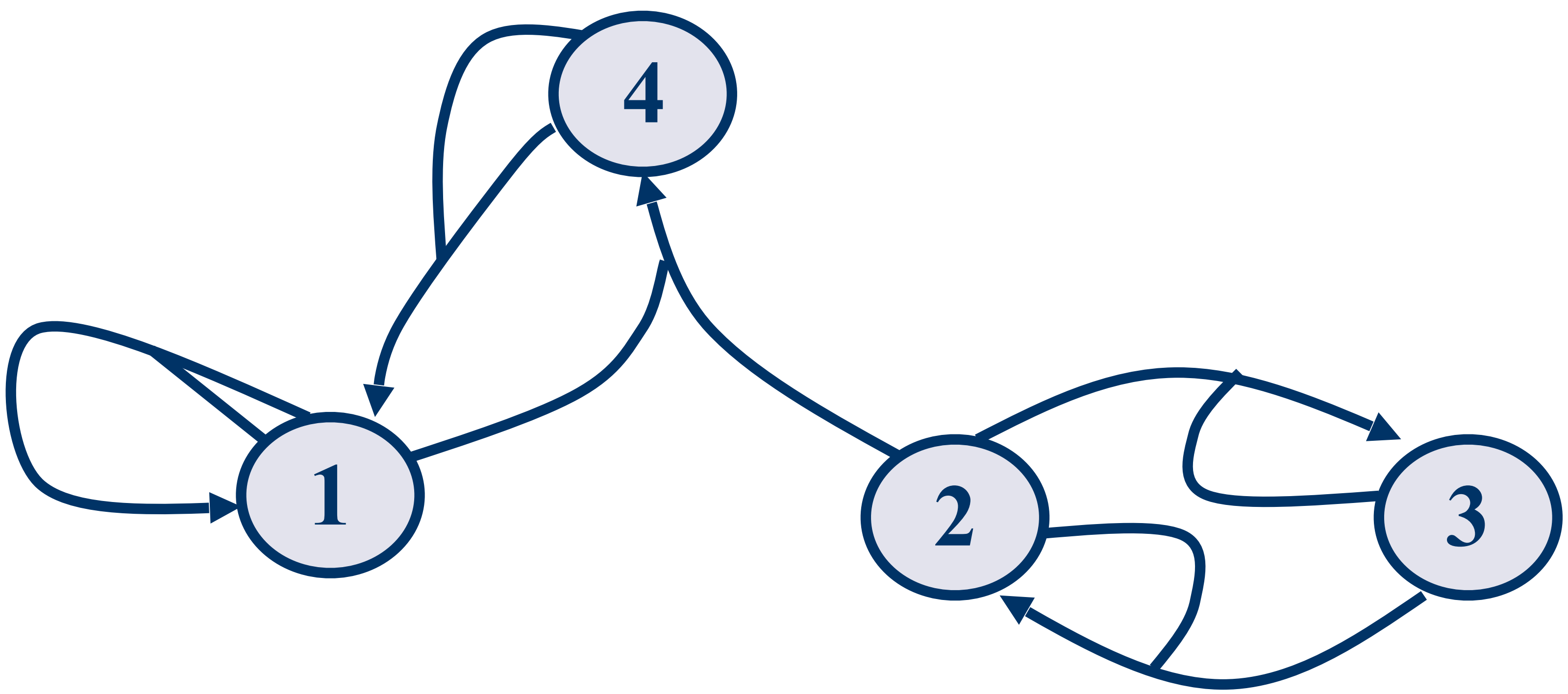


An Example

- Each molecule has also a first order outflow:

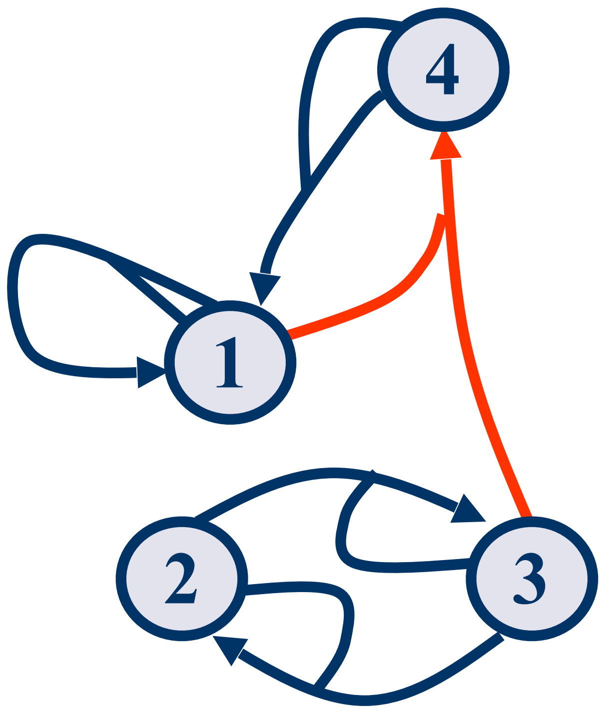


  - $1 \to \emptyset$
  - $2 \to \emptyset$
  - $3 \to \emptyset$
  - $4 \to \emptyset$

Network

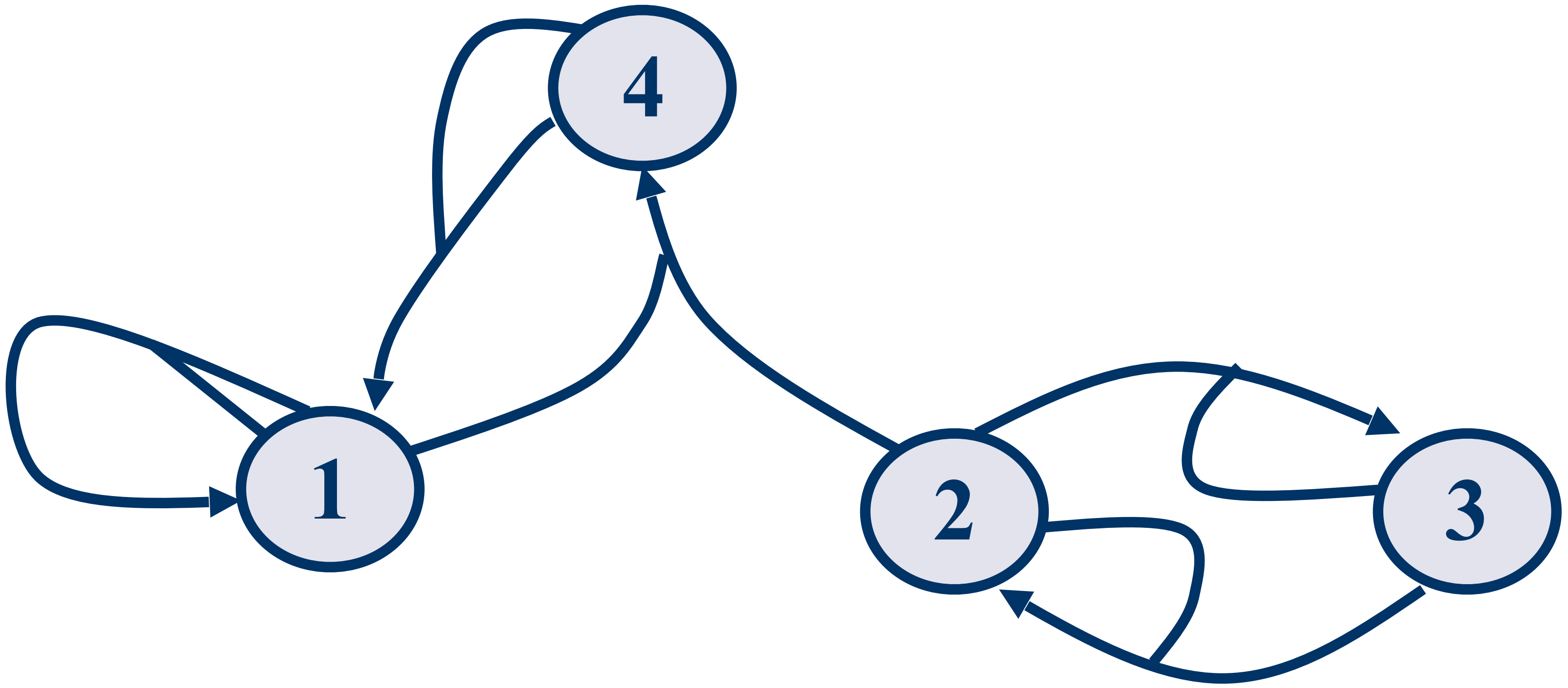
Node: molecular species

Arc: „If molecule 1 and 3 is present, then 4 can/will be produced“.



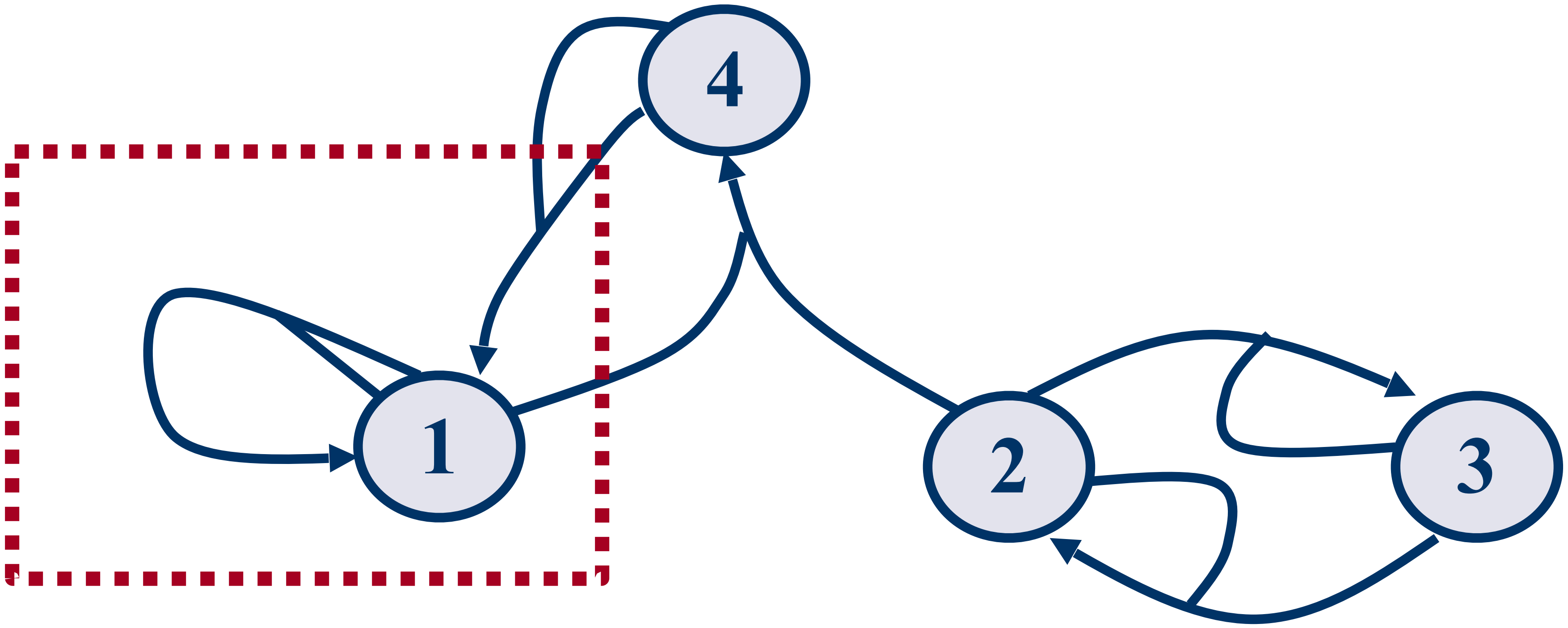
An Example

closed set



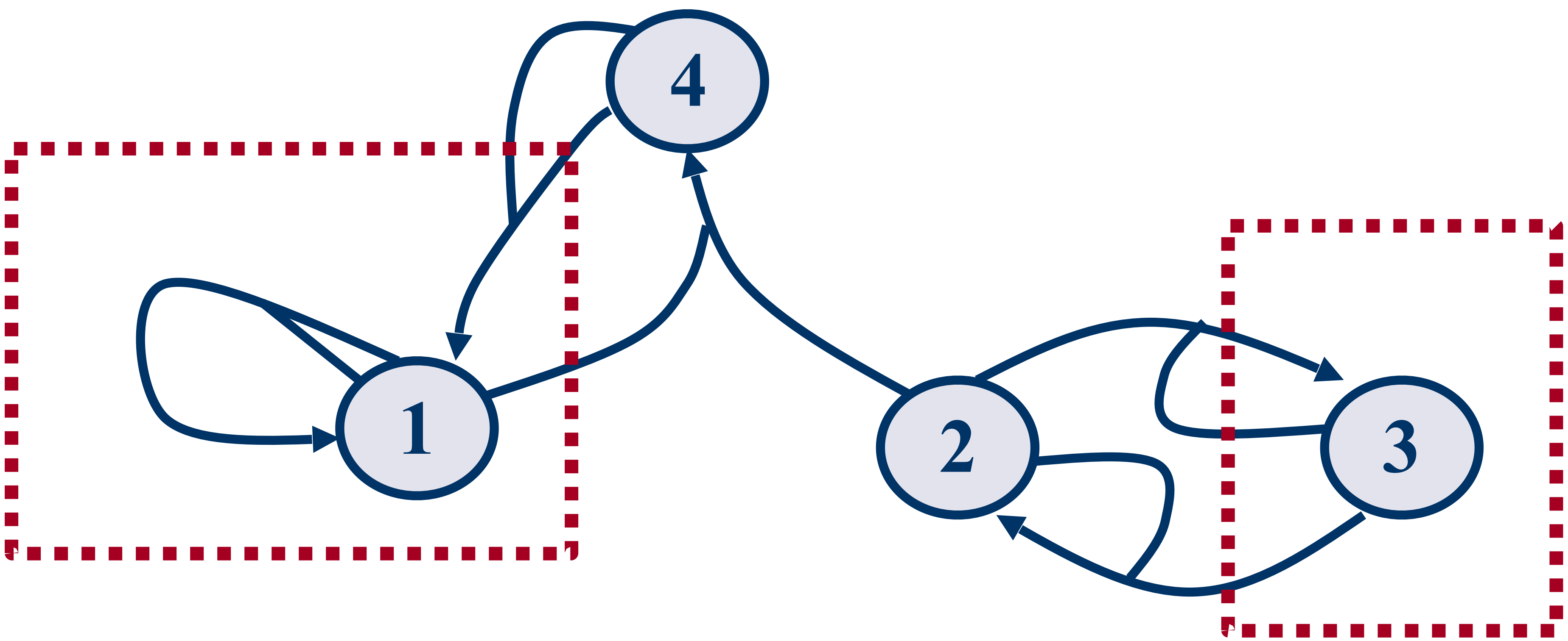
An Example

closed set



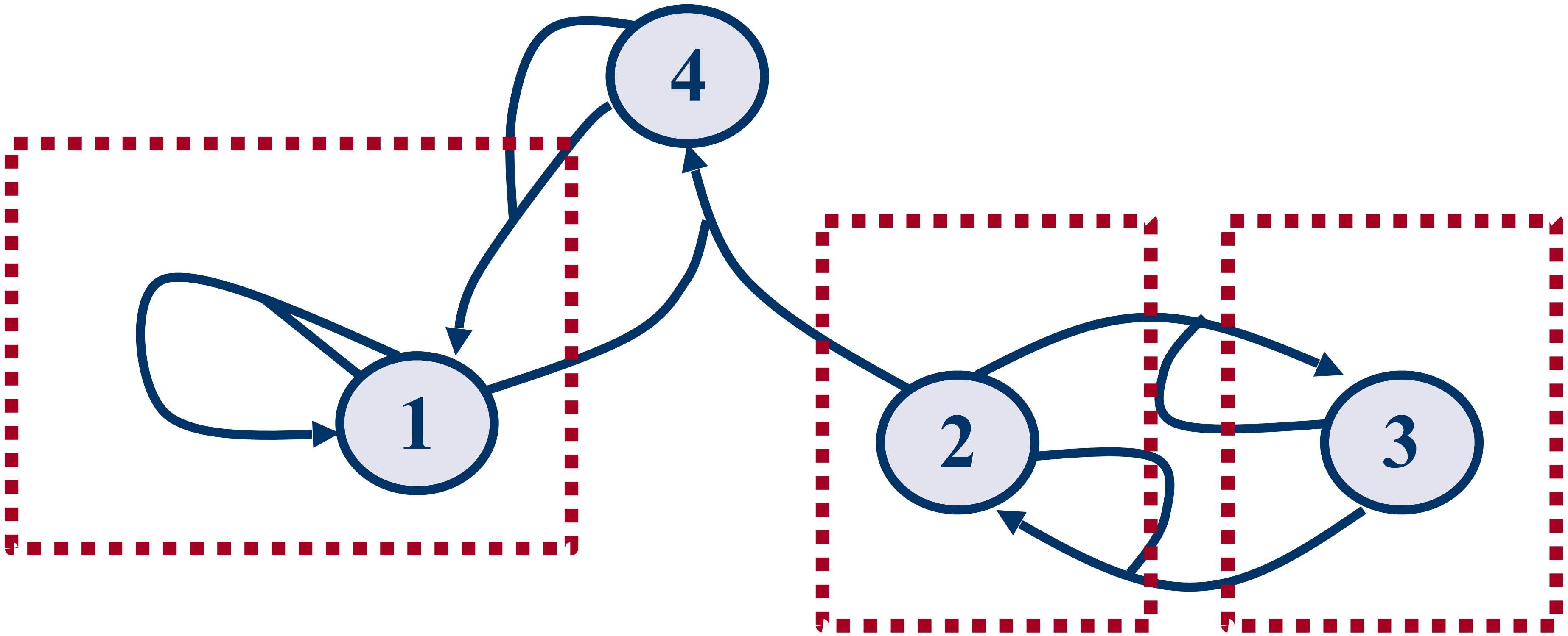
An Example

closed set



An Example

closed set



An Example

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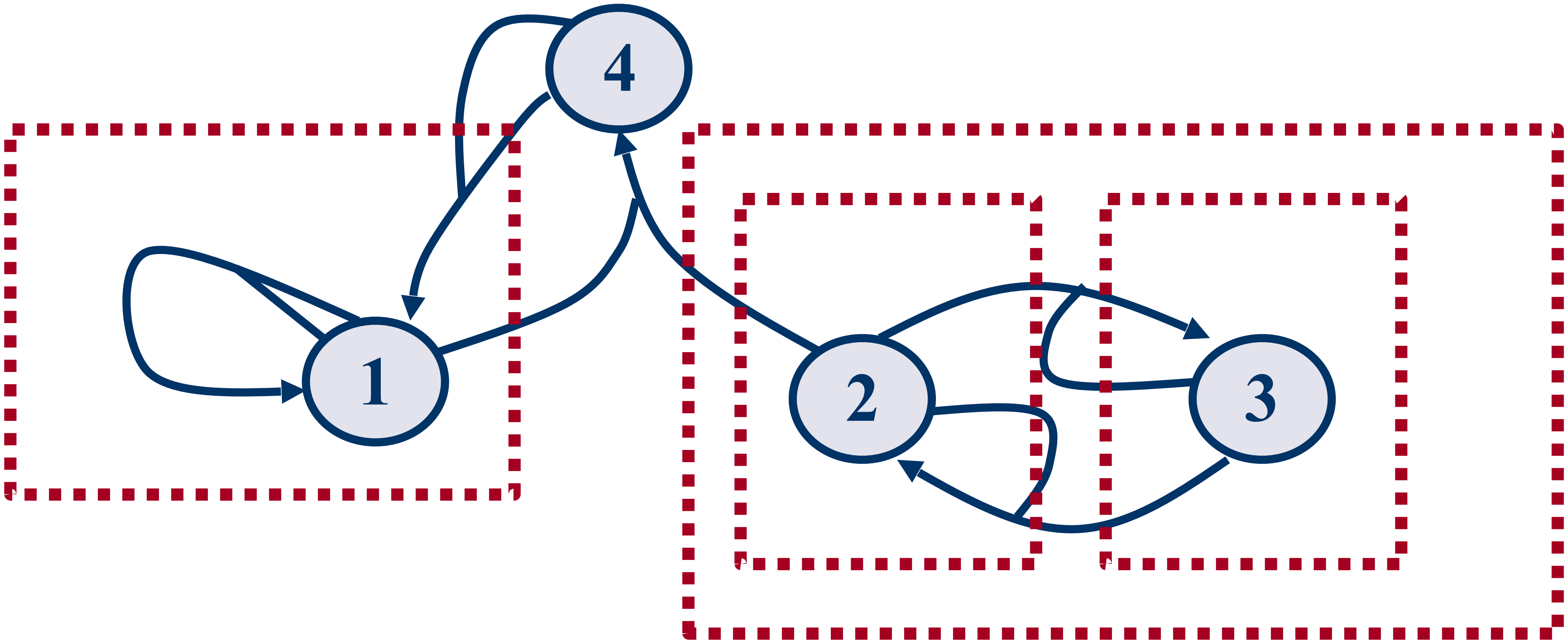
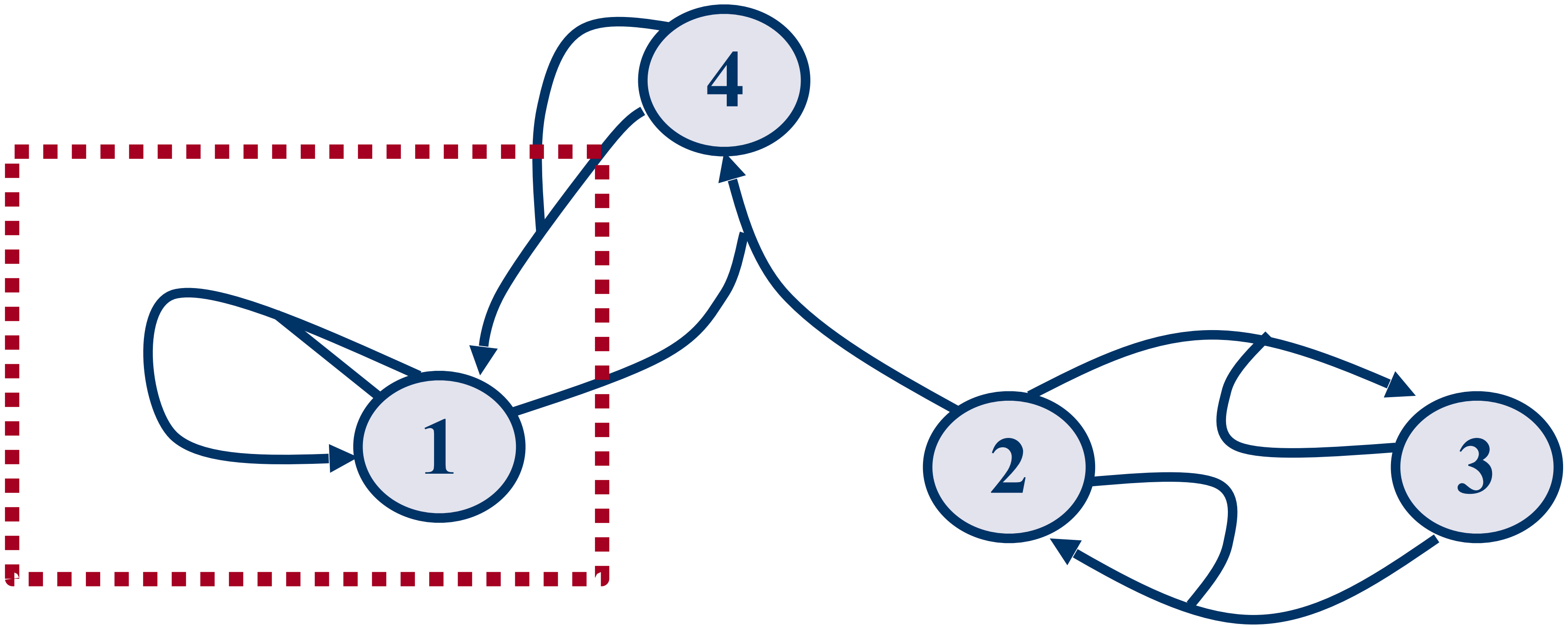


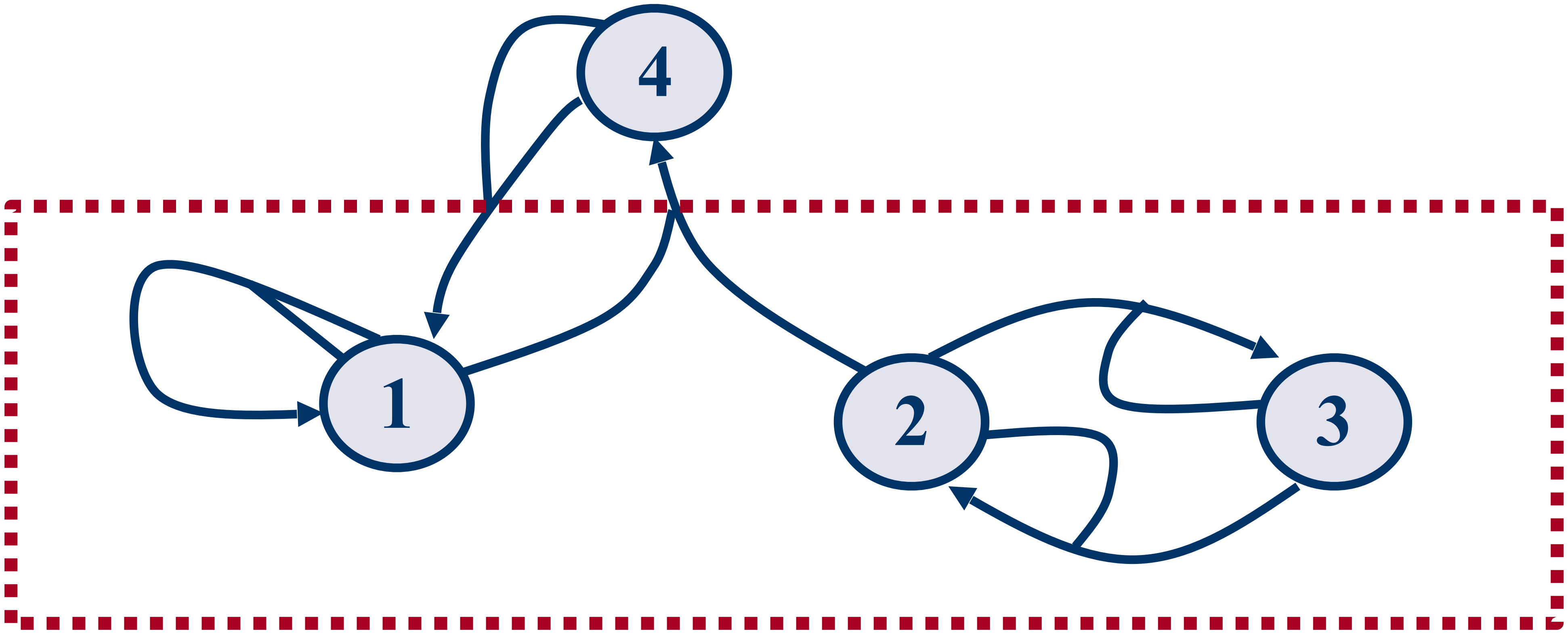
An Example

self-maintaining set



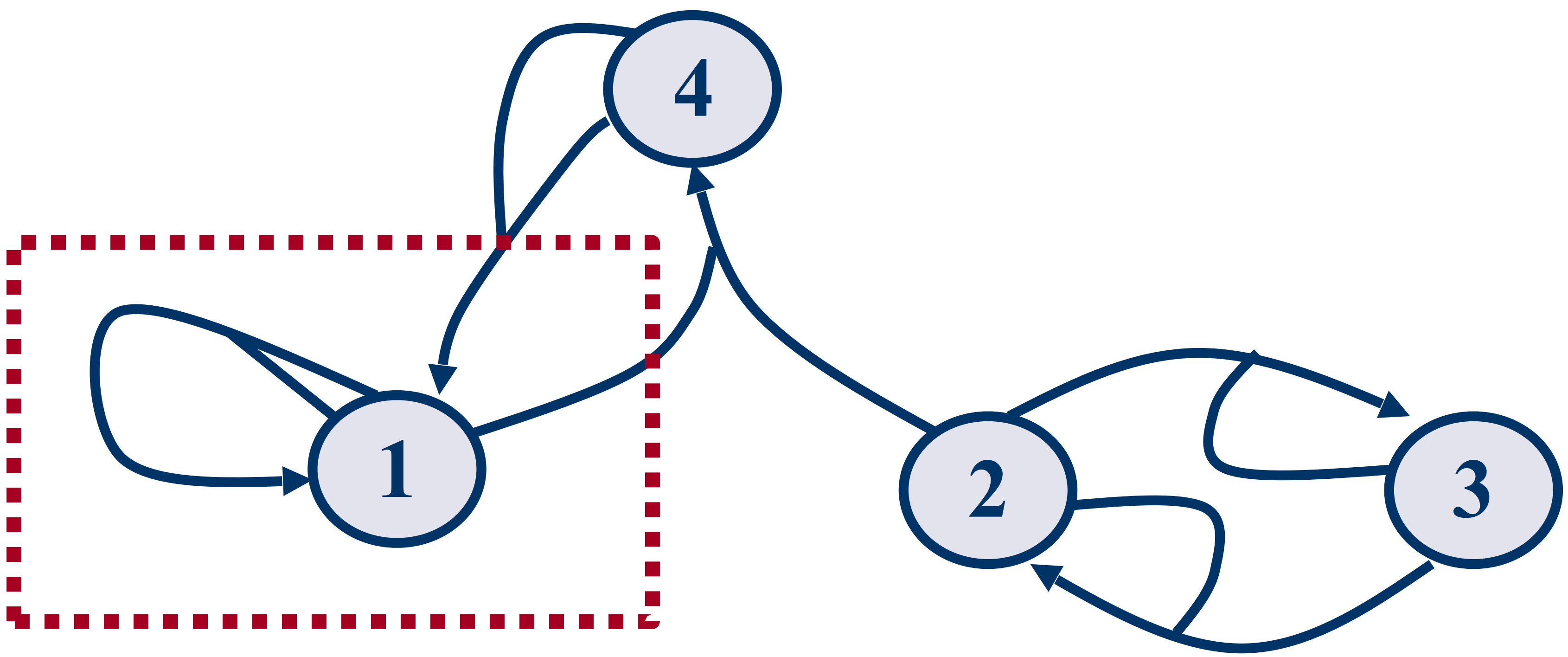
An Example

self-maintaining set



An Example

organisation = closed and self-maintaining



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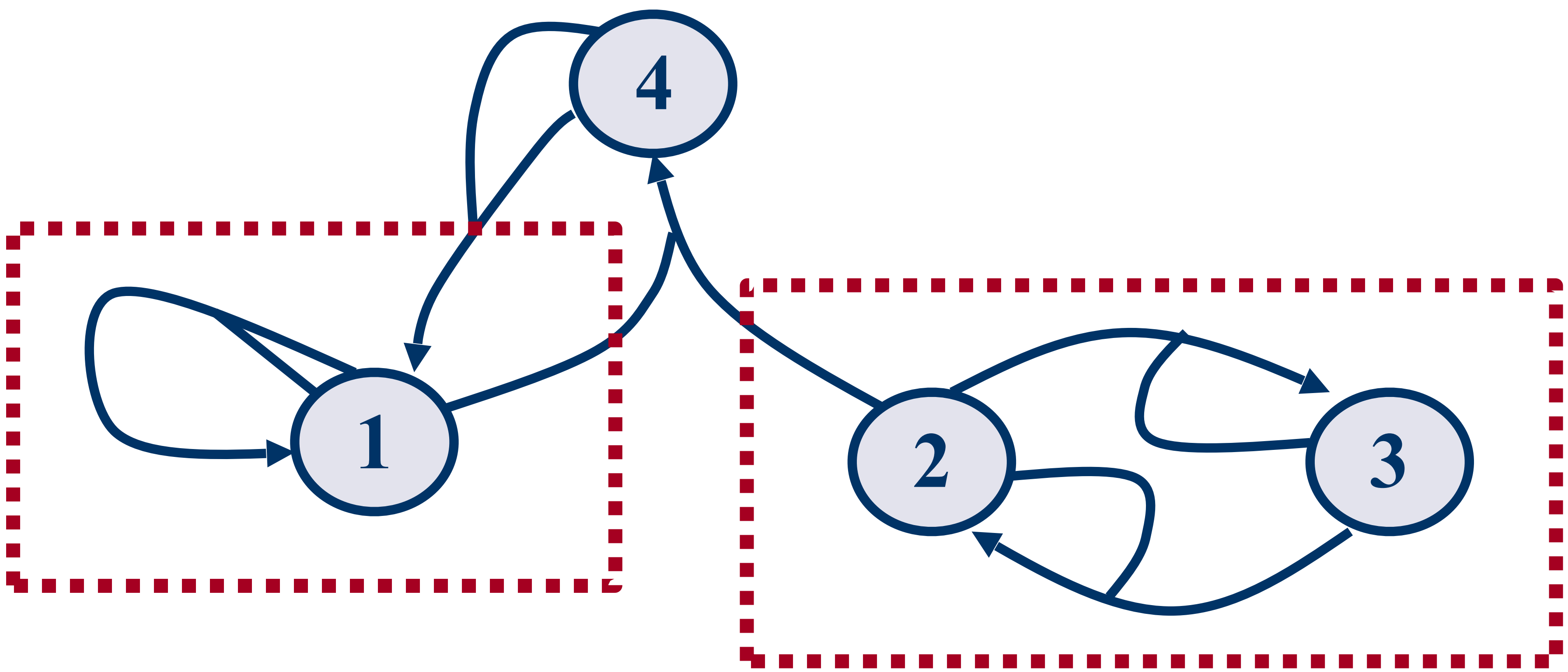

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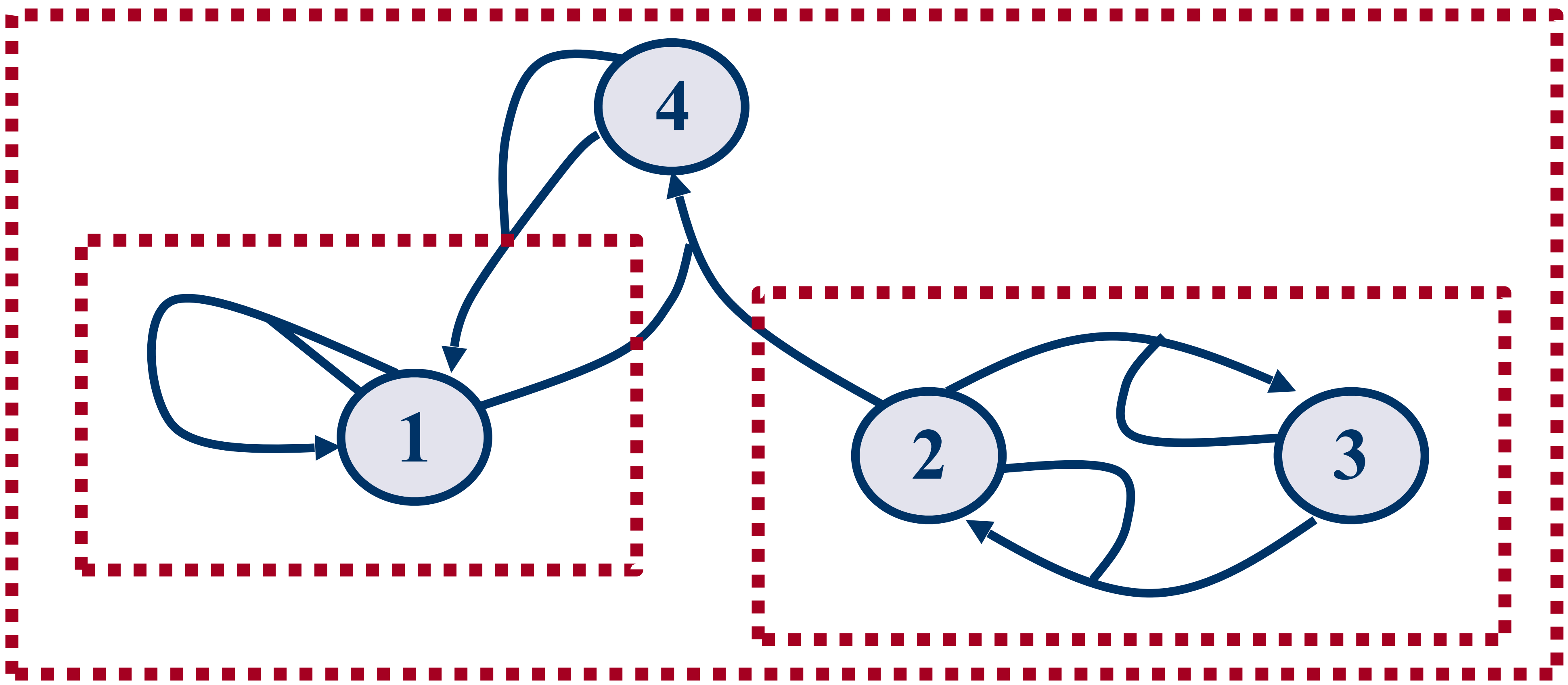
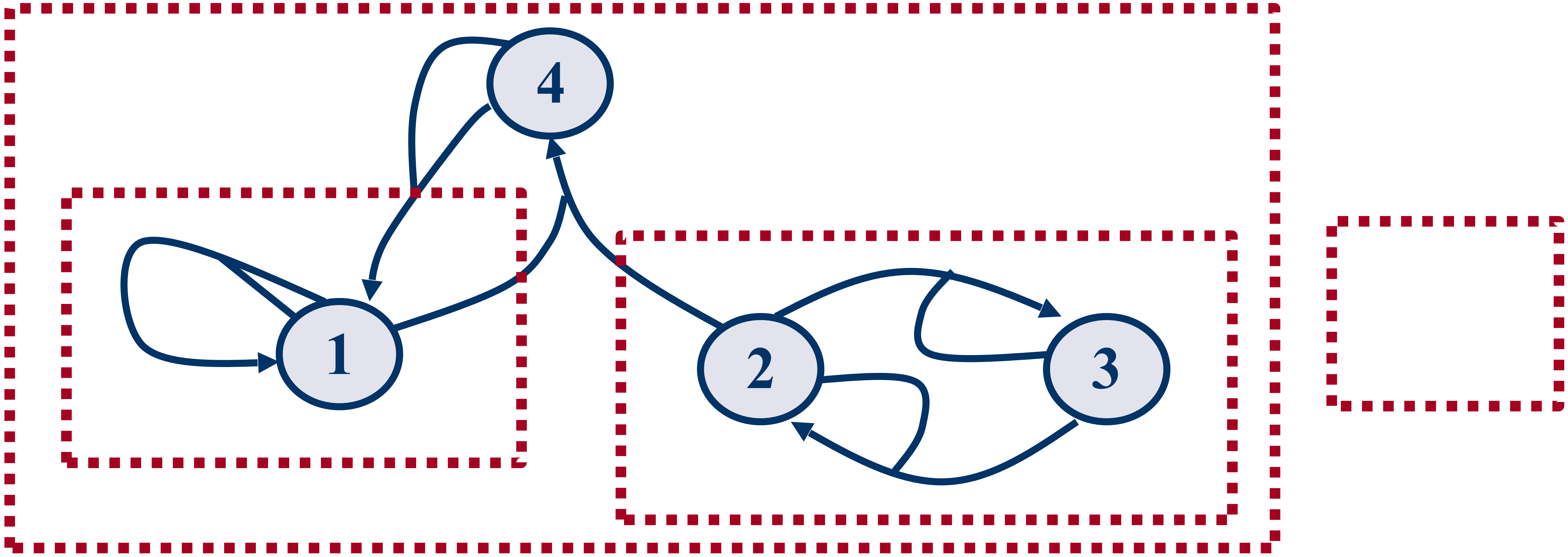


An Example

set of all organisations

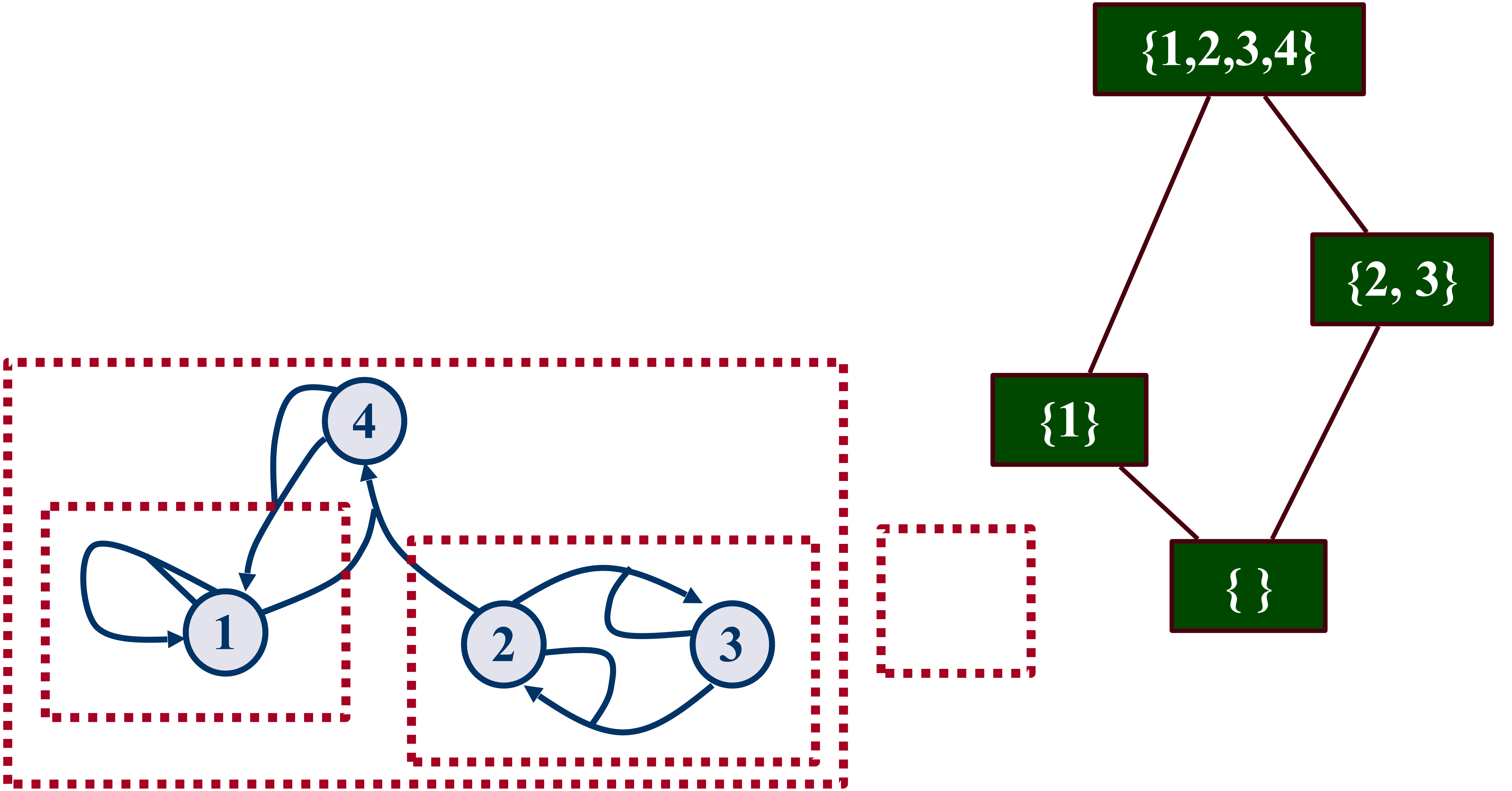


Lattice of organisations

Given the set of all organization (**O**),
given the operation organizational union (⊔),
given the operation organizational intersection (⊓),

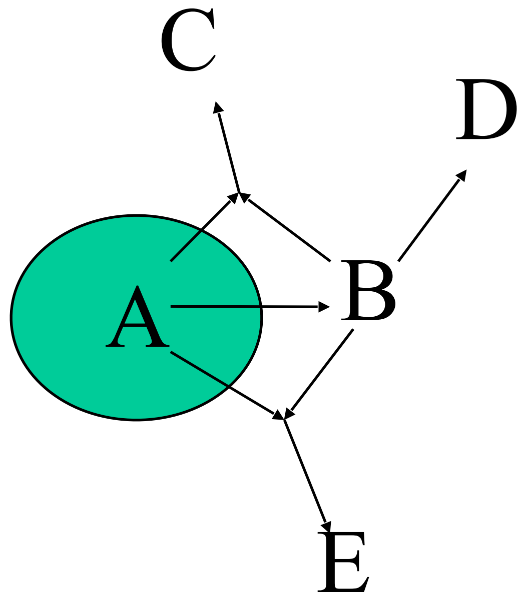
<O, ⊔, ⊓ > is a Lattice.

Lattice of organisations



Closed set generated by a set

- Given any set is possible to generate its closure. The smallest closed set containing it.



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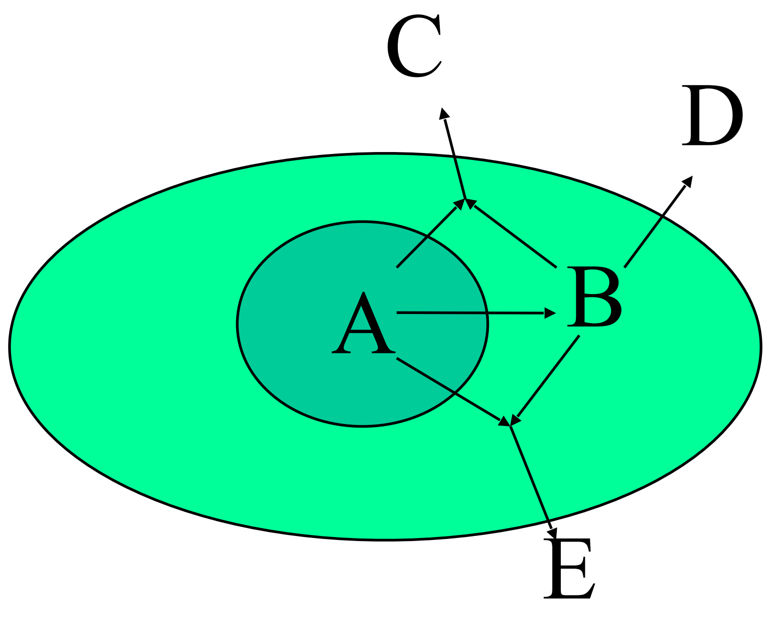

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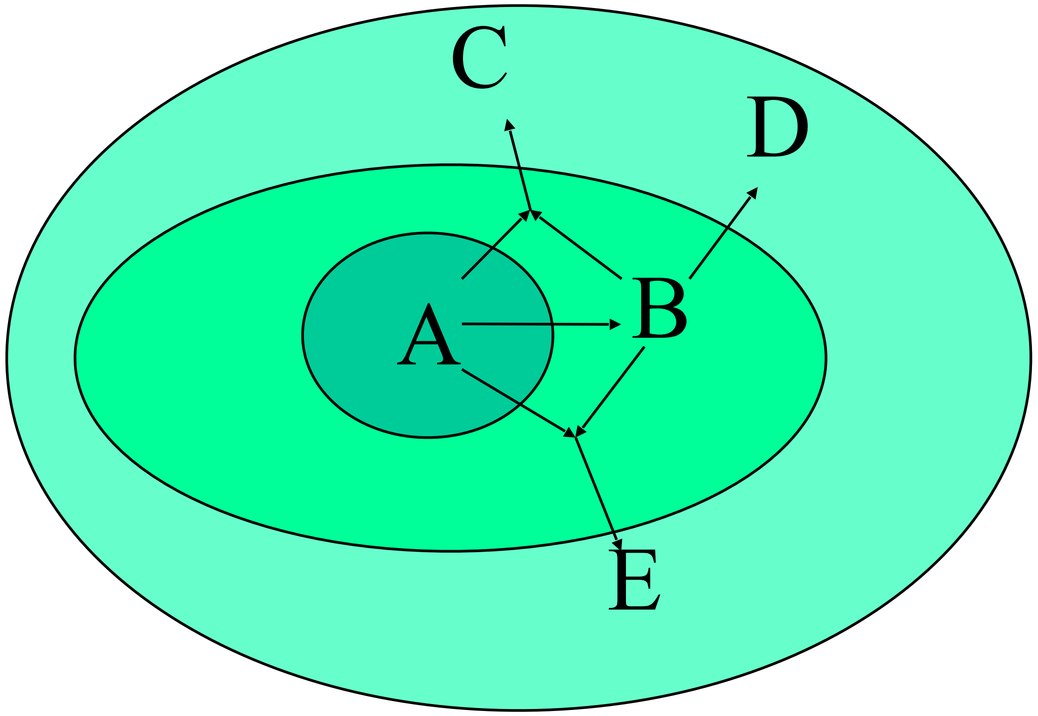

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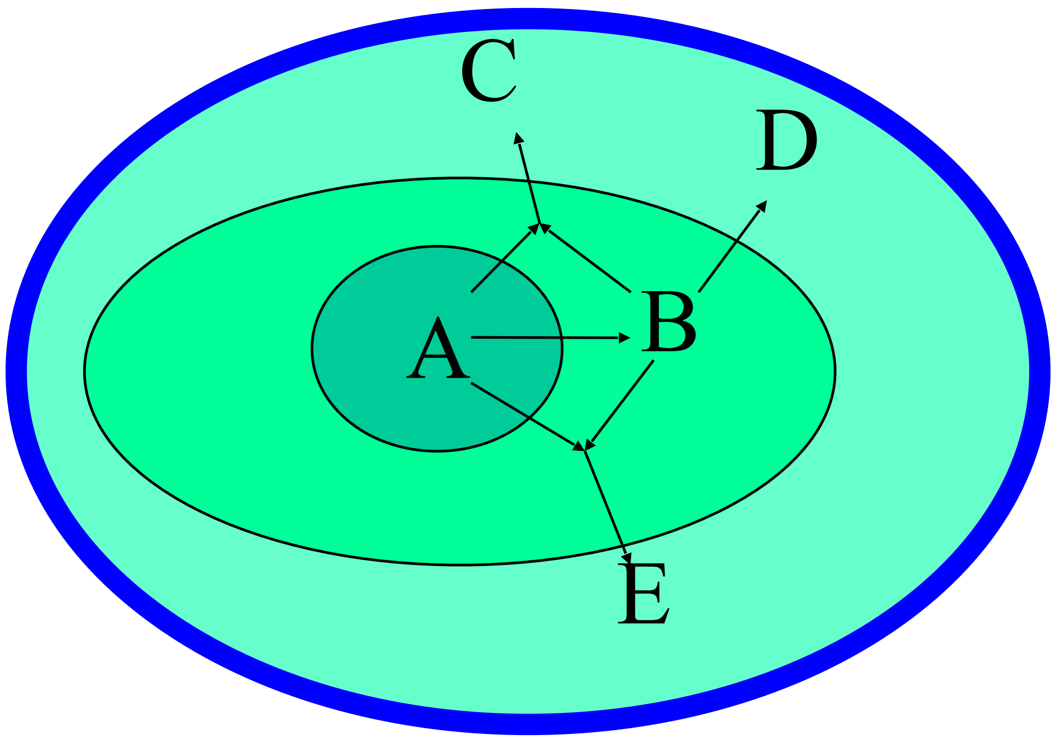
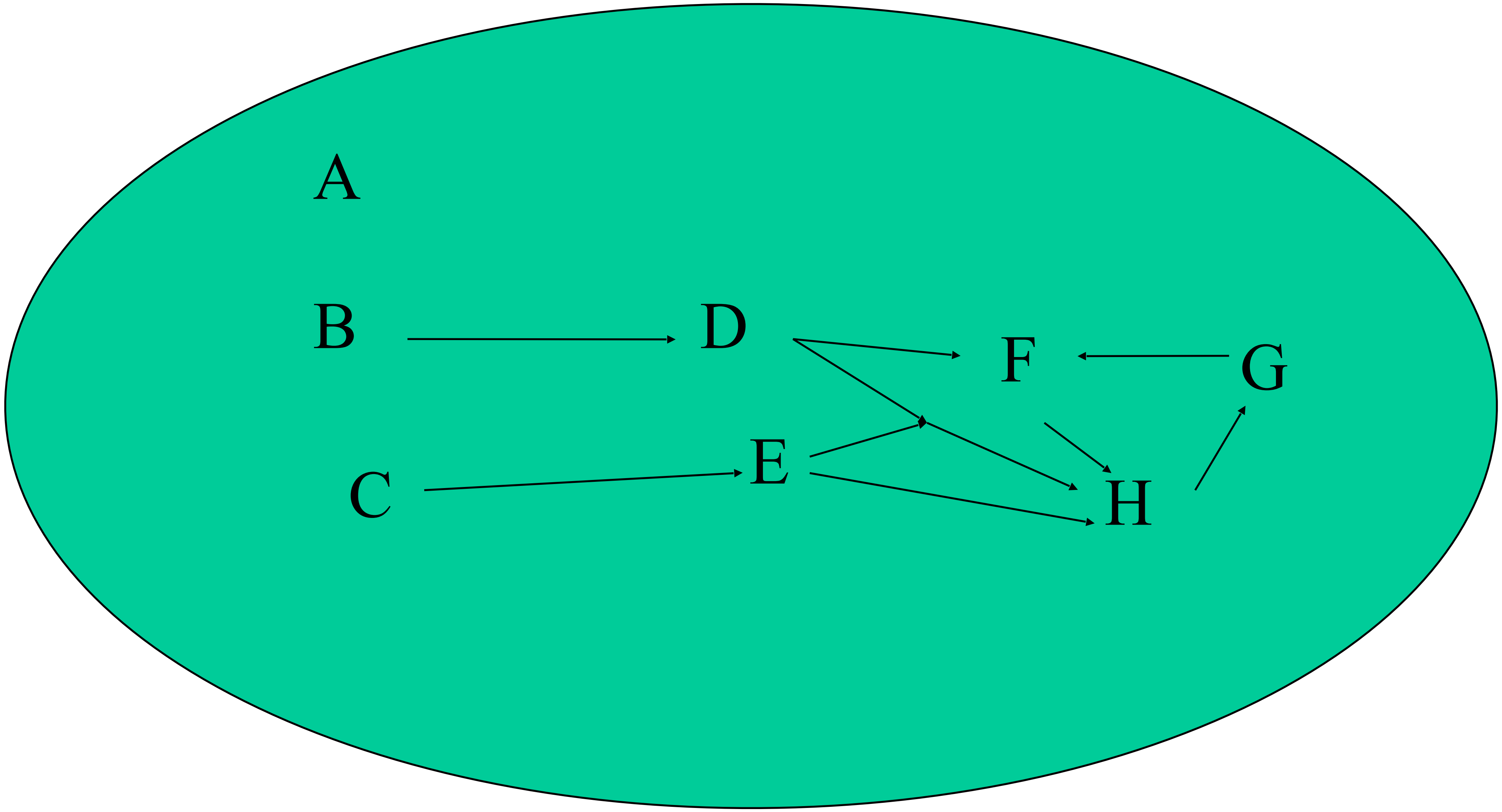


Self Maintaining Set generated by a set.

Given any set is possible to reduce to its self maintaining subset.



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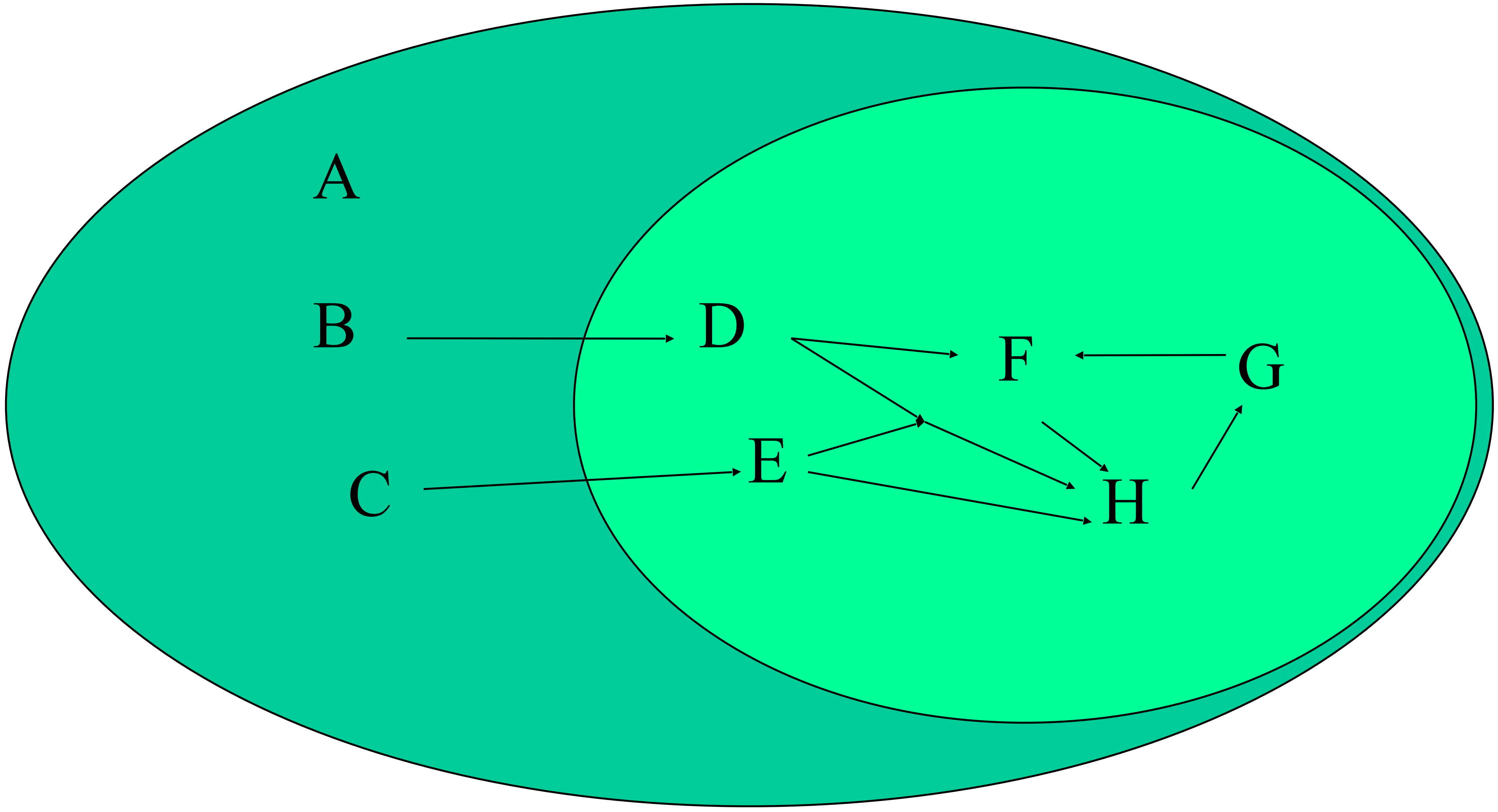

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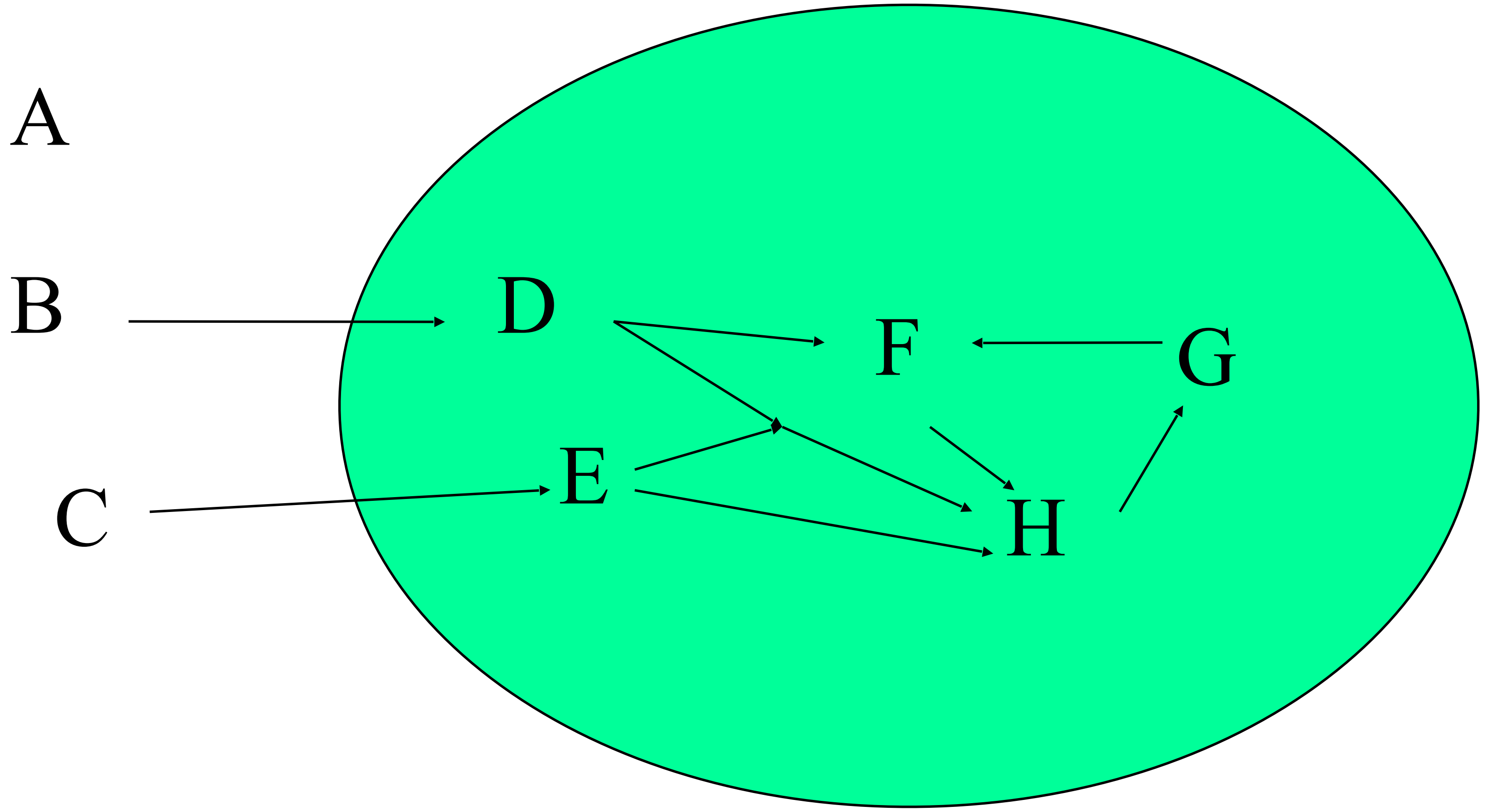

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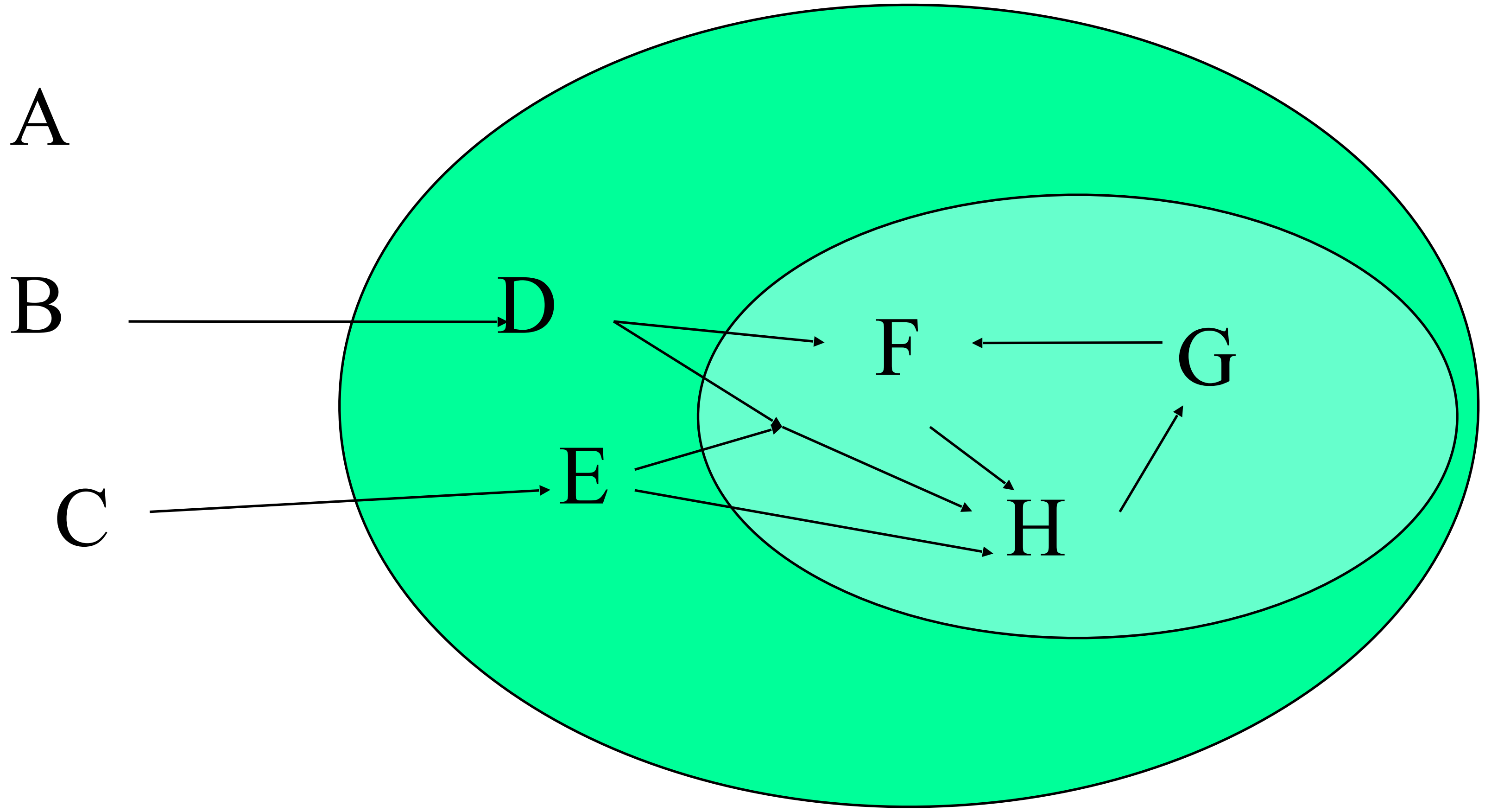

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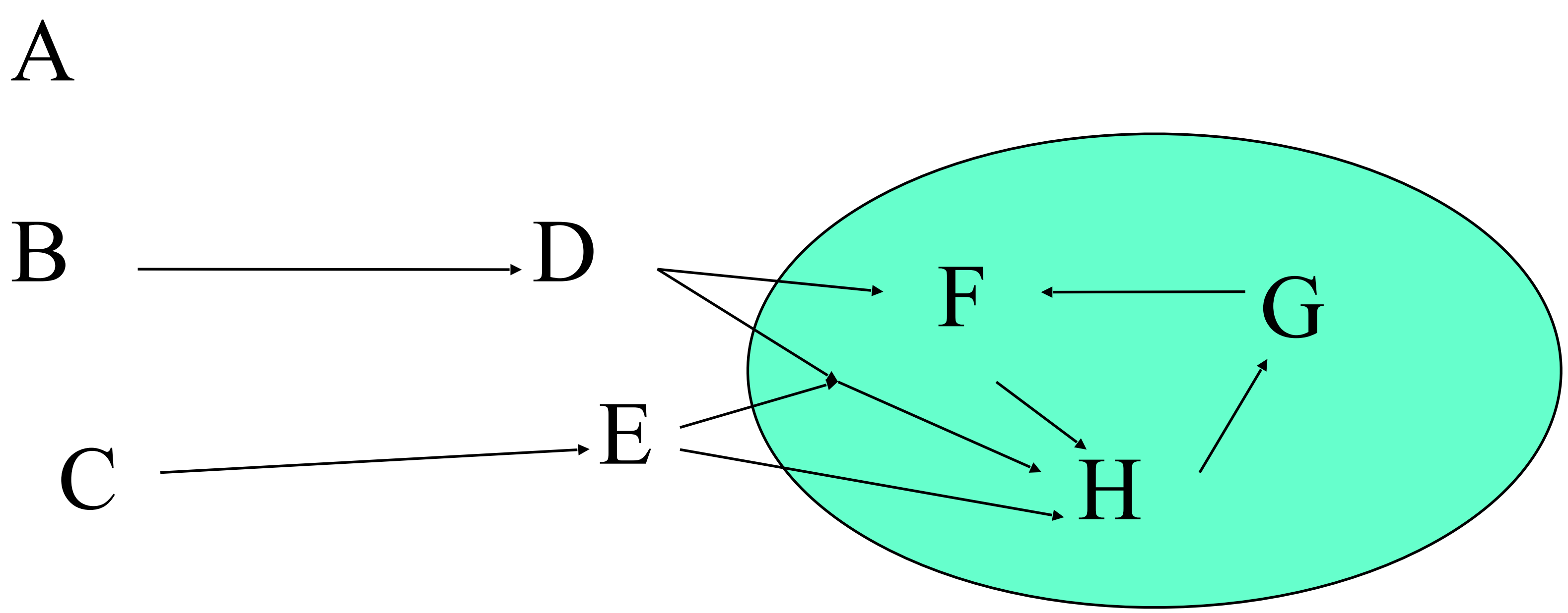

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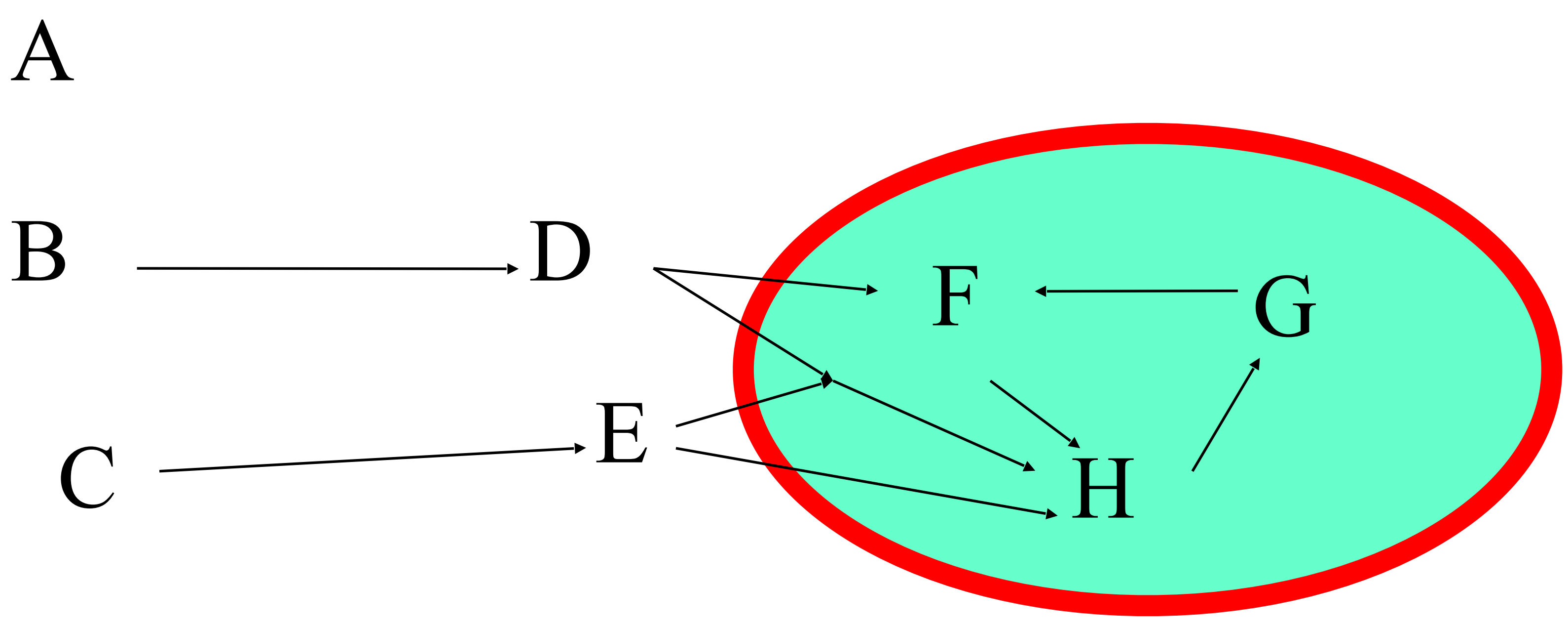


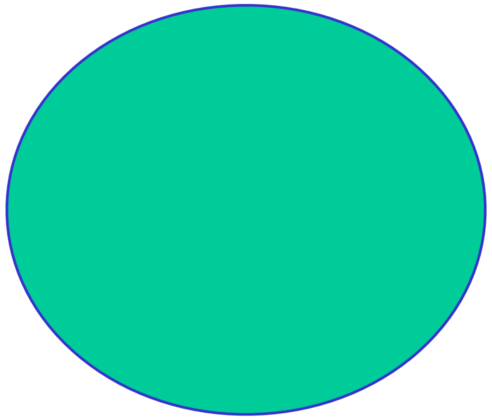
Organisation generated by a subset

- In the same way given any set it uniquely generates a Organisation.
- This is done by first taking the closure of the set
- then the biggest self maintaining set in the closed set.

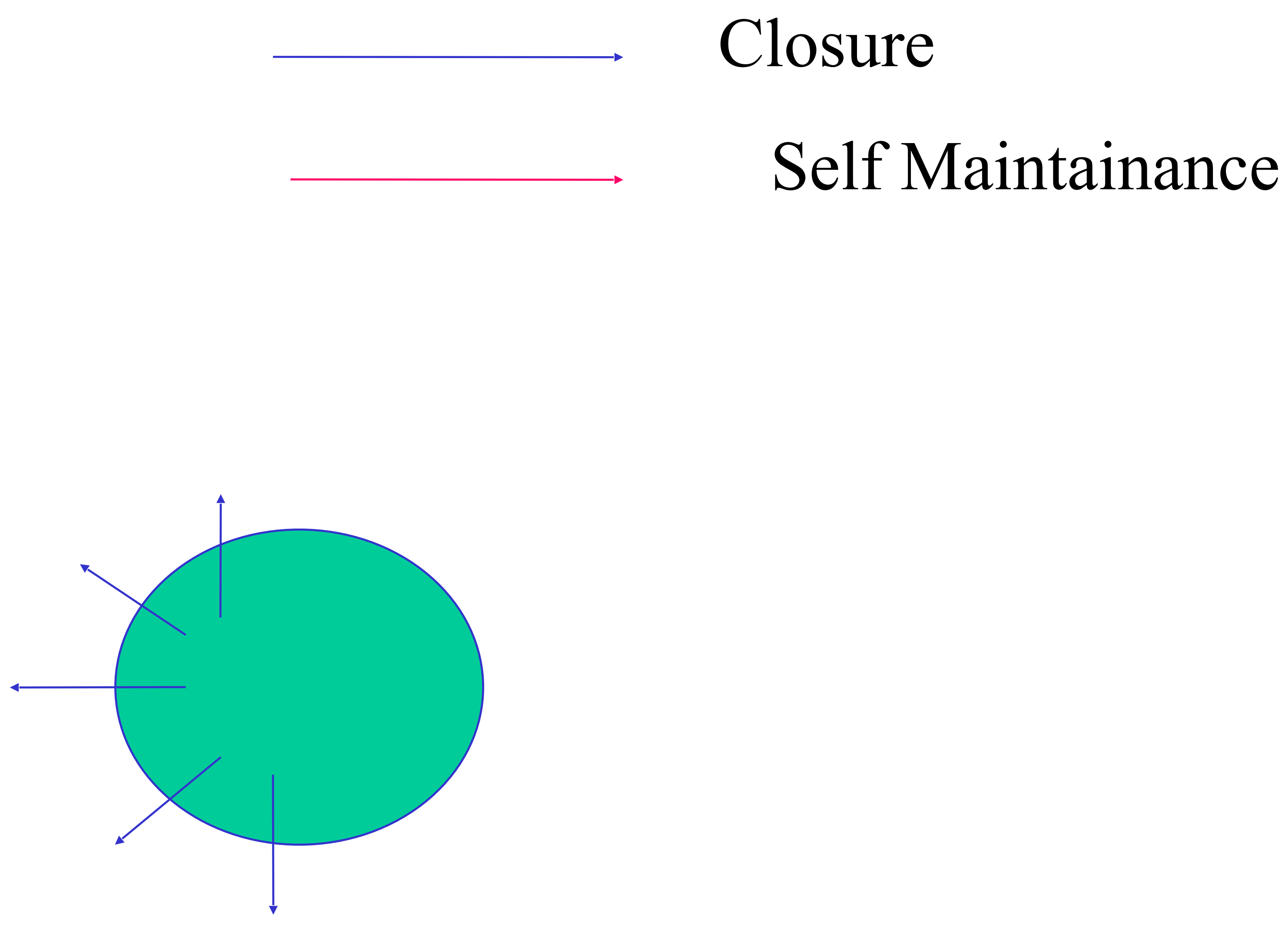
Organisation generated by a subset

Closure

Self Maintainance



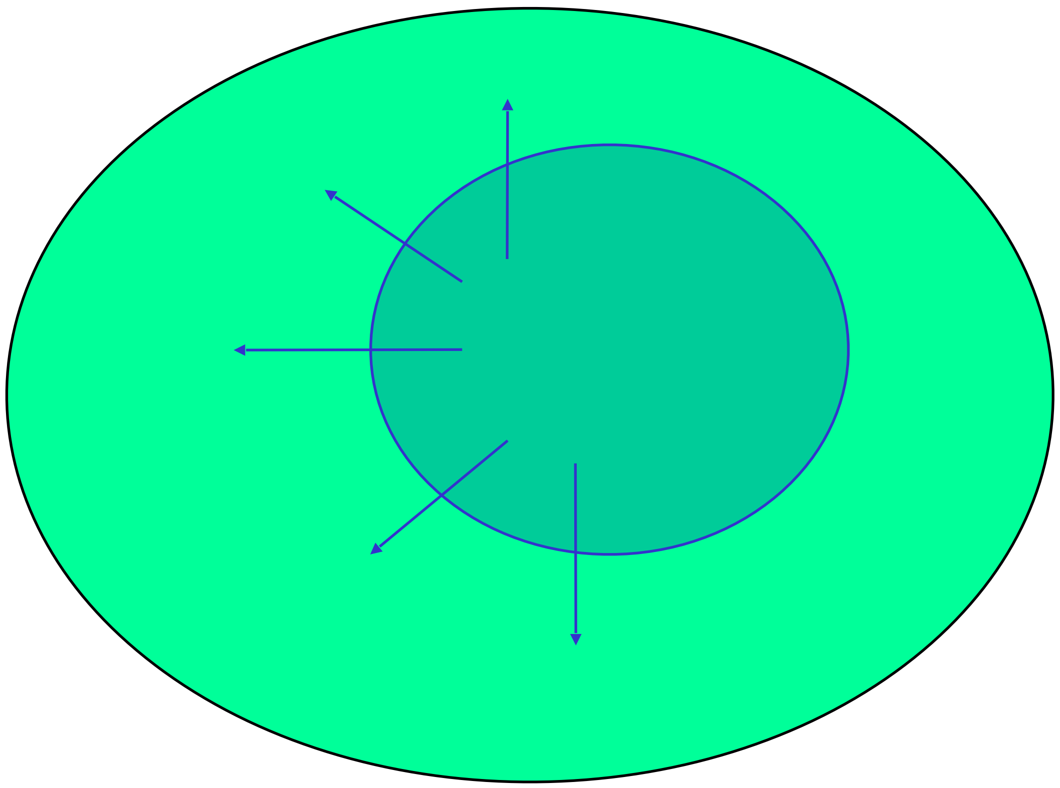
Organisation generated by a subset



Organisation generated by a subset

Closure

Self Maintainance



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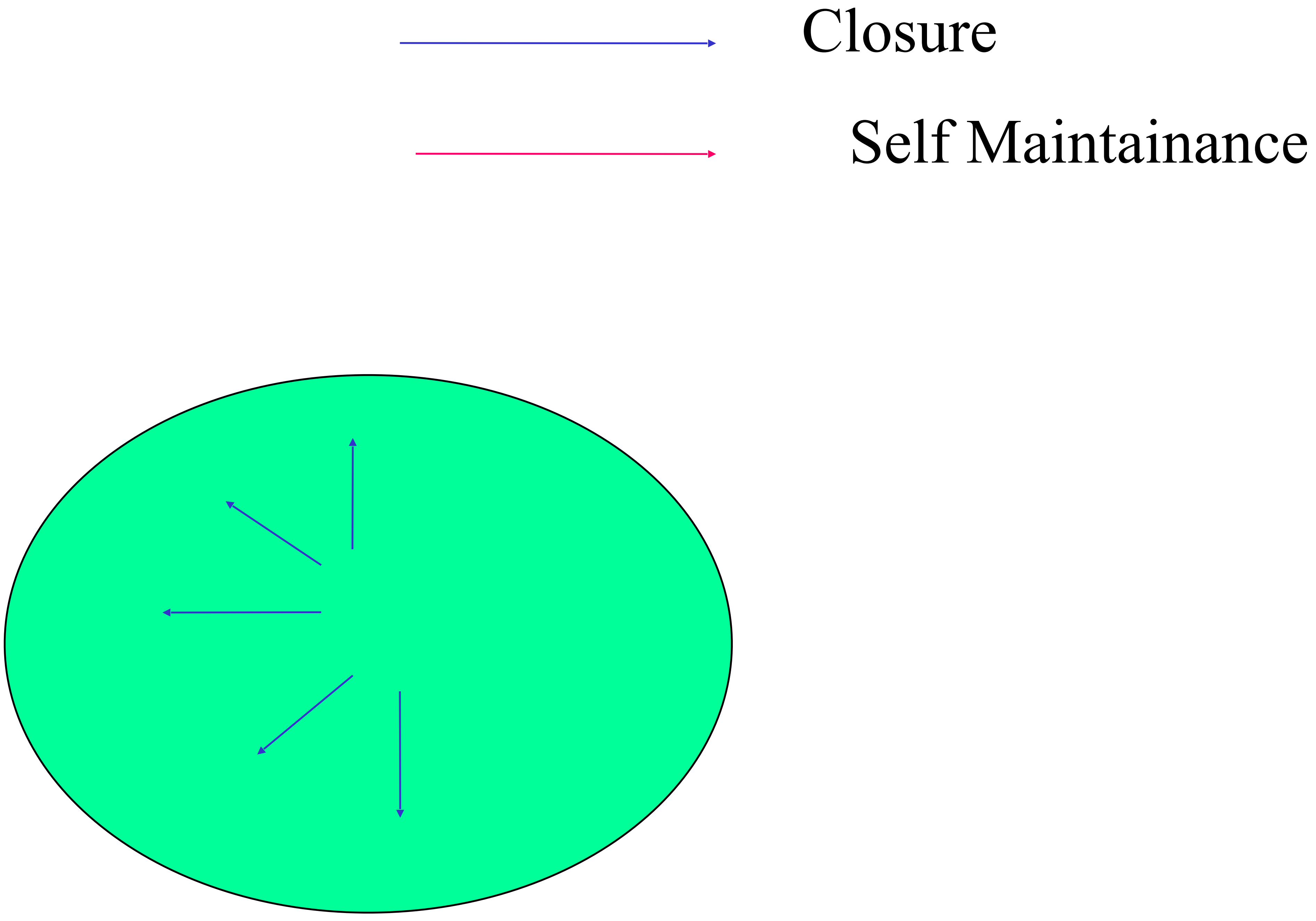

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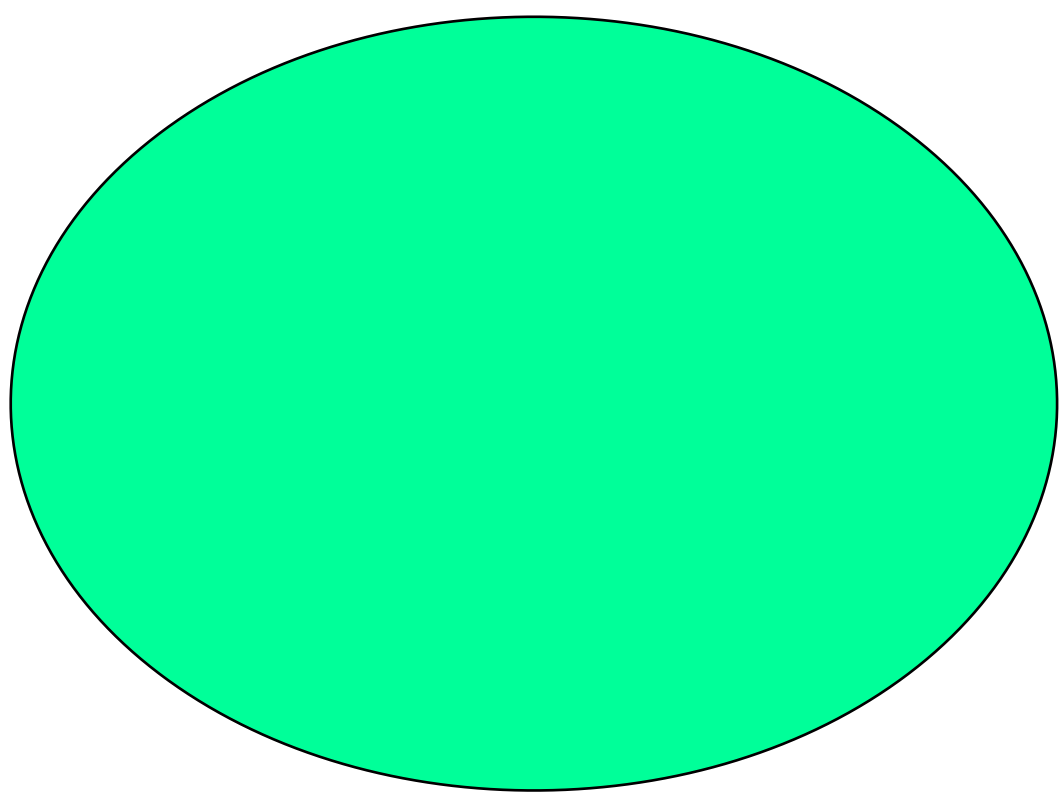

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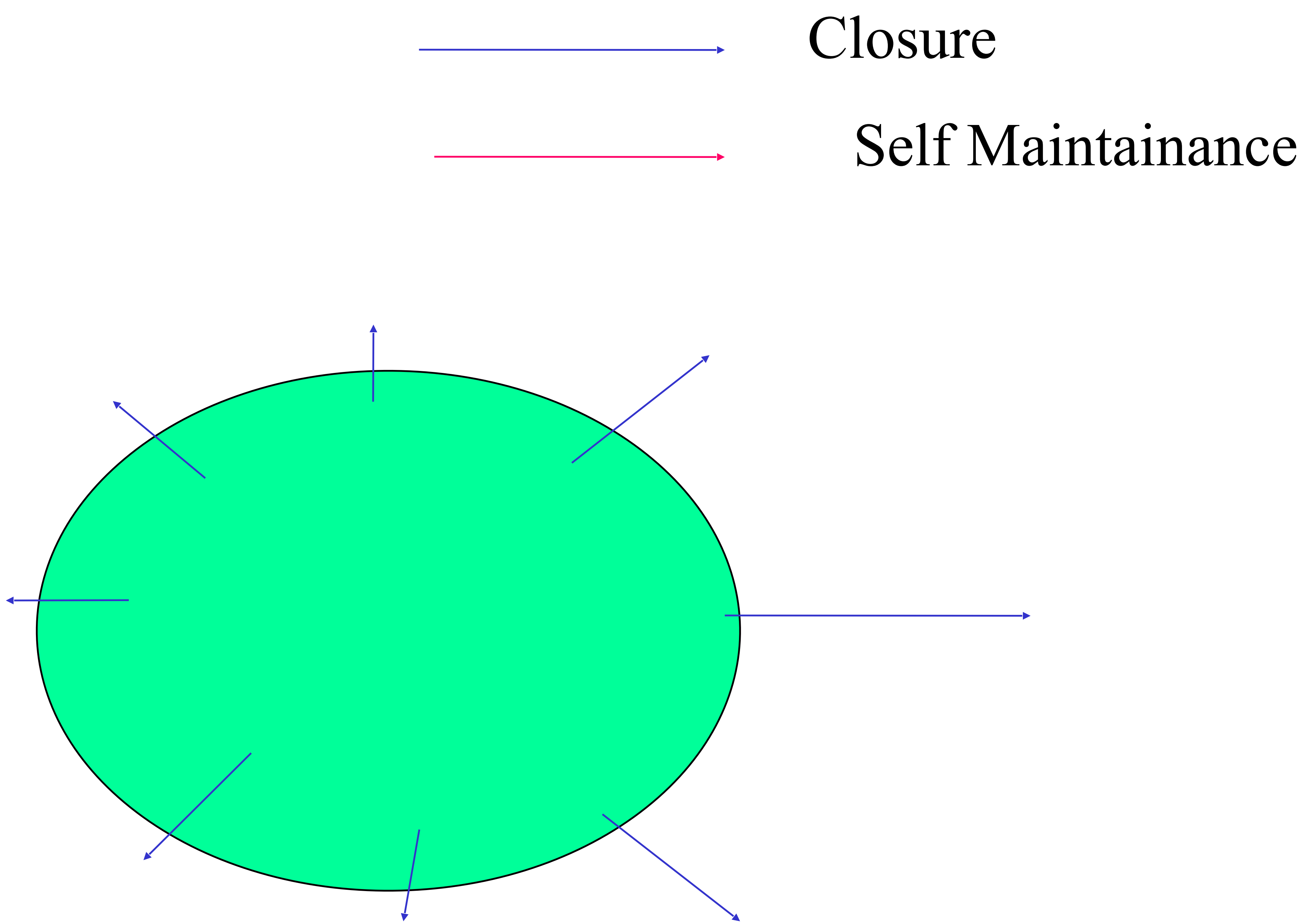

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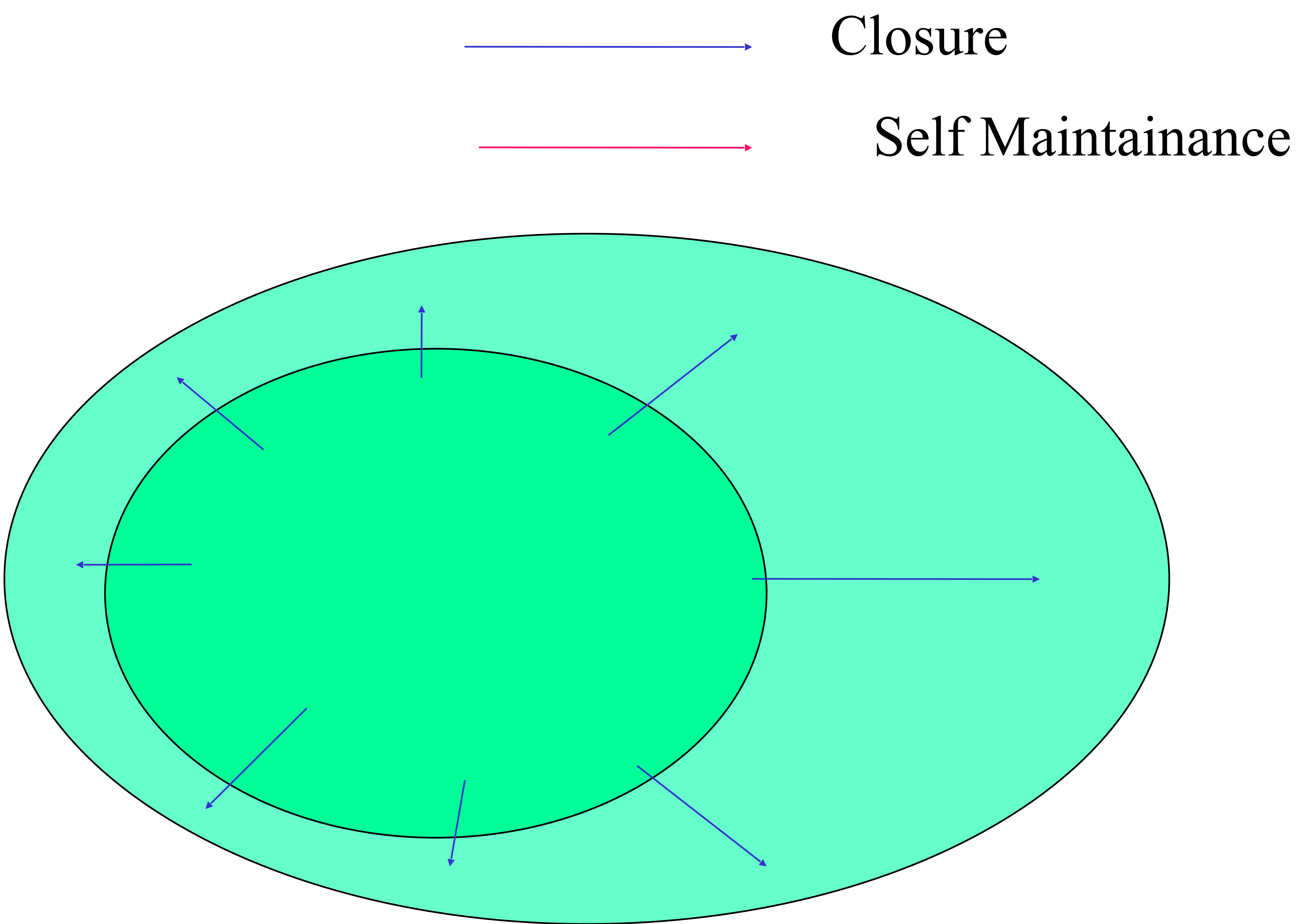

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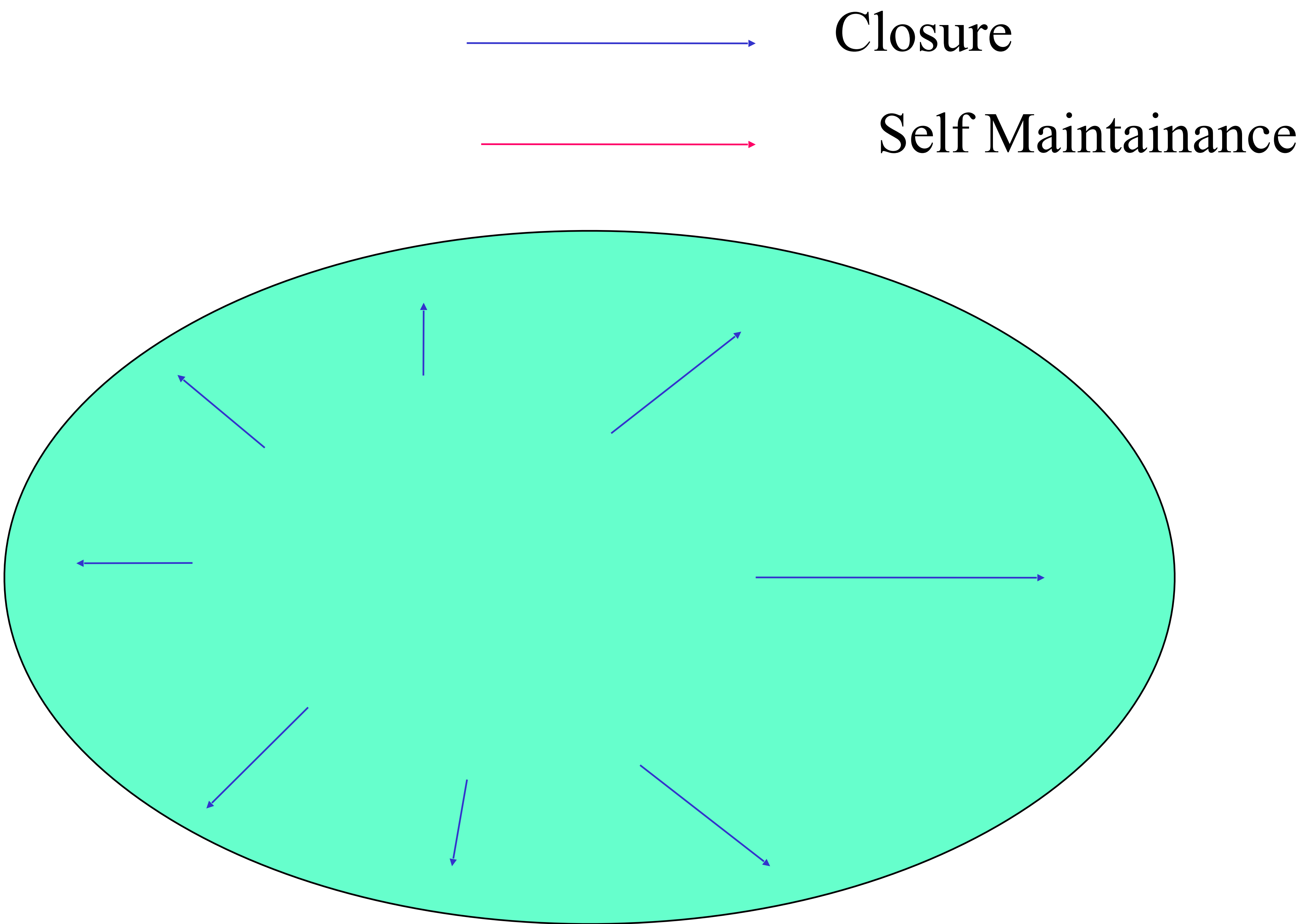

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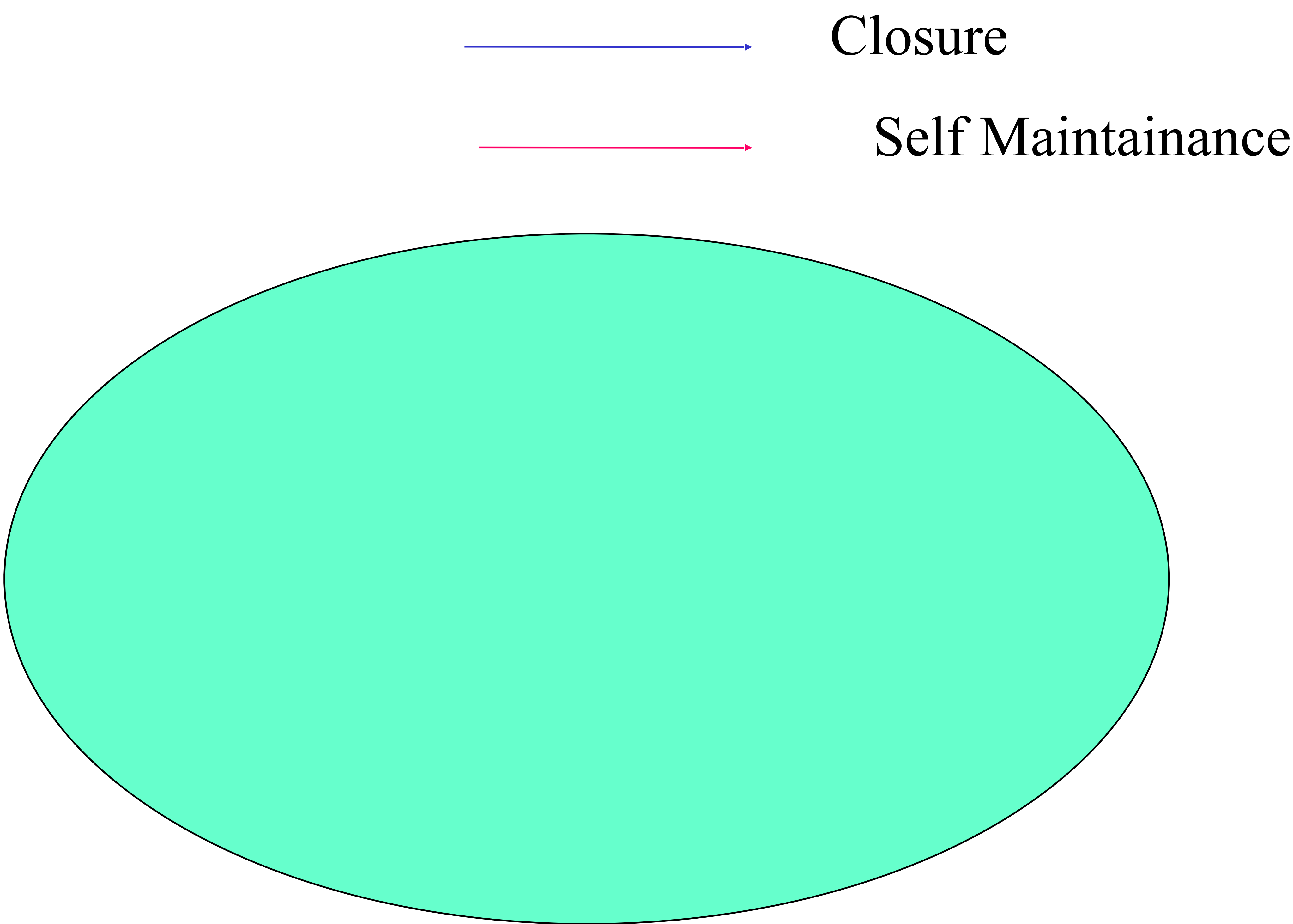

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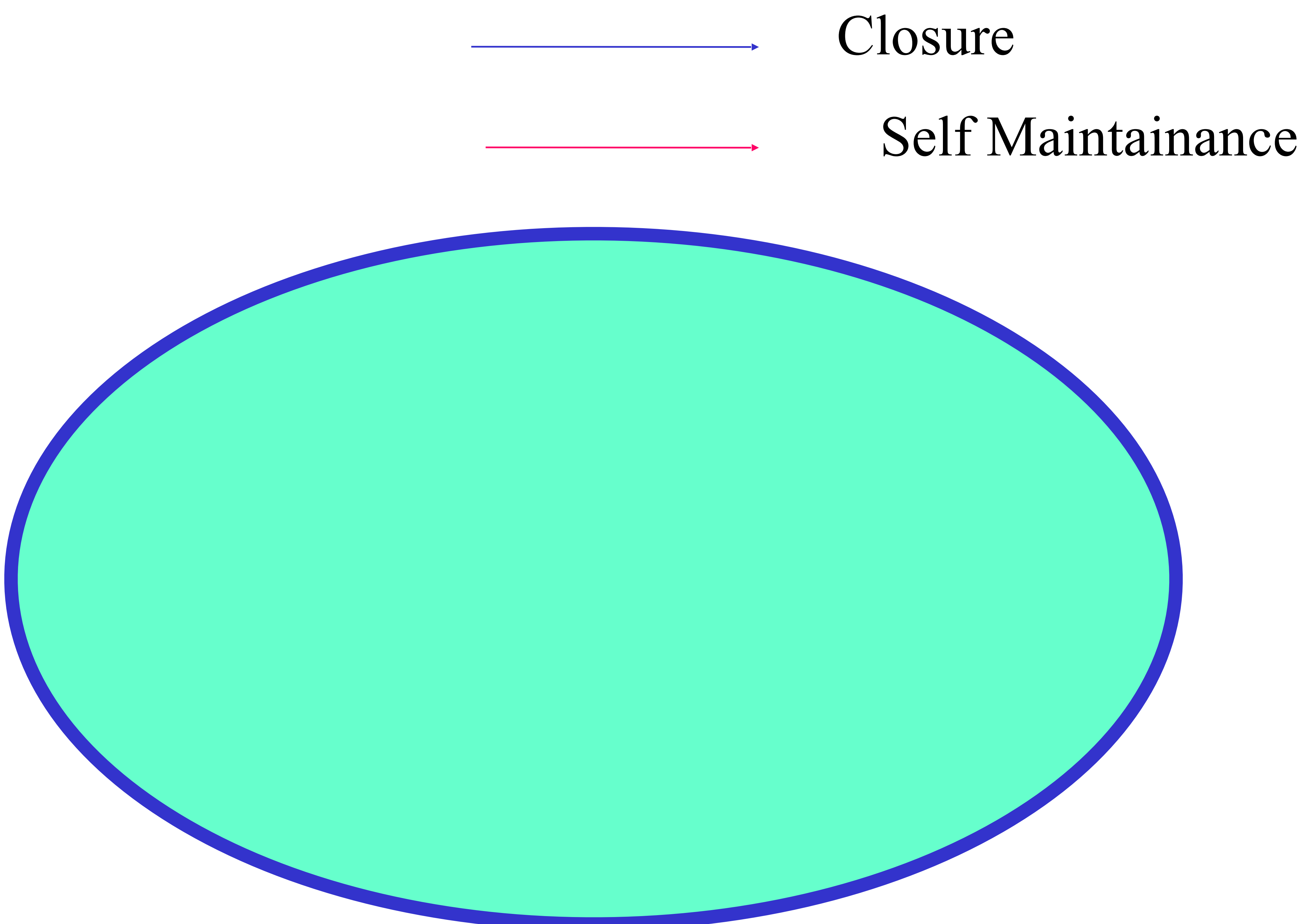

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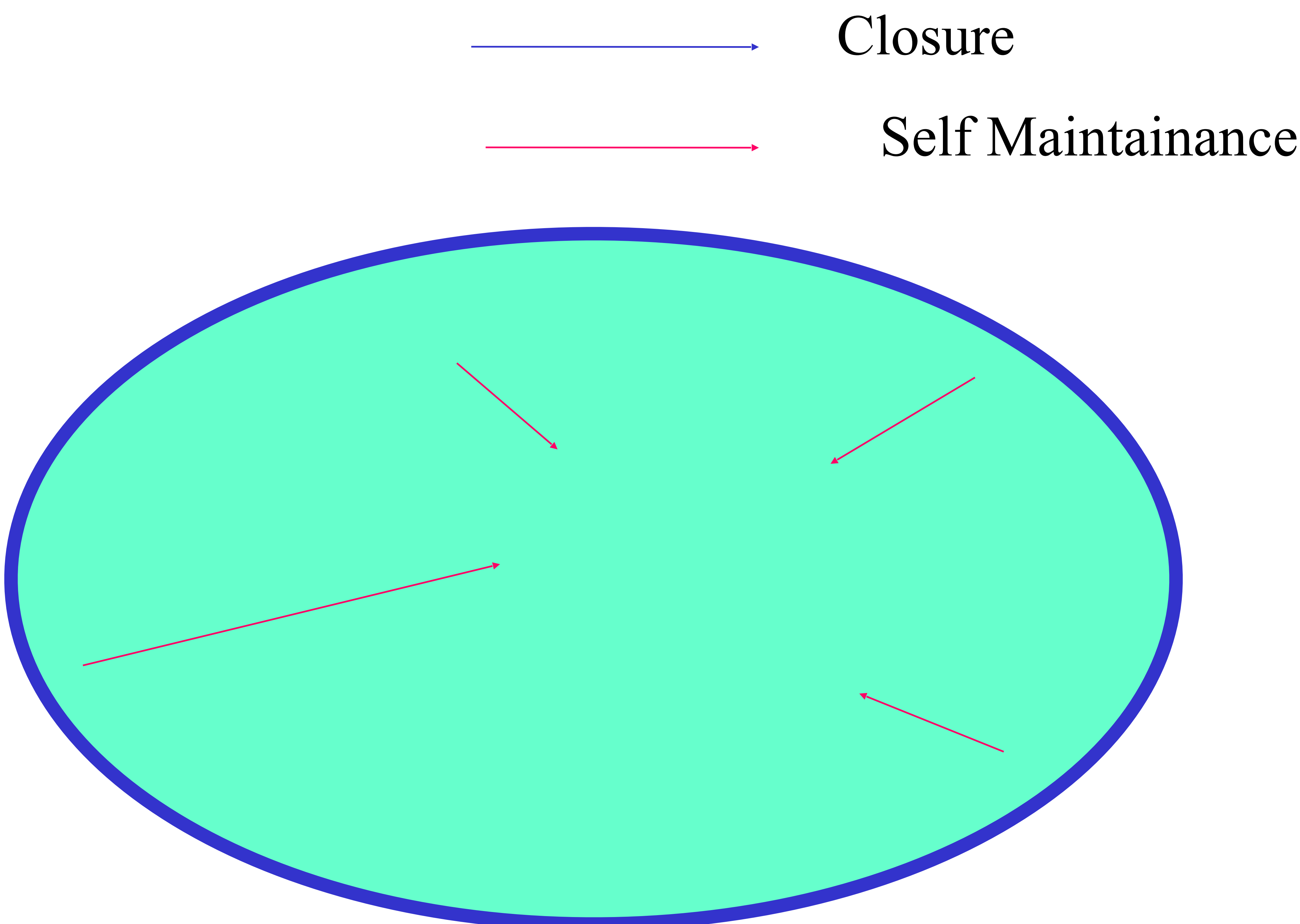

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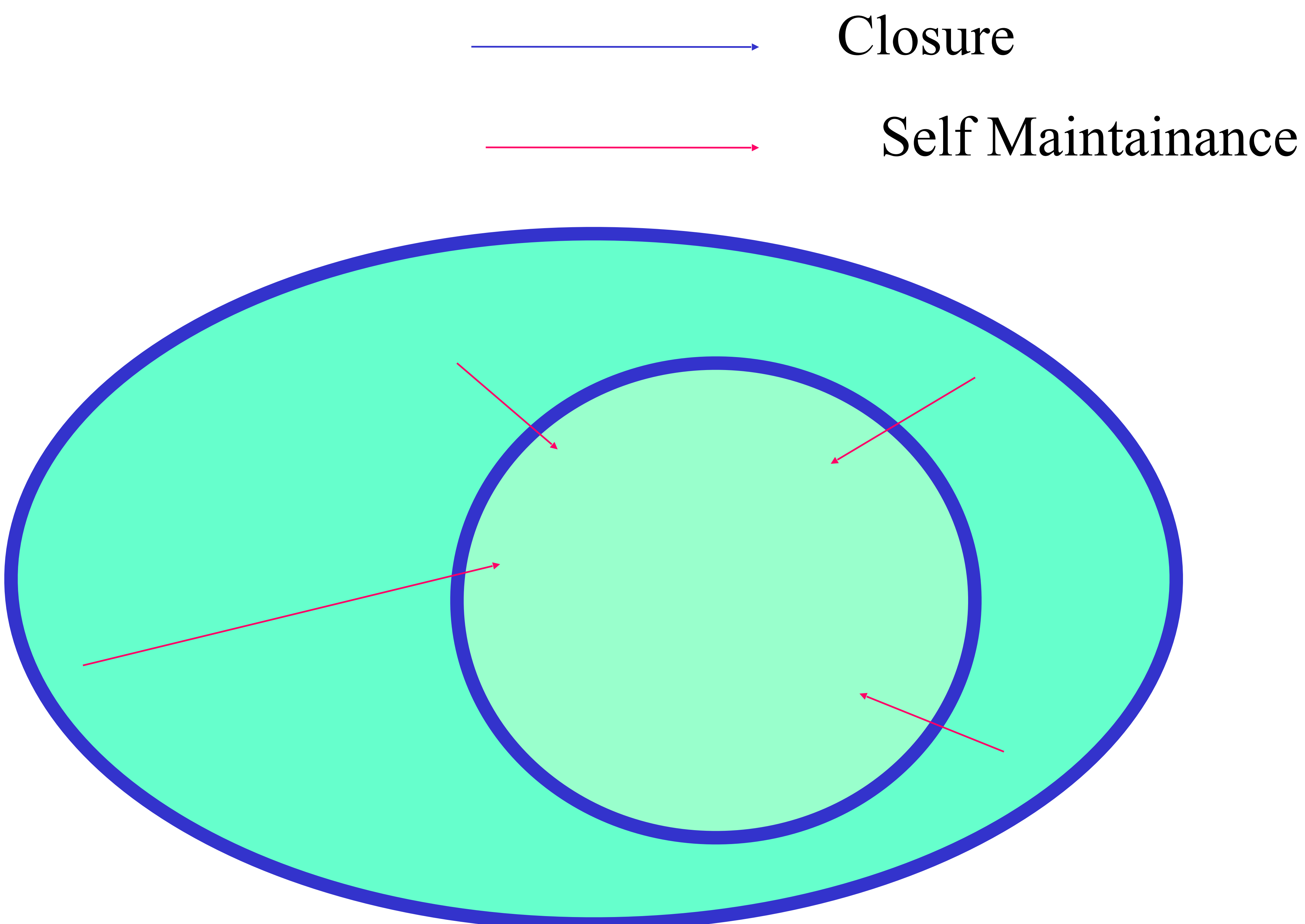

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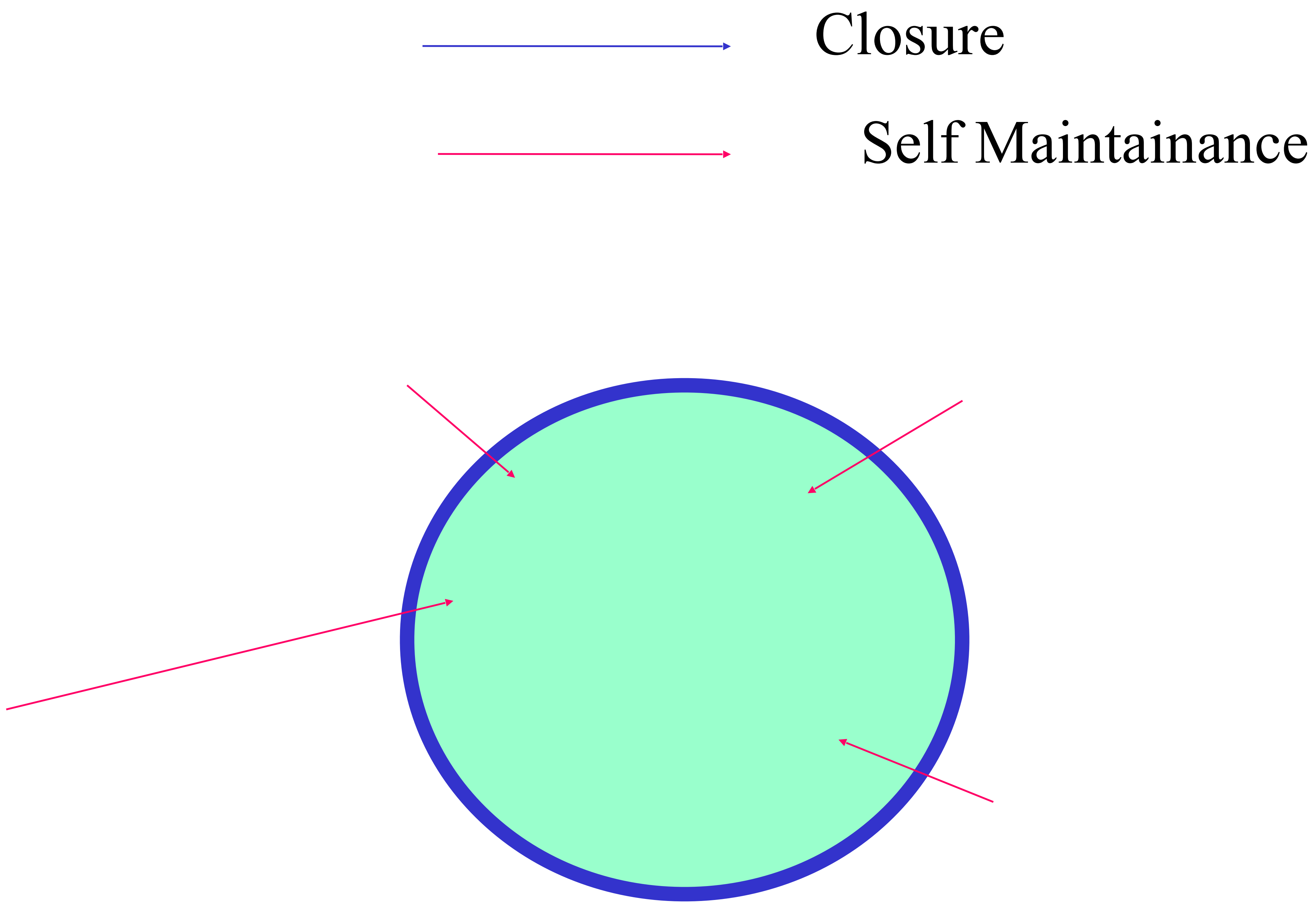

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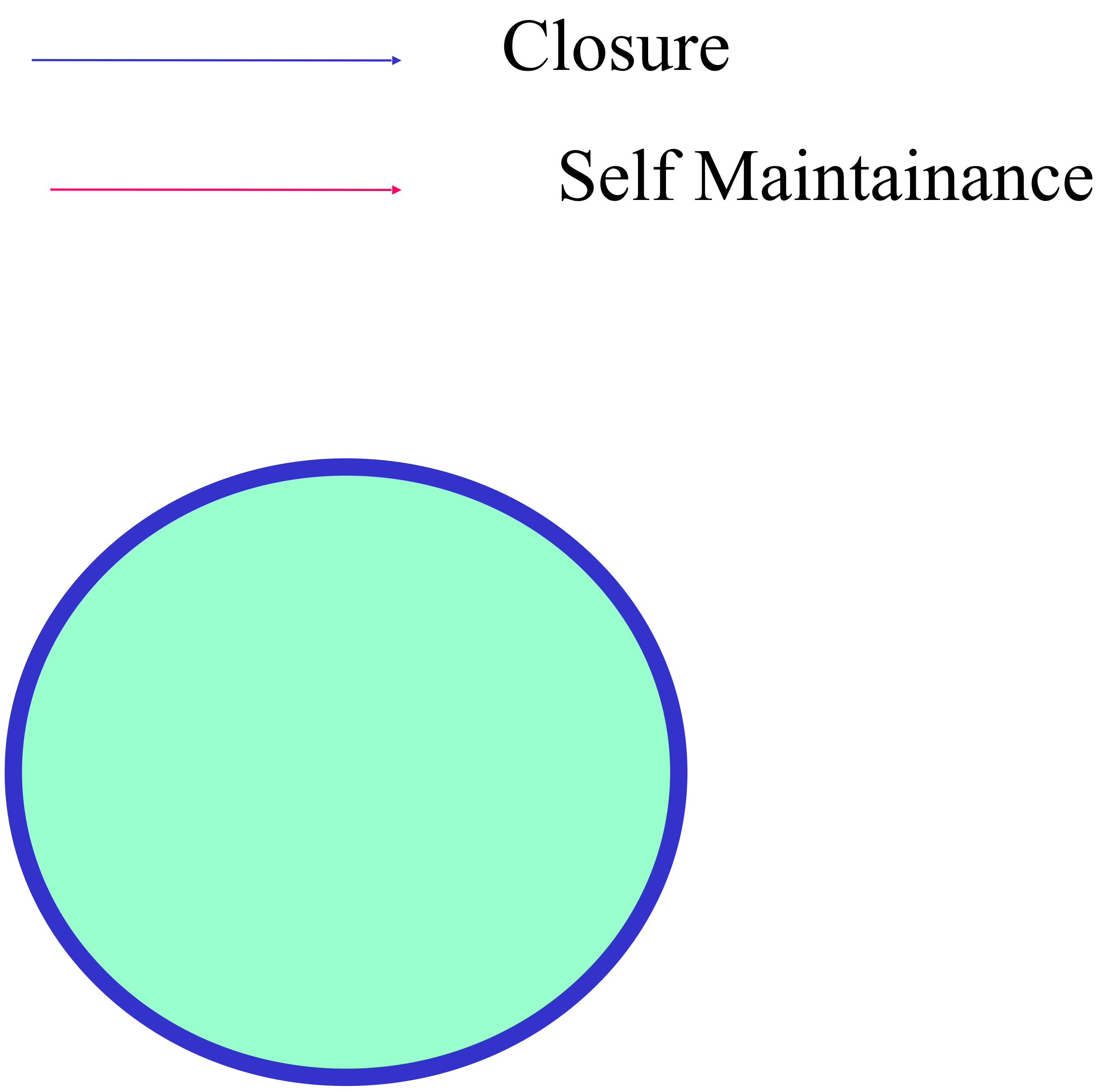
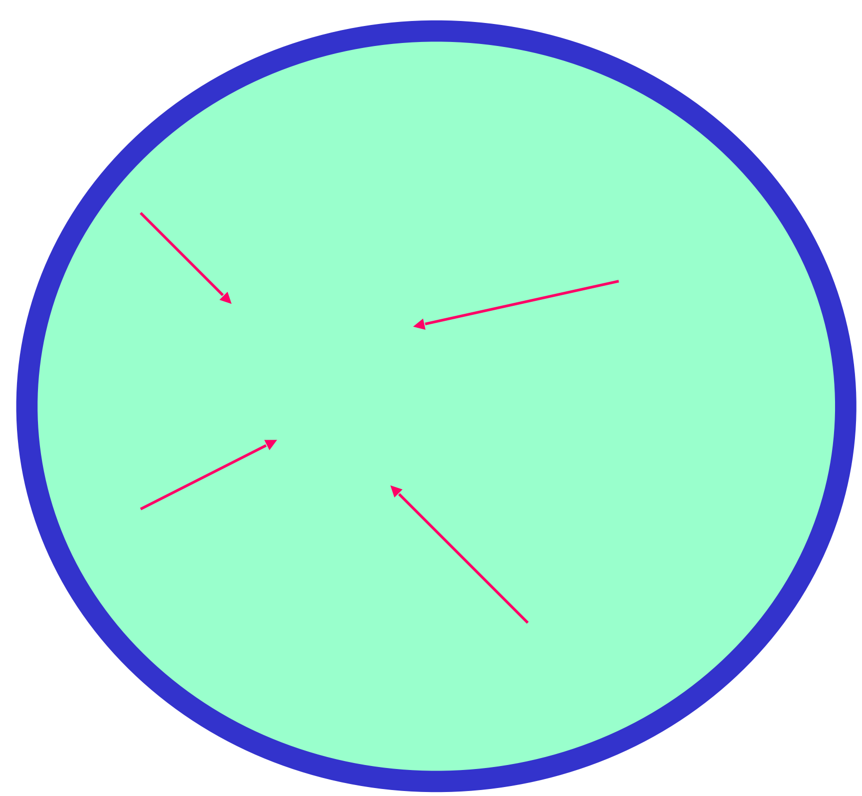


Organisation generated by a subset

Closure

Self Maintainance



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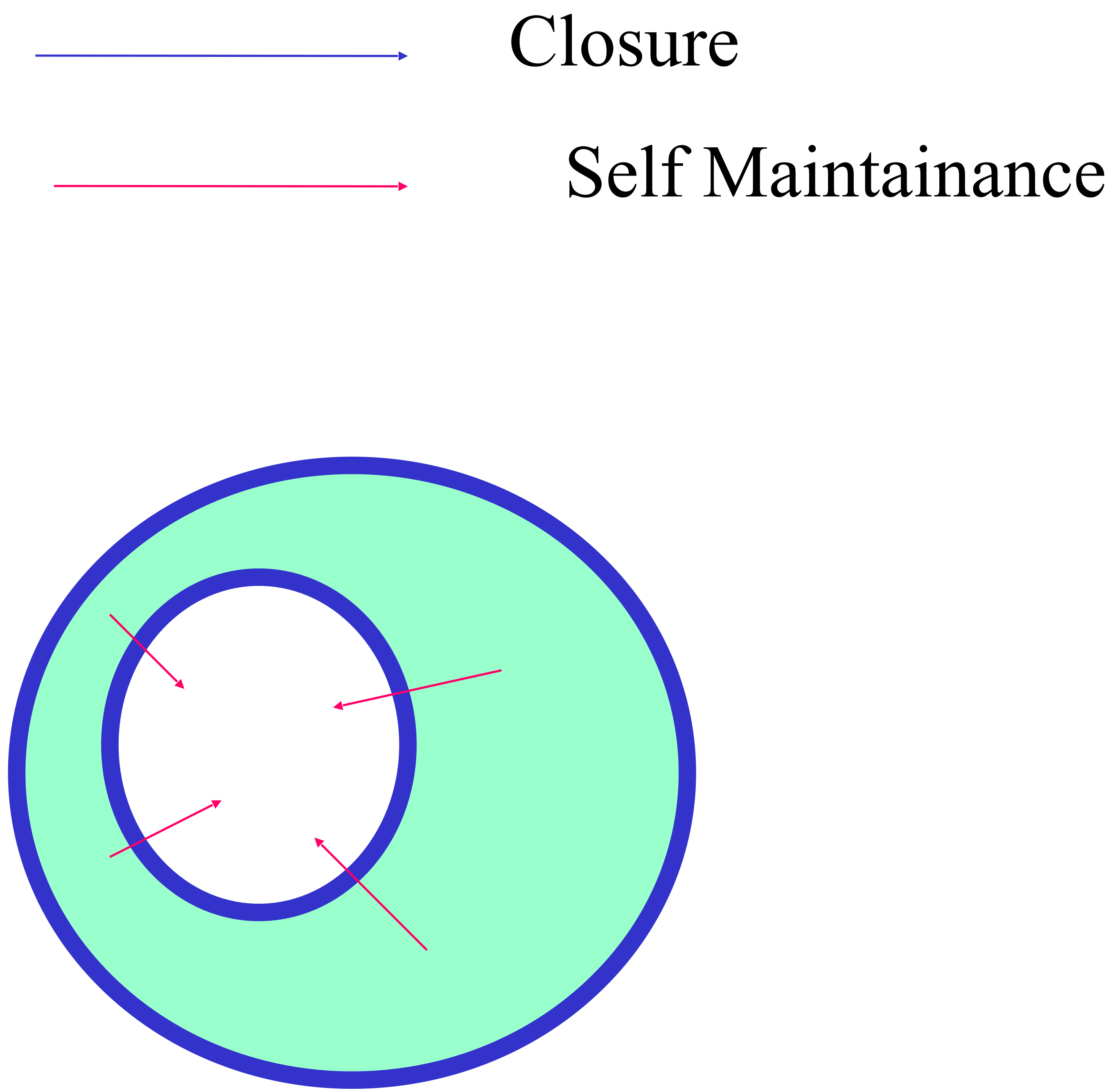

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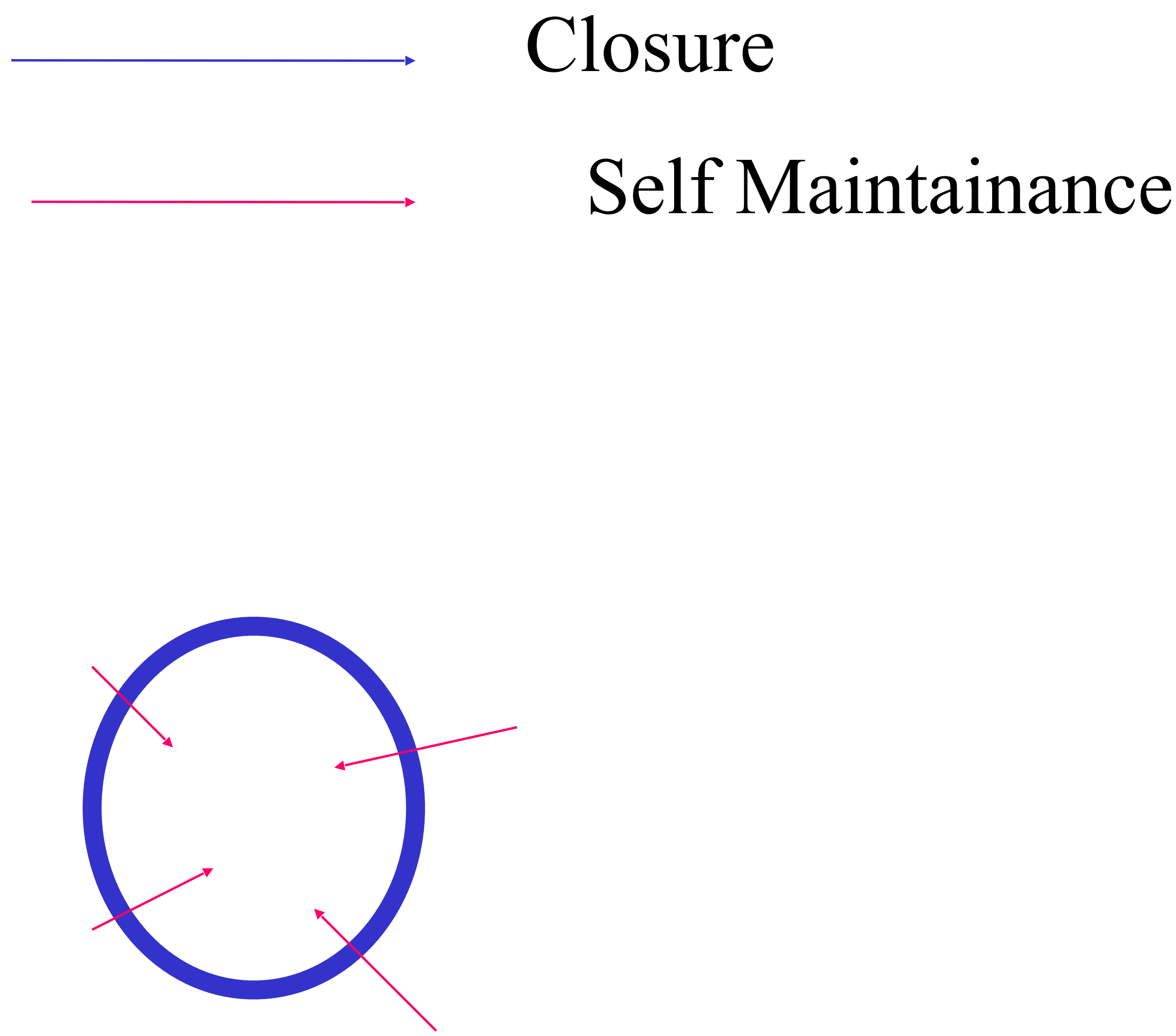

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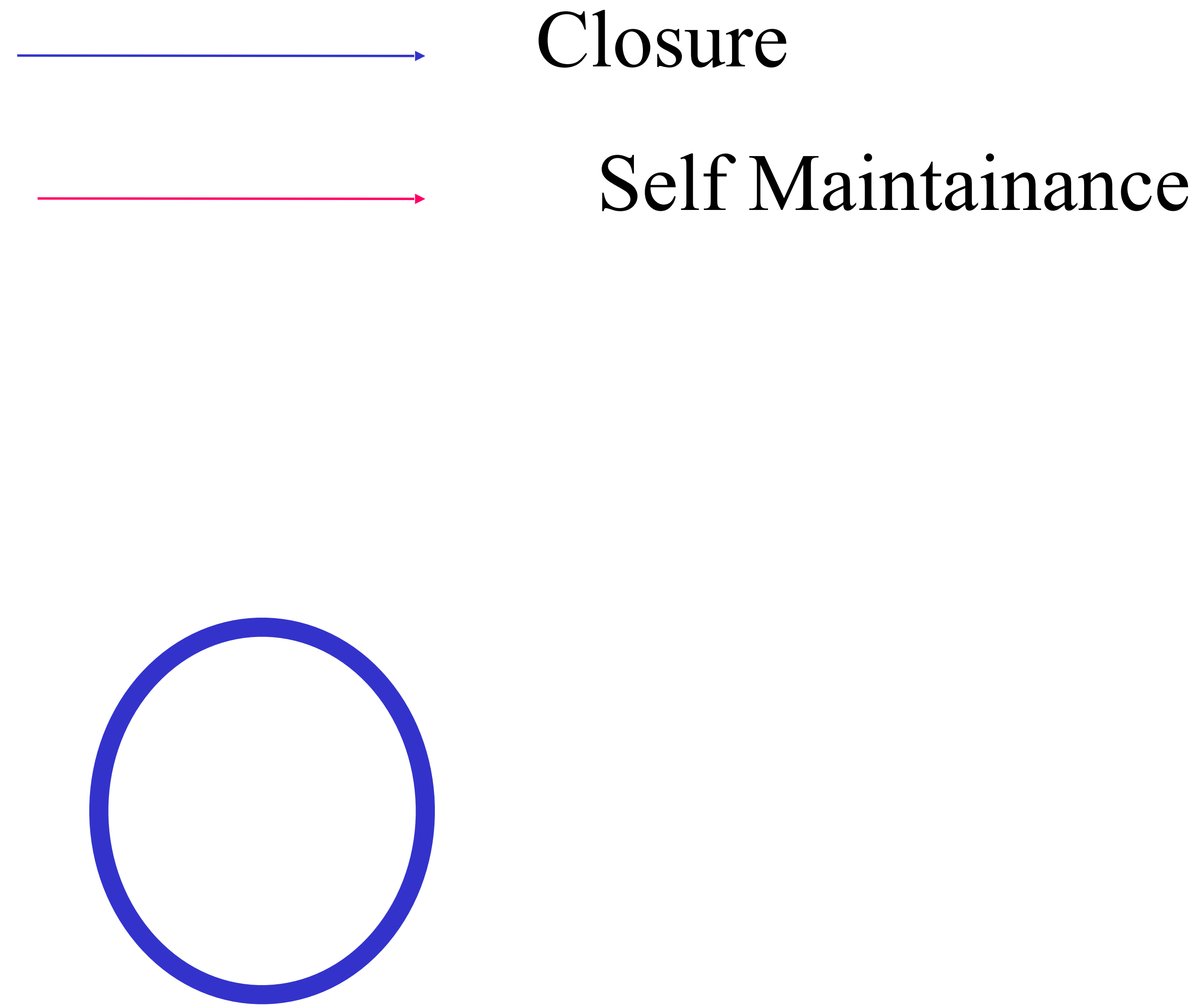

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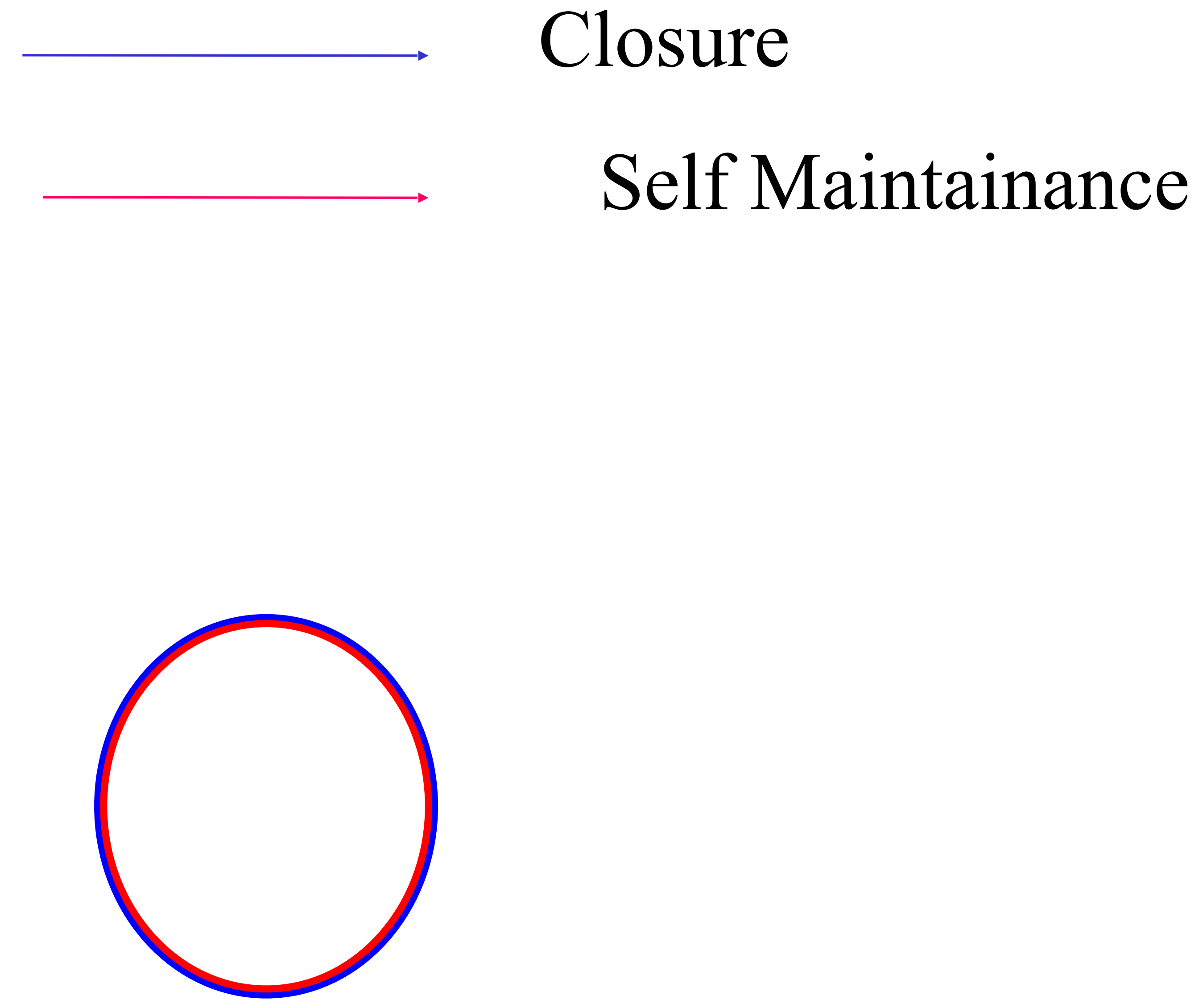


Organisation generated by a subset

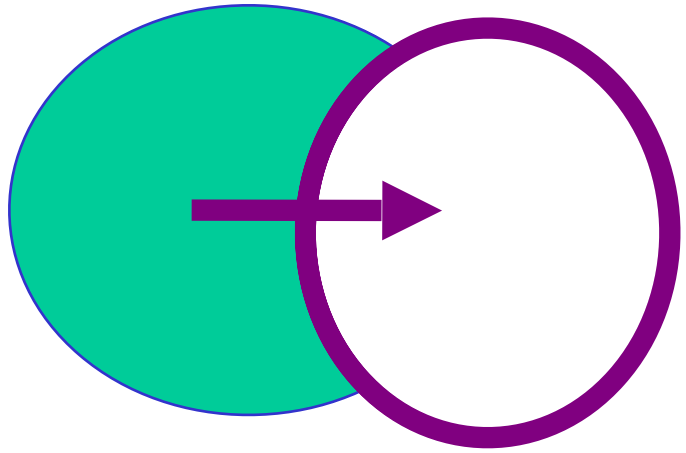
Closure

Self Maintainance

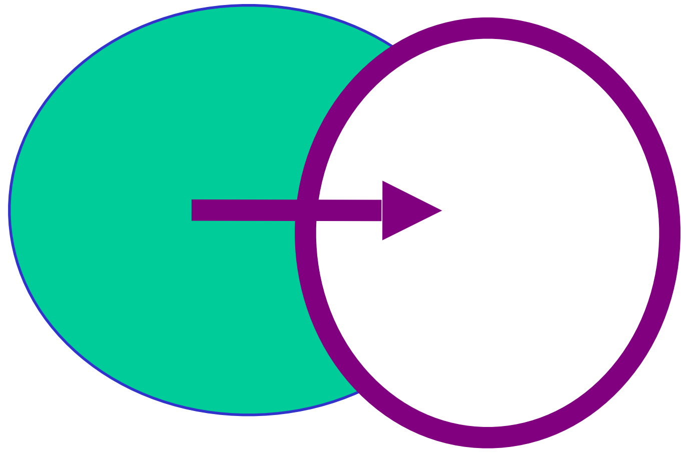
Organisation generated by a subset

Closure

Self Maintainance

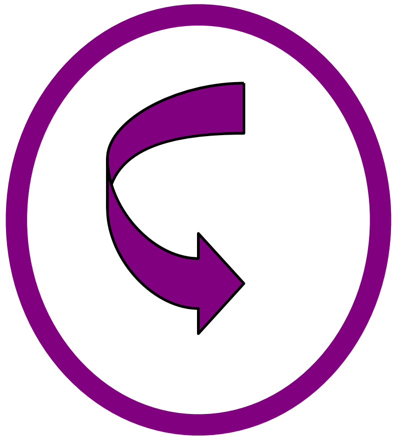


Organisation generated by a subset



Organisation generated by a subset

Of course if the starting subset is already a organization the we will just regenerate the same organization.
So organisations are the **fixed point**
of the "**generate organization**" operator.



Intersection of Organisation

- Of course given two organisations it is uniquely defined the organization generated by their intersection

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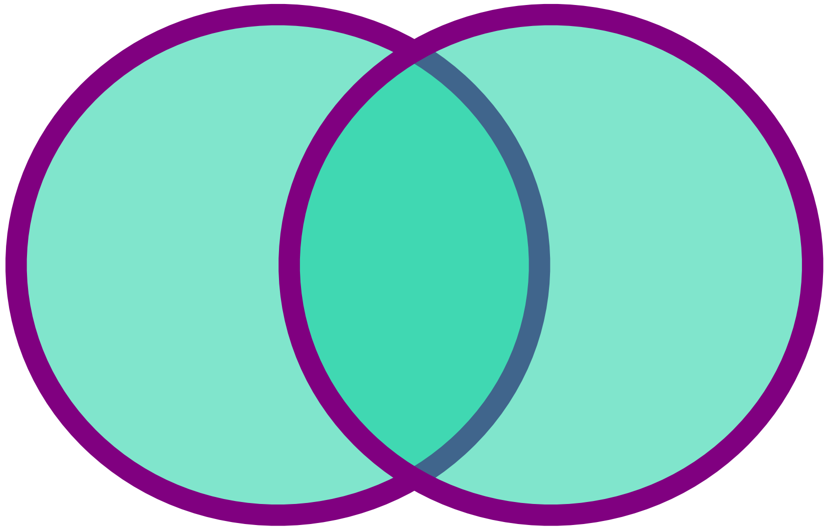

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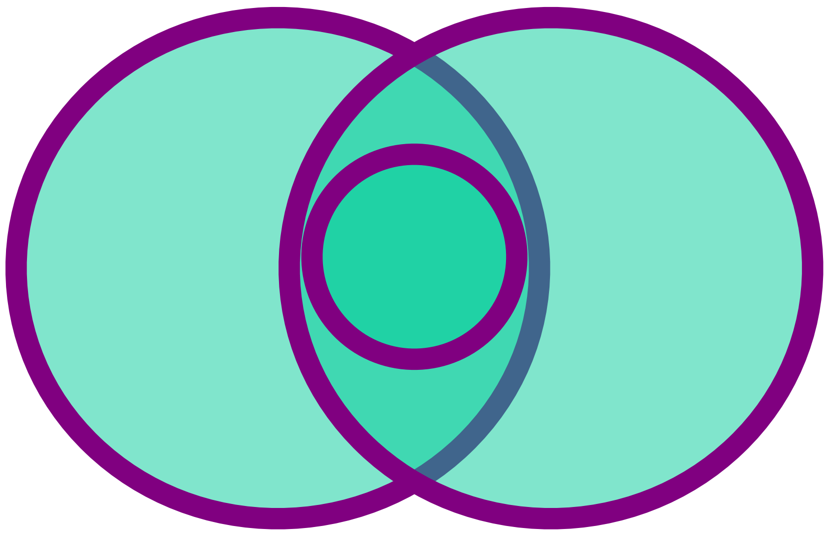

Intersection of organisations

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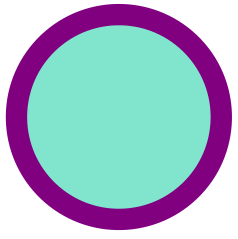

Union of organisations

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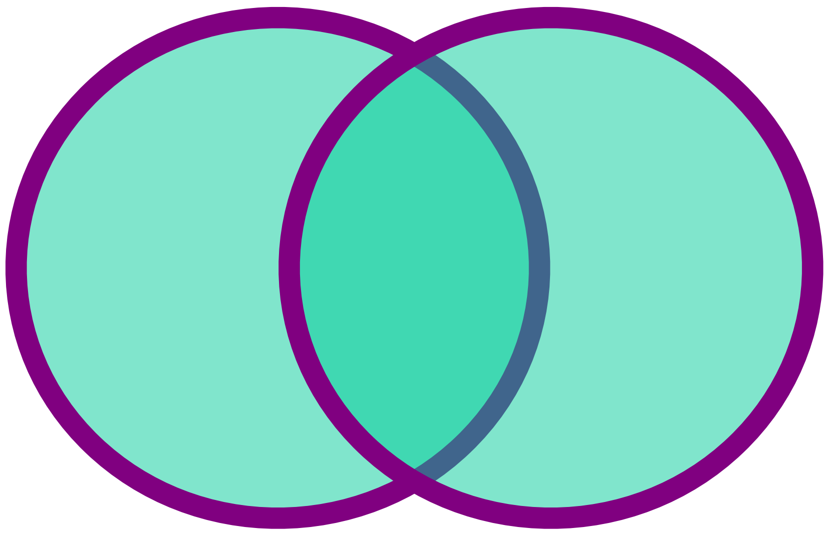

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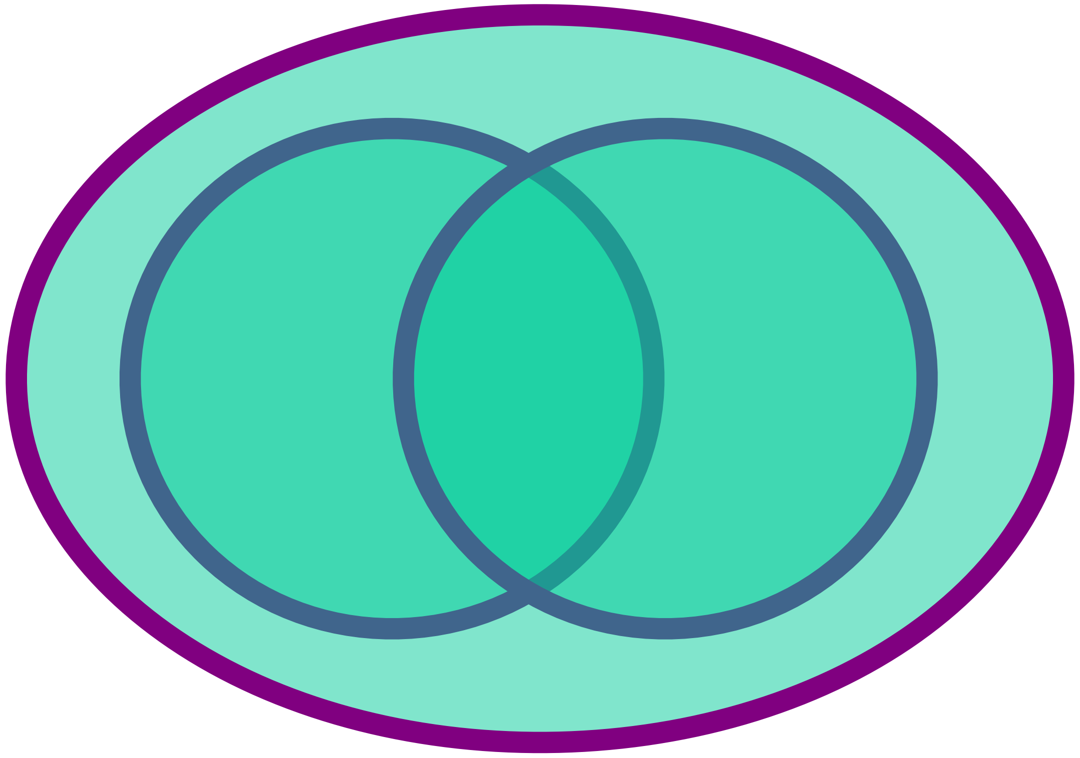

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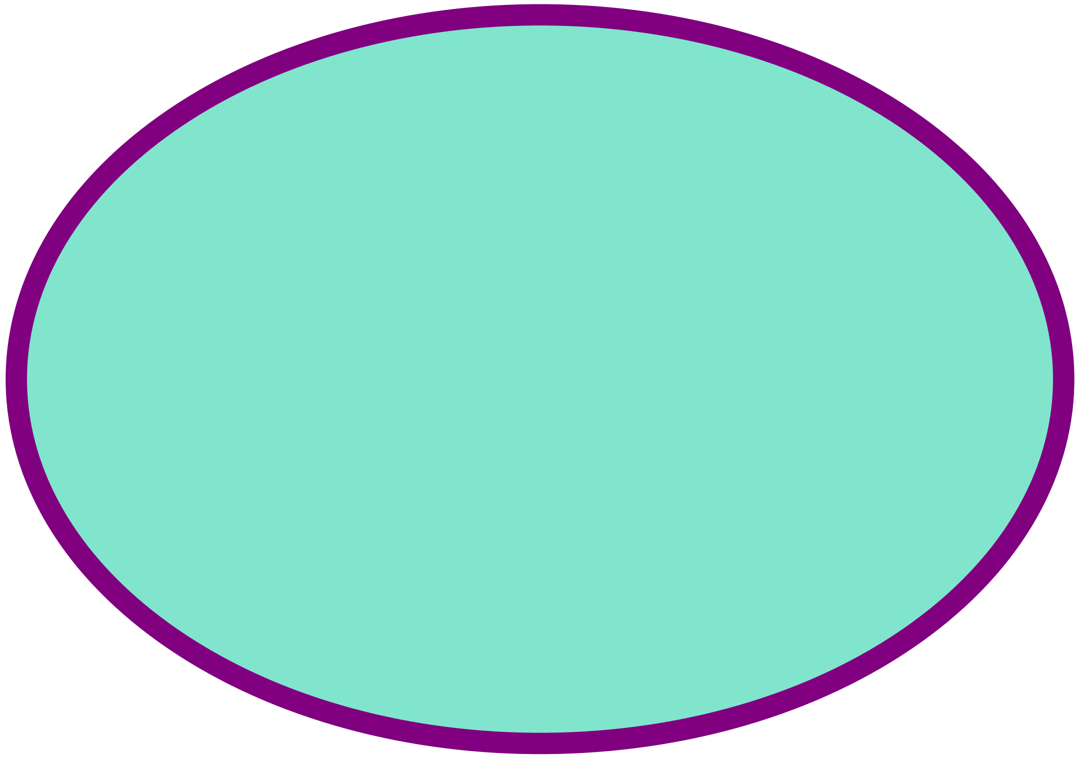

Self Organisation in a System of Binary Strings

Self-organisation in a system of binary strings

Wolfgang Banzhaf

Department of Computer Science, Dortmund University

Baroper Str. 301, 44221 Dortmund, GERMANY

banzhaf@tarantoga.informatik.uni-dortmund.de

Abstract

We discuss a system of autocatalytic sequences of binary numbers. Sequences come in two forms, a 1-dimensional form (operands) and a 2-dimensional form (operators) that are able to react with each other. The resulting reaction network shows signs of emerging metabolisms. We discuss the general framework and examine specific interactions for a system with strings of length 4 bits. A self-maintaining network of string types and parasitic interactions are shown to exist.

Introduction

Sequences of binary numbers are the most primitive form of information storage we know today. They are able to code any kind of man-made information, be it still or moving images, sound waves and other sensory stimulations, be it written language or the rules of mathematics, just to name a few. As the success of von-Neumann computers has shown over the last 50 years, binary sequences are also sufficient to store the commands that drive the execution of computer programs. In fact, part of the success of the digital computer was due to the universality of bits and their interchangeability between data and programs.

It is not far-fetched to expect that the physical identity between operators (programs) and operands (data) may also play an essential role in self-organisation. We have proposed to consider a simple self-organising system [1], in which sequences of binary numbers are able to react with each other and sometimes even to replicate themselves. This ability of binary strings was a result of the proposition to consider binary strings similar to sequences of nucleotides in RNA. RNA sequences which presumably stood at the cradle of life [2, 3], seem capable of self-organisation and come in at least two alternative forms, a one-dimensional genotypic form and a two or three-dimensional phenotypic form. We proposed to consider binary strings in analogy and to provide for a second, folded and operative form of strings. Technically, we considered as this alternative a two-dimensional matrix form that is able to perform operations on other one-dimensional binary strings.

Reactions between binary strings

The fundamental ideas of this model have been outlined elsewhere (see ref. [1],[4],[7] for details). Here we only give a brief overview of what has been learned so far.

Let us consider sequences

$$\vec{s} = (s_1, s_2, ..., s_i, ..., s_N)\,. \qquad (1)$$

of binary symbols $s_i \in \{0, 1\}, i = 1, ..., N$ organised in 1-dimensional strings.

Then we ask the question: Does there exist an alternative form of these strings, that is (i) reversibly transformable into the form (1), and is (ii) operative on form (1)? The answer is surprisingly simple and well known from mathematics: Yes, there are operators with the above capabilities, known as matrices.

Thus, we require the existence of a mapping $\mathcal{M}$

$$\mathcal{M} : \vec{s} \rightarrow \mathcal{P}_{\vec{s}} \qquad (2)$$

which transforms $\vec{s}$ into a corresponding 2-dimensional matrix form $\mathcal{P}_{\vec{s}}$ of the sequence which should be unique and reversible. This mapping is simply a spatial reorganisation of the information contained in a sequence and may be termed a *folding*, in close analogy to the notion used in molecular biology.

The most compact realization of such a 2-dimensional form would be a quadratic matrix. For a string with a quadratic number of components $N, N \in \mathcal{N}_{sq}$ with $\mathcal{N}_{sq} = \{1, 4, 9, 16, 25, ...\}$, the procedure is straightforward: Any systematic folding (examples are shown in Figure 1) would do. Since folding is not yet very sophisticated, and different configurations may be obtained by a renumbering of string components, we shall consider here the topological folding of Figure 1 (b) only.

In the more general case of N being a non-quadratic number, different generalizations are reasonable. Here

NTop

Boolean strings folded into matrix;

Matrix multiplication;

Result unfolded;


0
1
1
1
0
1
0 1 1 0
1 0 0 1
0 1 0 1


0 1 1 0 1
0 1 1 0
1 1 0 0 1
1 0 1 0 1
1
0
1


0
1
1
1
0
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0 1 1 0
1 0 0 1
0 1 0 1
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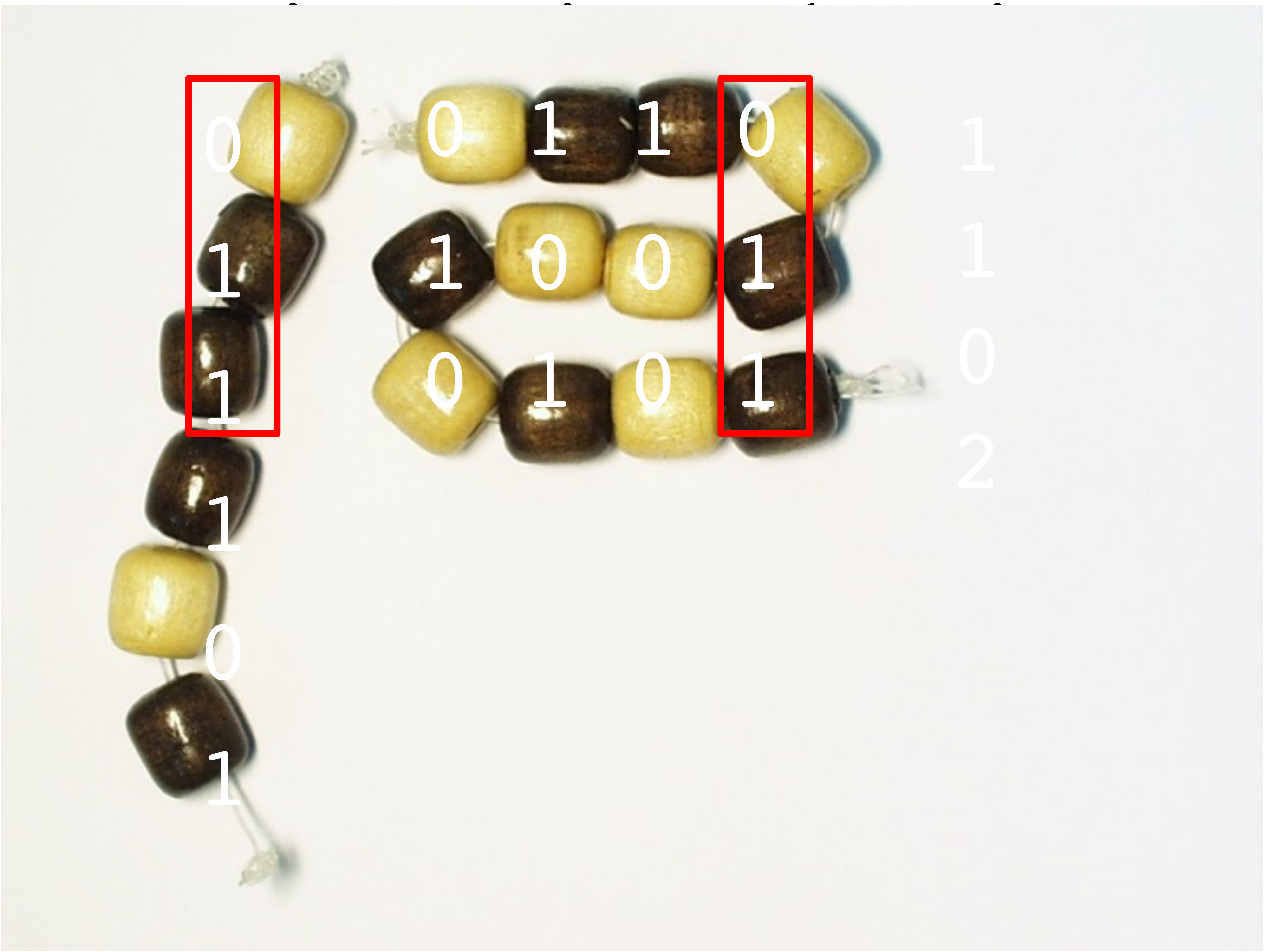
0 1 1 1 0 1
0 1 1 0
1 0 0 1
0 1 0 1
1 1 0



0 1 1 0
1 0 0 1
0 1 0 1
0 1 1 1 0 1
1 1 0 2

0
1
1
1
0
1
0 1 1 0
1 0 0 1
0 1 0 1
1
1
0
2


0
1
1
1
0
1
0 1 1 0
1 0 0 1
0 1 0 1
1
1
0
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Introduction

Sequences of binary numbers are the most primitive form of information storage we know today. They are able to code any kind of man-made information, be it still or moving images, sound waves and other sensory stimulations, be it written language or the rules of mathematics, just to name a few. As the success of von-Neumann computers has shown over the last 50 years, binary sequences are also sufficient to store the commands that drive the execution of computer programs. In fact, part of the success of the digital computer was due to the universality of bits and their interchangeability between data and programs.

It is not far-fetched to expect that the physical identity between operators (programs) and operands (data) may also play an essential role in self-organisation. We have proposed to consider a simple self-organising system [1], in which sequences of binary numbers are able to react with each other and sometimes even to replicate themselves. This ability of binary strings was a result of the proposition to consider binary strings similar to sequences of nucleotides in RNA. RNA sequences which presumably stood at the cradle of life [2, 3], seem capable of self-organisation and come in at least two alternative forms, a one-dimensional genotypic form and a two or three-dimensional phenotypic form. We proposed to consider binary strings in analogy and to provide for a second, folded and operative form of strings. Technically, we considered as this alternative a two-dimensional matrix form that is able to perform operations on other one-dimensional binary strings.

Reactions between binary strings

The fundamental ideas of this model have been outlined elsewhere (see ref. [1],[4],[7] for details). Here we only give a brief overview of what has been learned so far.

Let us consider sequences

$$\vec{s} = (s_1, s_2, ..., s_i, ..., s_N). \quad (1)$$

of binary symbols $s_i \in \{0, 1\}, i = 1, ..., N$ organised in 1-dimensional strings.

Then we ask the question: Does there exist an alternative form of these strings, that is (i) reversibly transformable into the form (1), and is (ii) operative on form (1)? The answer is surprisingly simple and well known from mathematics: Yes, there are operators with the above capabilities, known as matrices.

Thus, we require the existence of a mapping $\mathcal{M}$

$$\mathcal{M} : \vec{s} \to \mathcal{P}_{\vec{s}} \quad (2)$$

which transforms $\vec{s}$ into a corresponding 2-dimensional matrix form $\mathcal{P}_{\vec{s}}$ of the sequence which should be unique and reversible. This mapping is simply a spatial reorganisation of the information contained in a sequence and may be termed a *folding*, in close analogy to the notion used in molecular biology.

The most compact realization of such a 2-dimensional form would be a quadratic matrix. For a string with a quadratic number of components $N, N \in \mathcal{N}_{sq}$ with $\mathcal{N}_{sq} = \{1, 4, 9, 16, 25, ...\}$, the procedure is straightforward: Any systematic folding (examples are shown in Figure 1) would do. Since folding is not yet very sophisticated, and different configurations may be obtained by a renumbering of string components, we shall consider here the topological folding of Figure 1 (b) only.

In the more general case of N being a non-quadratic number, different generalizations are reasonable. Here

NTop

Boolean strings folded into matrix;

Matrix multiplication;

Result unfolded;

15 Molecules

53 Organisations

s_1 s_2	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
0	0	1	0	1	4	0	0	7	4	1	7	1	4	7	4	7
1	2	3	2	3	8	2	2	10	8	3	10	3	8	10	8	10
2	0	1	0	1	4	0	0	7	4	1	7	1	4	7	4	7
3	2	3	2	3	8	2	2	10	8	3	10	3	8	10	8	10
4	5	9	5	9	12	5	5	13	12	9	13	9	12	13	12	13
5	0	1	0	1	4	0	0	7	4	1	7	1	4	7	4	7
6	0	1	0	1	4	0	0	7	4	1	7	1	4	7	4	7
7	6	11	6	11	14	6	6	15	14	11	15	11	14	15	14	15
8	5	9	5	9	12	5	5	13	12	9	13	9	12	13	12	13
9	2	3	2	3	8	2	2	10	8	3	10	3	8	10	8	10
10	6	11	6	11	14	6	6	15	14	11	15	11	14	15	14	15
11	2	3	2	3	8	2	2	10	8	3	10	3	8	10	8	10
12	5	9	5	9	12	5	5	13	12	9	13	9	12	13	12	13
13	6	11	6	11	14	6	6	15	14	11	15	11	14	15	14	15
14	5	9	5	9	12	5	5	13	12	9	13	9	12	13	12	13
15	6	11	6	11	14	6	6	15	14	11	15	11	14	15	14	15

Toward a Theory of Organisations

Towards a Theory of Organizations

Pietro Speroni di Fenizio, Peter Dittrich, Wolfgang Banzhaf, and Jens Ziegler

University of Dortmund, Dept. of Computer Science, D-44221 Dortmund

Abstract

In this paper we develop an algebra to describe organizations. Its application is demonstrated with five examples. We start from definitions given by Fontana (1992) of an organization as a closed and self-maintaining set of interacting objects. We develop a formal framework to describe the inner structure of an organization and a relationship between different organizations. The definitions of intersection and union of organizations are developed. Those definitions naturally give rise to a lattice (an algebraic structure over a partially ordered set) which provides a precise basis to study the hierarchical nature of organizations. Some fundamental properties are described and the usefulness of the mathematical concepts demonstrated by application.

1 Introduction

The term *organization* is widely used in science, starting from social sciences and economy to physics and computer science. In nearly all these areas *organization* has a specific meaning, which is sufficient for qualitative statements on a system embedded in a specific context. But once quantitative measurements are sought, an exact definition of organization is required.

This paper tries to define the term organization using precise mathematical and algebraic statements. It intends to give a means for describing organization in systems with a maximum of accuracy, independent of their constituting parts, be they molecules, stars of a galaxy, or departments of a company. These exact statements shall be applied to five examples of systems, stemming from the field af artificial chemistry (AC). Artificial chemistries are able to generate organizations with different characteristics. The concept of an artificial chemistry is an elegant means for dealing with structures that are able to change or maintain themselves, and especially with systems that are able to create new components.

Varela, Maturana, and Uribe (1974) investigate the basic organization of living systems with simple autopoietic models. Their approach can be seen as one of the early works in artificial chemistry that in the 1980s contributed to the formation of the field *Artificial Life* (AL), an interdisciplinary area of research that deals with the abstract foundations of living systems. Many AL researcher investigated the theory of organizations of artificial living systems (e.g. (Kampis 1991; Fontana and Buss 1994; Szathmary 1995)). It soon emerged that properties like *self-maintenance, self-creation, seclusion, and openness*, observable in different artificial (and natural) chemical systems, are crucial to understand the structure and dynamics of organizations, independent from their instantiating structure. In order to investigate these phenomena artificial chemistries have been proven to be important constructive and analytical tools. McCaskill (1988), Banzhaf (1993b), Ikegami and Hashimoto (1995), Ehricht, Ellinger, and McCaskill (1997), Dittrich and Banzhaf (1998), Breyer, Ackermann, and McCaskill (1999), and Ono and Ikegami (1999) for instance, studied different artificial chemistries, ranging from abstract automata to rewriting systems; whereas Hjelmfelt, Weinberger, and Ross (1991), Adleman (1994), Rambidi and Maximychev (1997), Segré, Lancet, Kedem, and Pilpel (1998) analyzed natural

1

Given any set of molecules you can define the organisation generated by this set

for all sets of molecules T,
exists O_T
(that can be generated in this way….)
such that O_T is an Organisation.

If T, S sets, with T>S
Then $O_T \geq O_S$

Organisations form an algebra,
a *Lattice* in particular

The Lattice of Organizations

Lattice of Organizations

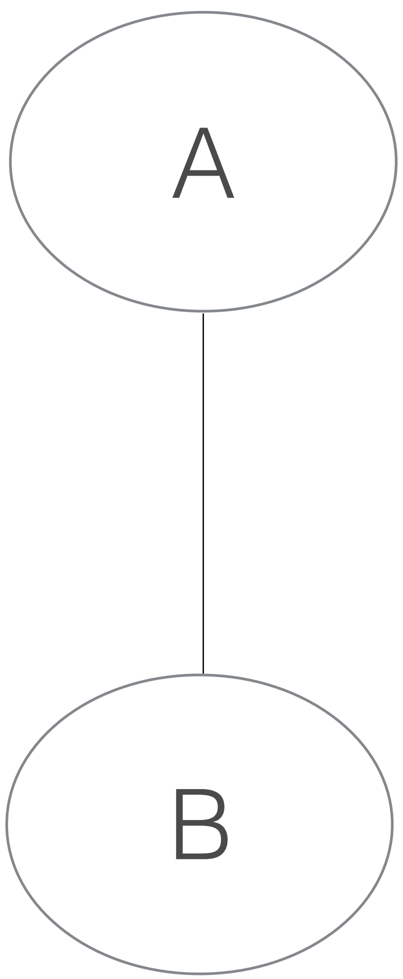
Given the set of all organization (**O**),

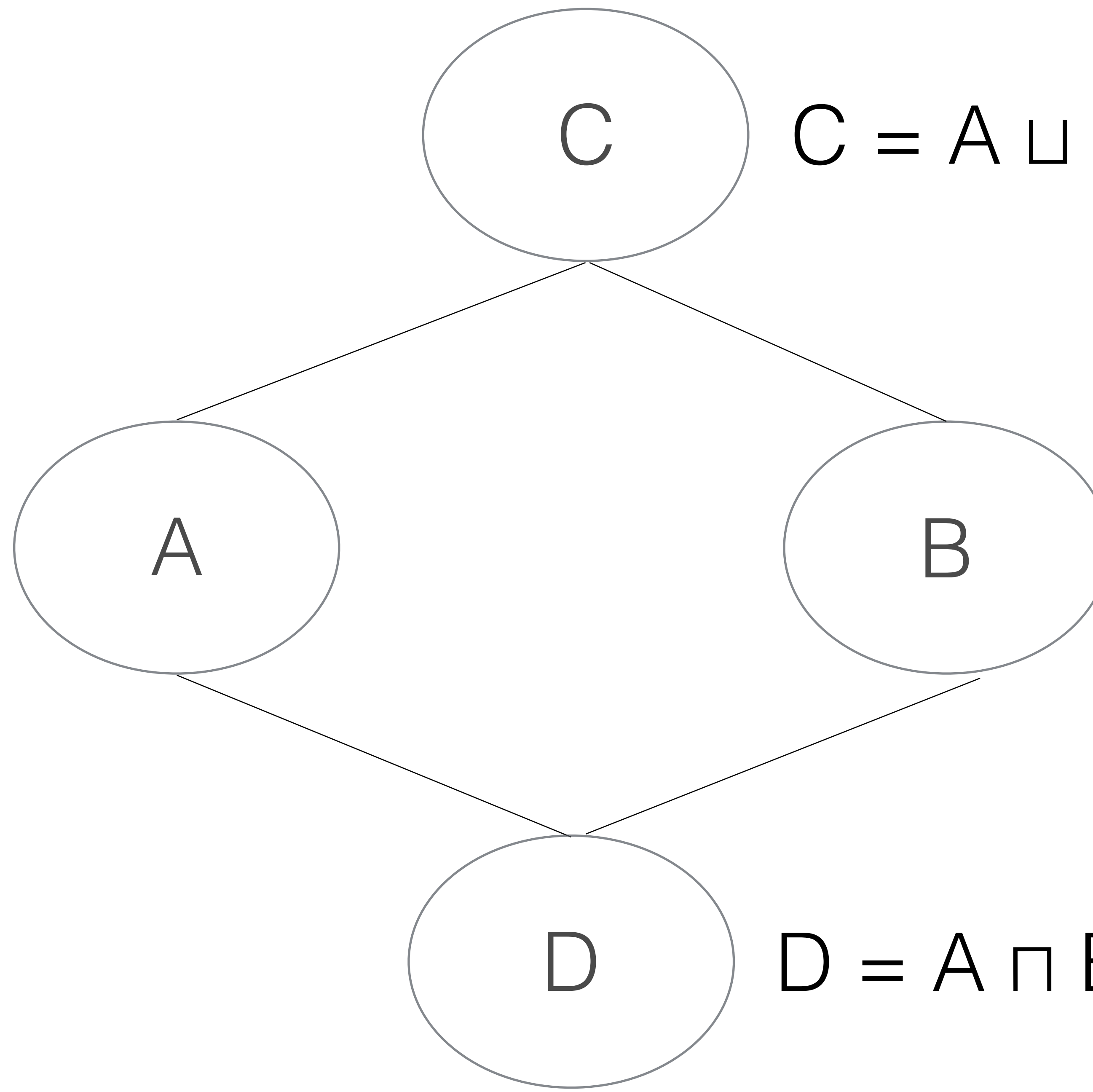
given the operation organizational union ($\cup$),

given the operation organizational intersection ($\cap$),

<O, $\cup$, $\cap$> is a Lattice.

Example of Lattice

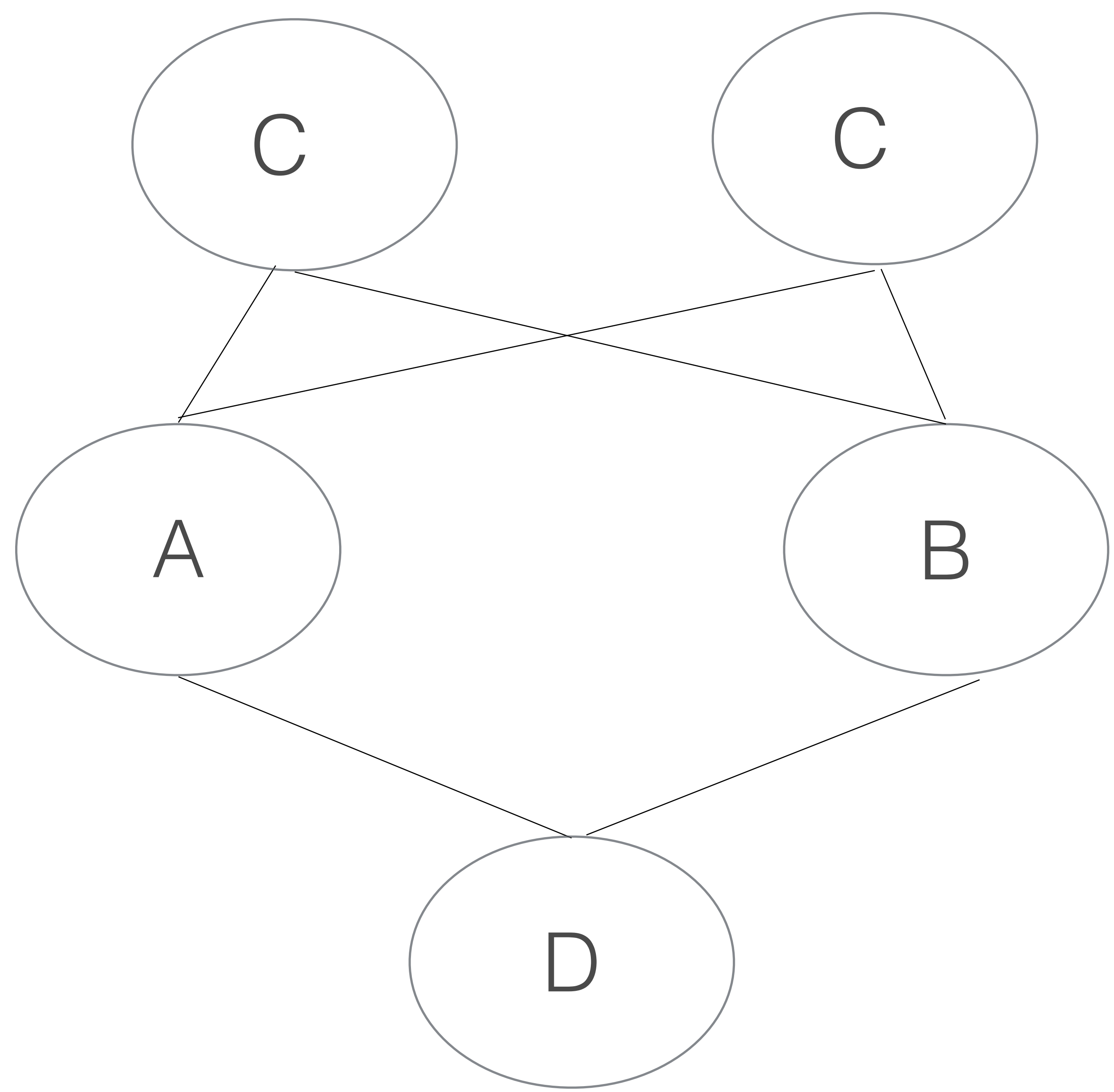




$C = A \sqcup B$

$D = A \sqcap B$

Example of not a Lattice

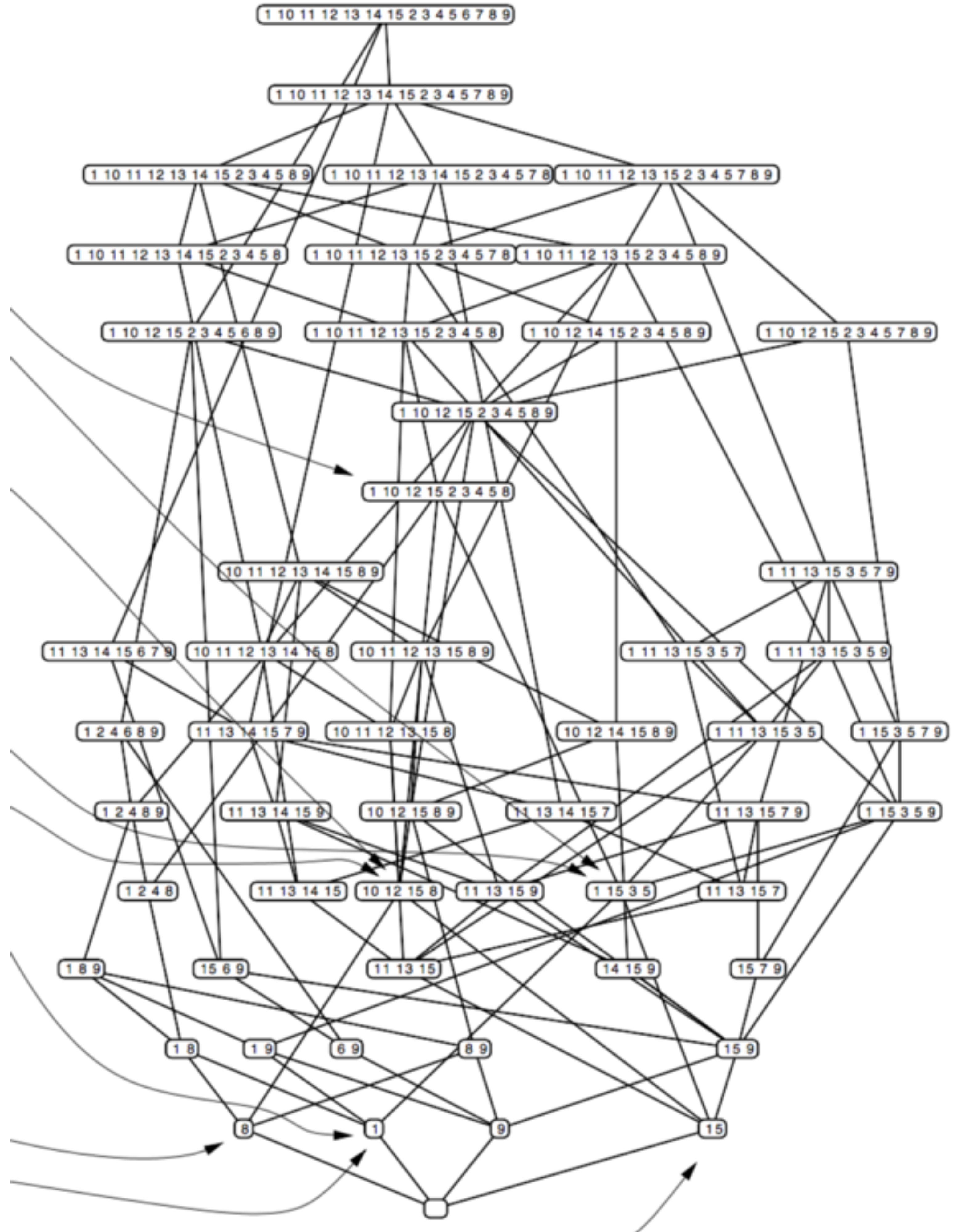


NTop

15 Molecules

~~53 Organisations~~

54 Organisations



Artificial Chemistry's Global Dynamic.
Movements in the Lattice of Organisation

in: Journal of Three Dimensional Images, 16(4):160-163

Artificial Chemistry's Global Dynamic. Movements in the Lattice of Organisation

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Abstract

As *artificial life* is the study of life as it could be, *artificial chemistry* can be seen as the study of chemistry as it could be. In such systems molecules interact to generate new molecules, possibly different from the original ones. Here, we will focus on a general theoretical approach to study artificial chemistries. In this approach we consider the set of all possible organisations (closed and self-maintaining sets) in an artificial chemistry. As was shown in [2, 3] this set generates a lattice. We consider the dynamical movement of a system in this lattice, under the influence of its inner dynamic and random noise. We notice that some organisations, while being algebraically closed, are not stable under the influence of random external noise. While others, while being algebraically self-maintaining, do not dynamically self-maintain all their elements. This leads to a definition of attractive organisations.

1 Introduction

Artificial chemistries (AC) are a way to model natural systems. They have been used to model chemical systems, biochemical, ecological, sociological, and linguistic systems (refs. in [1]).

With the term artificial chemistry we refer to a system that can be described by three parts: the molecules $\mathcal{M}$, the operation $\oplus$, and the dynamic. The molecules are a set of elements[1]. Depending on the modelling aim, those elements can represent atoms, real molecules, animals, communication symbols, etc. Common in all those systems is that from the interaction of those elements new elements are generated. From this follows that in artificial chemistries the operation (the exact law that describes, given a set of interacting elements what comes out) is also important. In mathematical terms, if $\mathcal{M}$ is the set of all possible molecules, the operation is a reaction that (usually) goes from $\oplus : \mathcal{M} \times \mathcal{M} \longrightarrow \mathcal{M} \cup \{\emptyset\}$. In other words the operation does not need to return a molecule for all possible couples. Some couples do not react, thus are called elastic. Some artificial chemistries use a more general product, where the product takes more than two elements, or returns more than one element. The last important element in an AC is the dynamic. The dynamic is an algorithm or formal system that specifies how the molecules are to be handled. In general the molecules are considered to live in a reaction vessel (e.g., a multiset, which is a set where the same element can appear multiple times). This reaction vessel is often called the soup or population, but the exact procedure that governs how the soup should be handled may vary from interaction to interaction. For example the soup could be a well stirred reactor, or from another medium. The dynamic also describes how the new molecule should enter the soup. Should they substitute the interacting ones, should they just be added to the set of existing molecules, or should they substitute another molecule randomly taken from the soup. In this paper we will not focus on a particular system, but we will investigate some characteristics common to many artifi-

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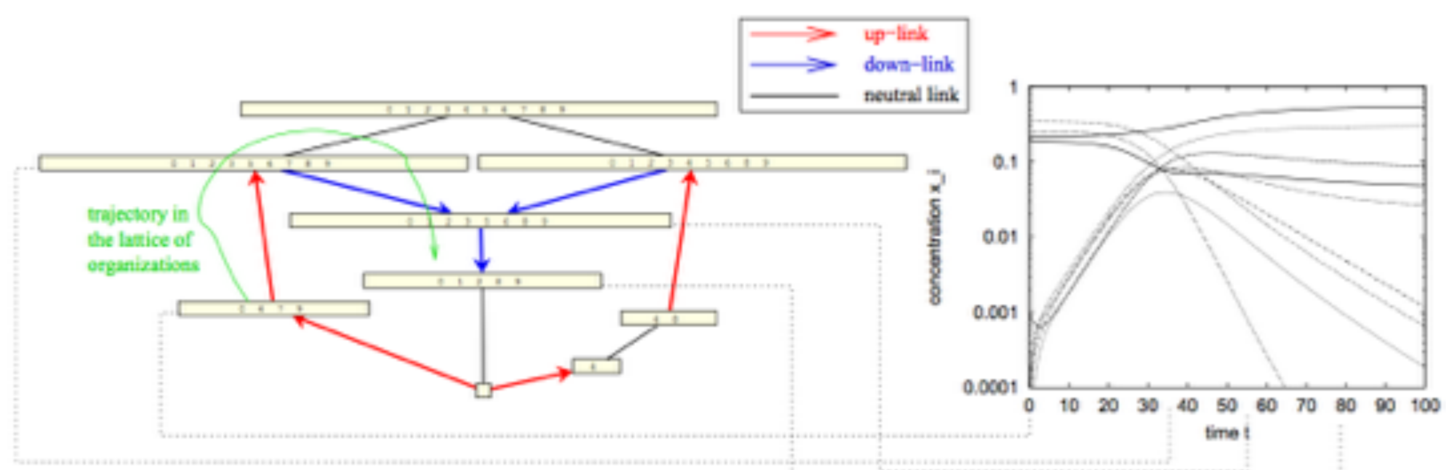
[1]Not to be confused with chemical elements.

…we consider the set of all possible organisations in an artificial chemistry.
…this set generates a lattice.

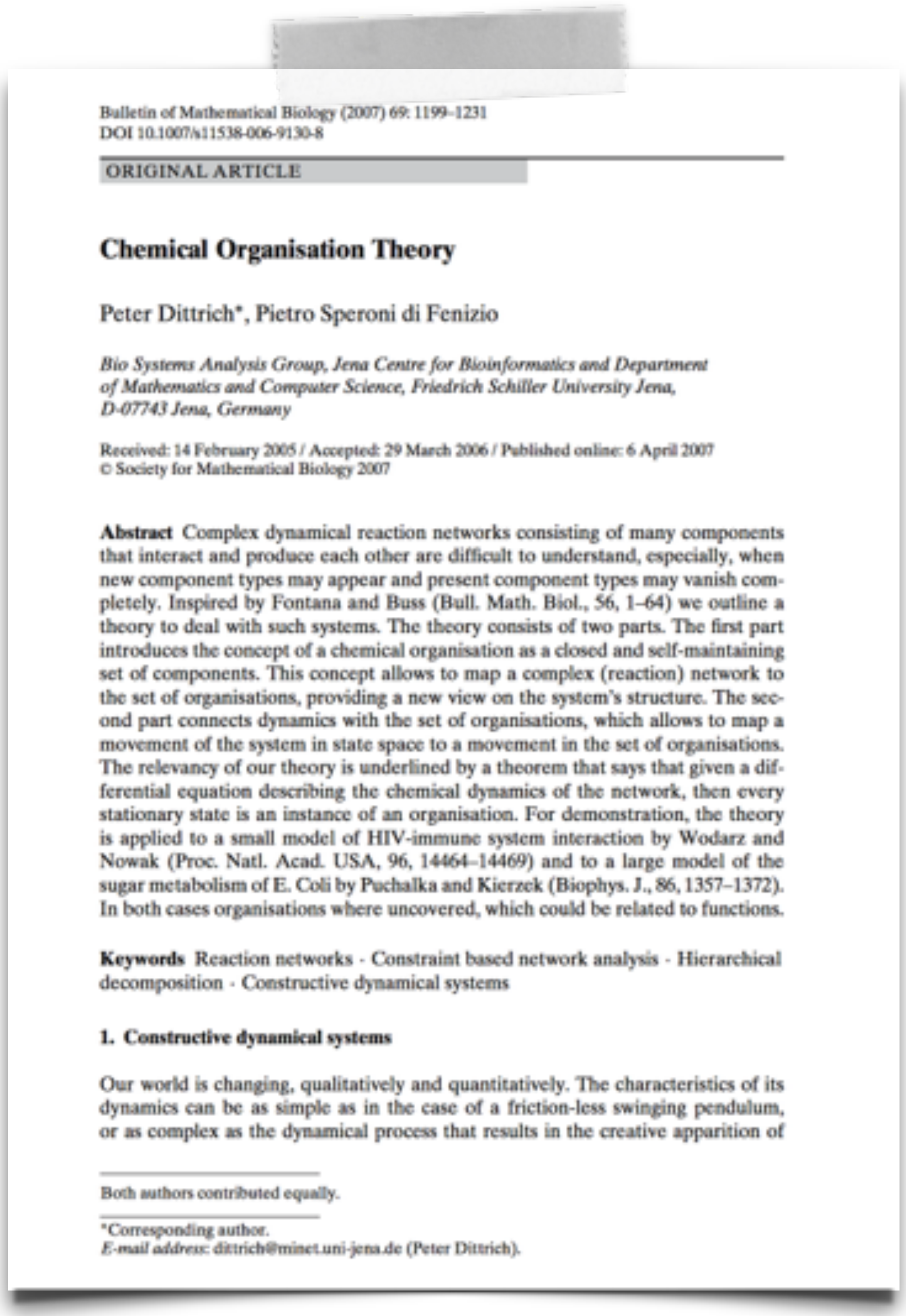
We consider the dynamical movement of a system in this lattice, under the influence of its inner dynamic and random noise.

We notice that some organisations, while being algebraically closed, are not stable under the influence of random external noise. While others, while being algebraically self-maintaining, do not dynamically self-maintain all their elements. This leads to a definition of attractive organisations.



Problems: Find the Lattice of organisations

Chemical Organisation Theory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ORIGINAL ARTICLE

Chemical Organisation Theory

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Abstract Complex dynamical reaction networks consisting of many components that interact and produce each other are difficult to understand, especially, when new component types may appear and present component types may vanish completely. Inspired by Fontana and Buss (Bull. Math. Biol., 56, 1–64) we outline a theory to deal with such systems. The theory consists of two parts. The first part introduces the concept of a chemical organisation as a closed and self-maintaining set of components. This concept allows to map a complex (reaction) network to the set of organisations, providing a new view on the system's structure. The second part connects dynamics with the set of organisations, which allows to map a movement of the system in state space to a movement in the set of organisations. The relevancy of our theory is underlined by a theorem that says that given a differential equation describing the chemical dynamics of the network, then every stationary state is an instance of an organisation. For demonstration, the theory is applied to a small model of HIV-immune system interaction by Wodarz and Nowak (Proc. Natl. Acad. USA, 96, 14464–14469) and to a large model of the sugar metabolism of E. Coli by Puchalka and Kierzek (Biophys. J., 86, 1357–1372). In both cases organisations where uncovered, which could be related to functions.

Keywords Reaction networks · Constraint based network analysis · Hierarchical decomposition · Constructive dynamical systems

1. Constructive dynamical systems

Our world is changing, qualitatively and quantitatively. The characteristics of its dynamics can be as simple as in the case of a friction-less swinging pendulum, or as complex as the dynamical process that results in the creative apparition of

Both authors contributed equally.

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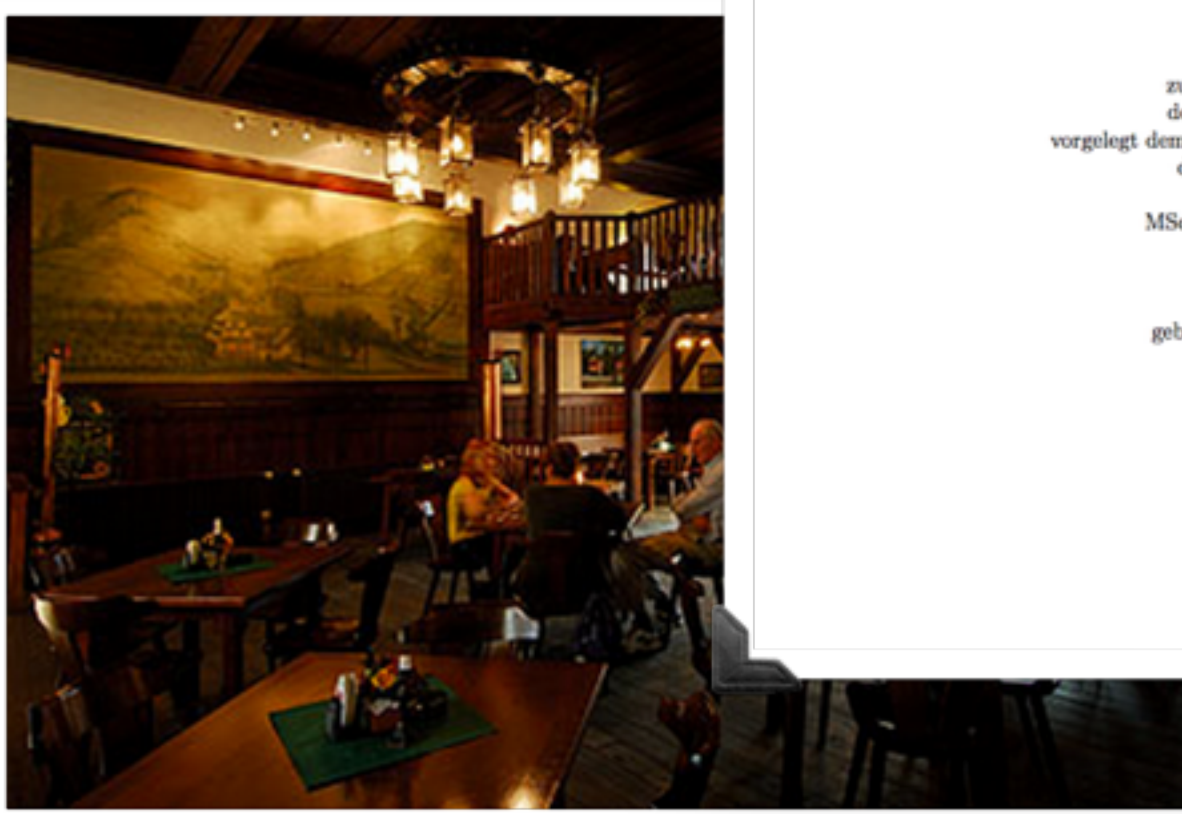
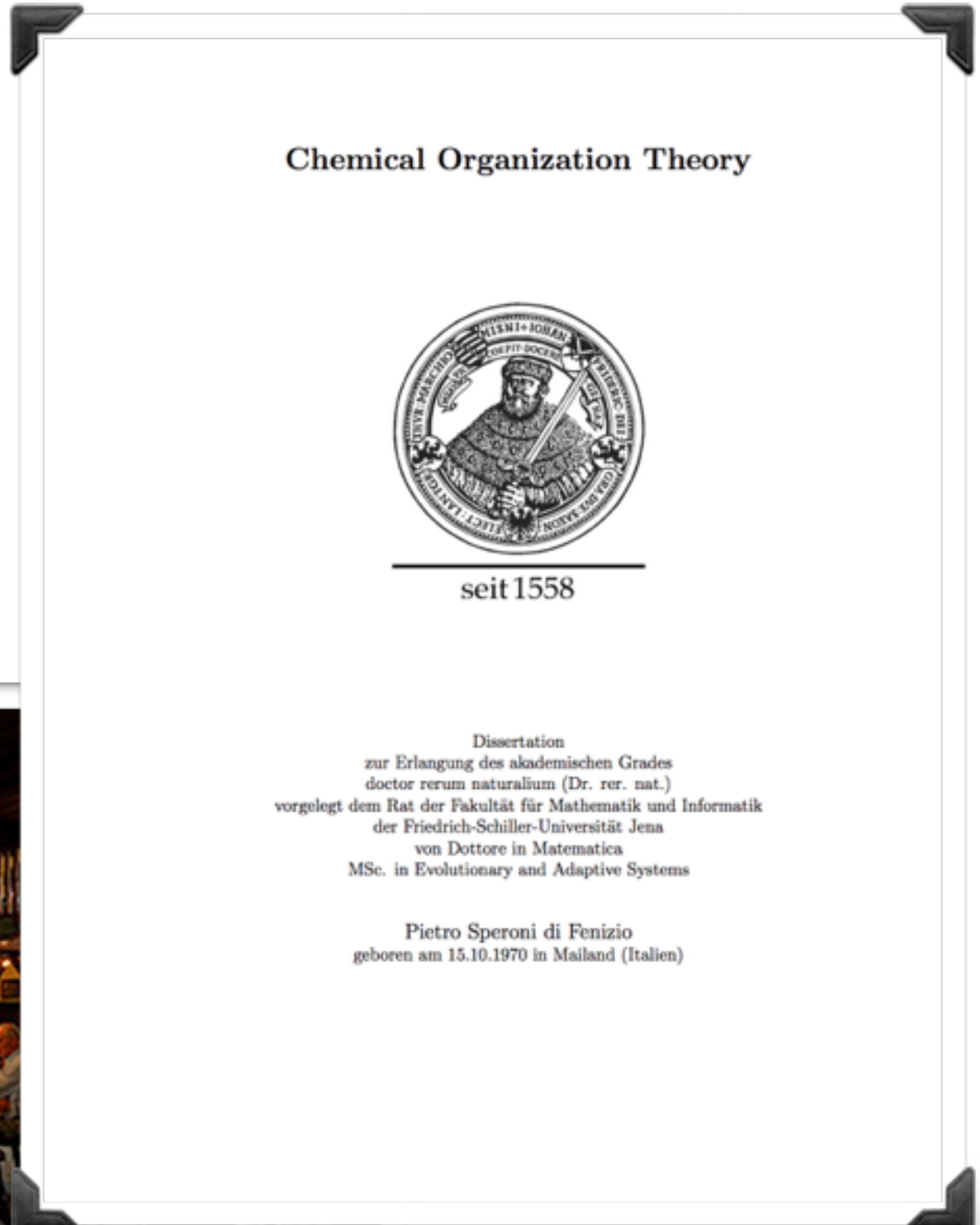
Formal Definition of Organisation that can be applied to
-Chemistry
-Biology
-Systems Biology
-Atmospheric Chemistry
-Engineering
-…

When is it a Lattice
When it is not

Chemical Organisation Theory





Chemical Organization Theory

seit 1558

Dissertation
zur Erlangung des akademischen Grades
doctor rerum naturalium (Dr. rer. nat.)
vorgelegt dem Rat der Fakultät für Mathematik und Informatik
der Friedrich-Schiller-Universität Jena
von Dottore in Matematica
MSc. in Evolutionary and Adaptive Systems

Pietro Speroni di Fenizio
geboren am 15.10.1970 in Mailand (Italien)

Understanding an Artificial Chemistry

Problems: Find the Lattice of organisations

Understanding an Artificial Chemistry means at least:

- know the lattice of Organisations:
  - know all the organisations;
  - given any two organisations A, B,
    know what is: $A \sqcup B$, $A \sqcap B$

A list, and 2 tables

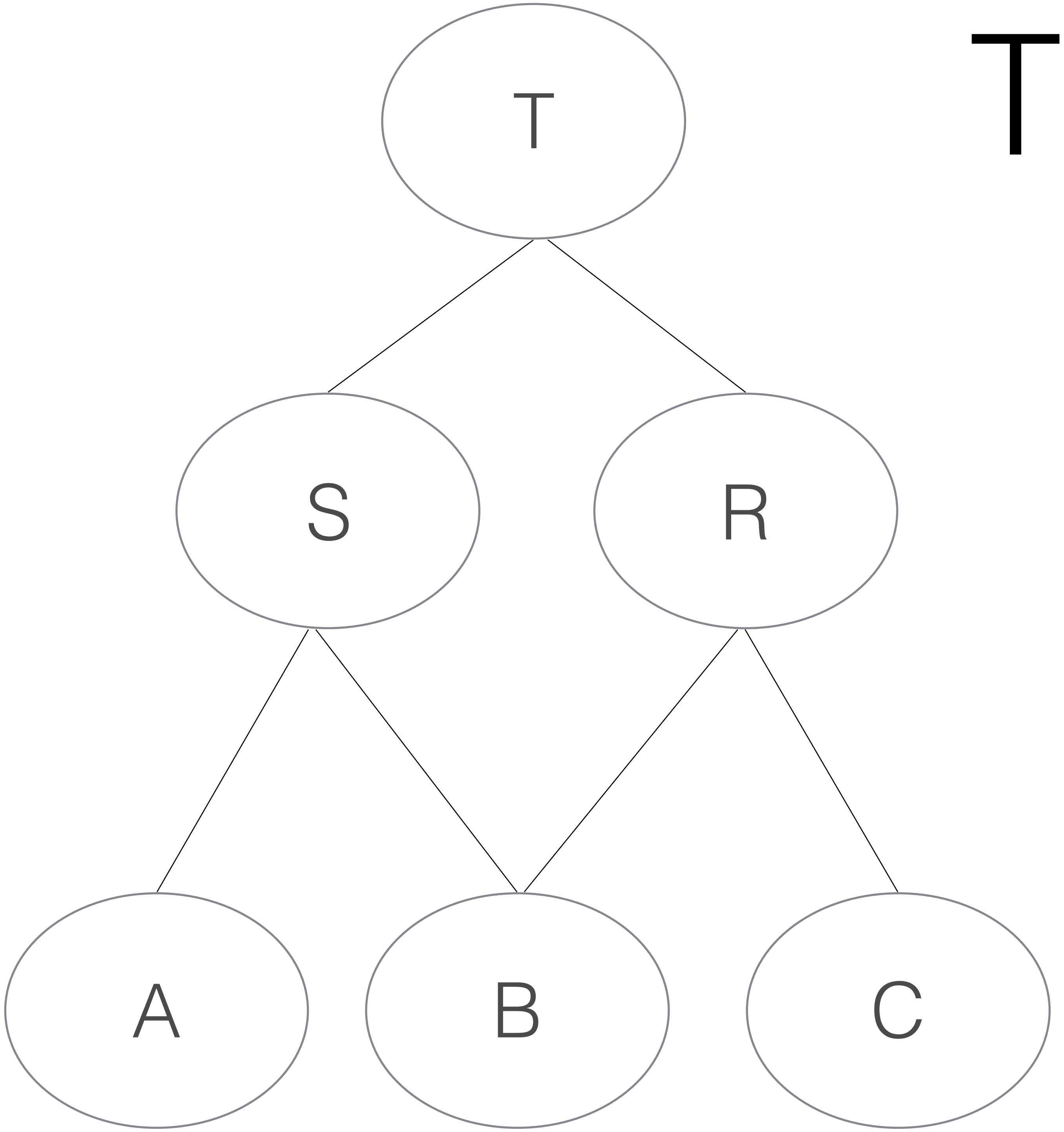
Applying the Lattice

- Start with a set of organisations.
- Calculate all the union and intersections and add them;
- Until you cannot add anything anymore;
    - Now you have a sub-lattice
- Take an Org, add *some* molecules to find a new Organisation

- Go from sub lattice to sub lattice

- …until you have found all the organisations.

Theorem 1



In a lattice:
(A U B) U C = A U (B U C);

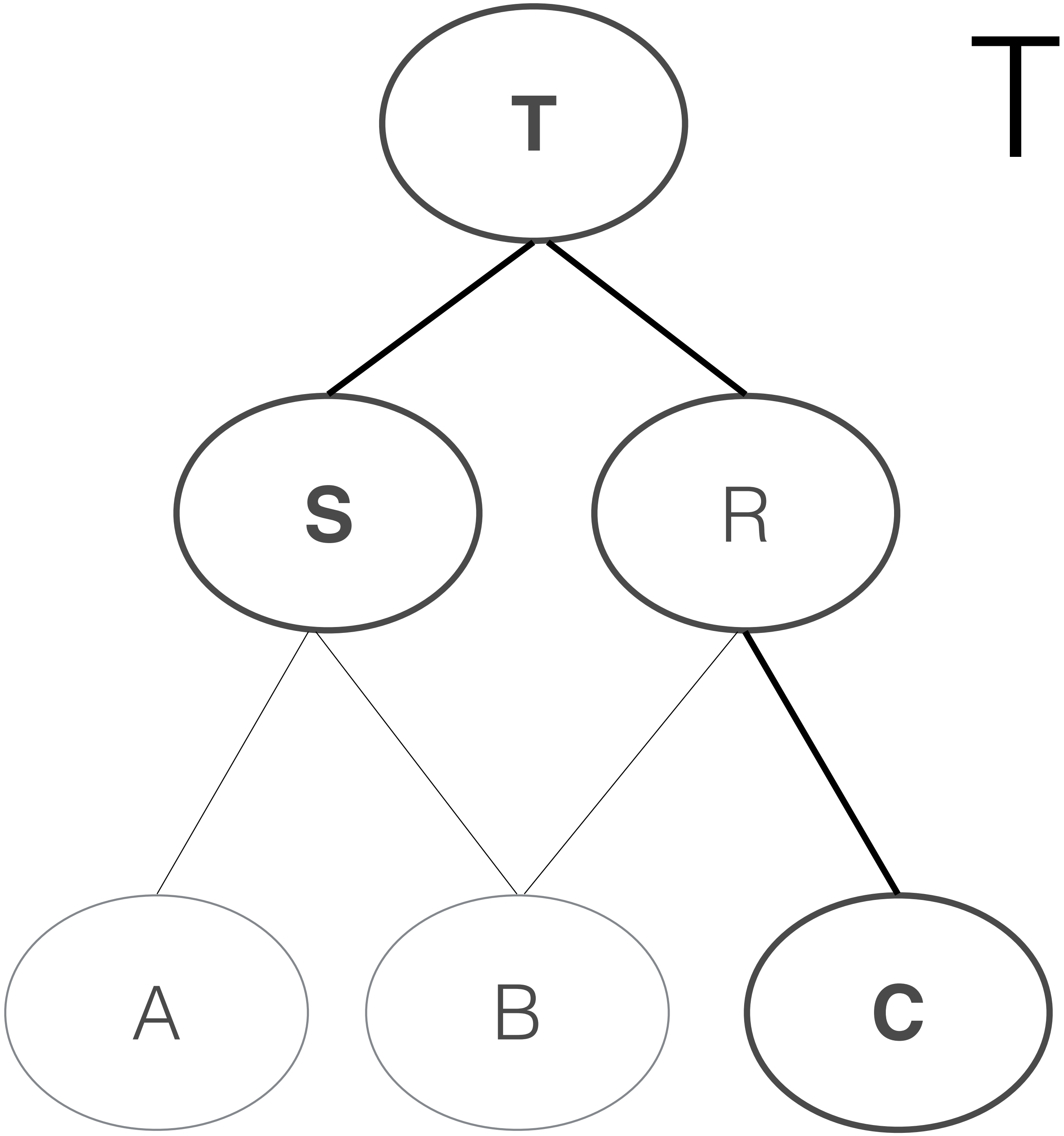
We have 2 Organisations S, C;
We are looking for T with T = S U C,

If exist 2 Organisations A, B
such that S = A U B

Then:
T = A U (B U C).

We might know R = B U C.
In which case
T = S U C = A U R

Theorem 1



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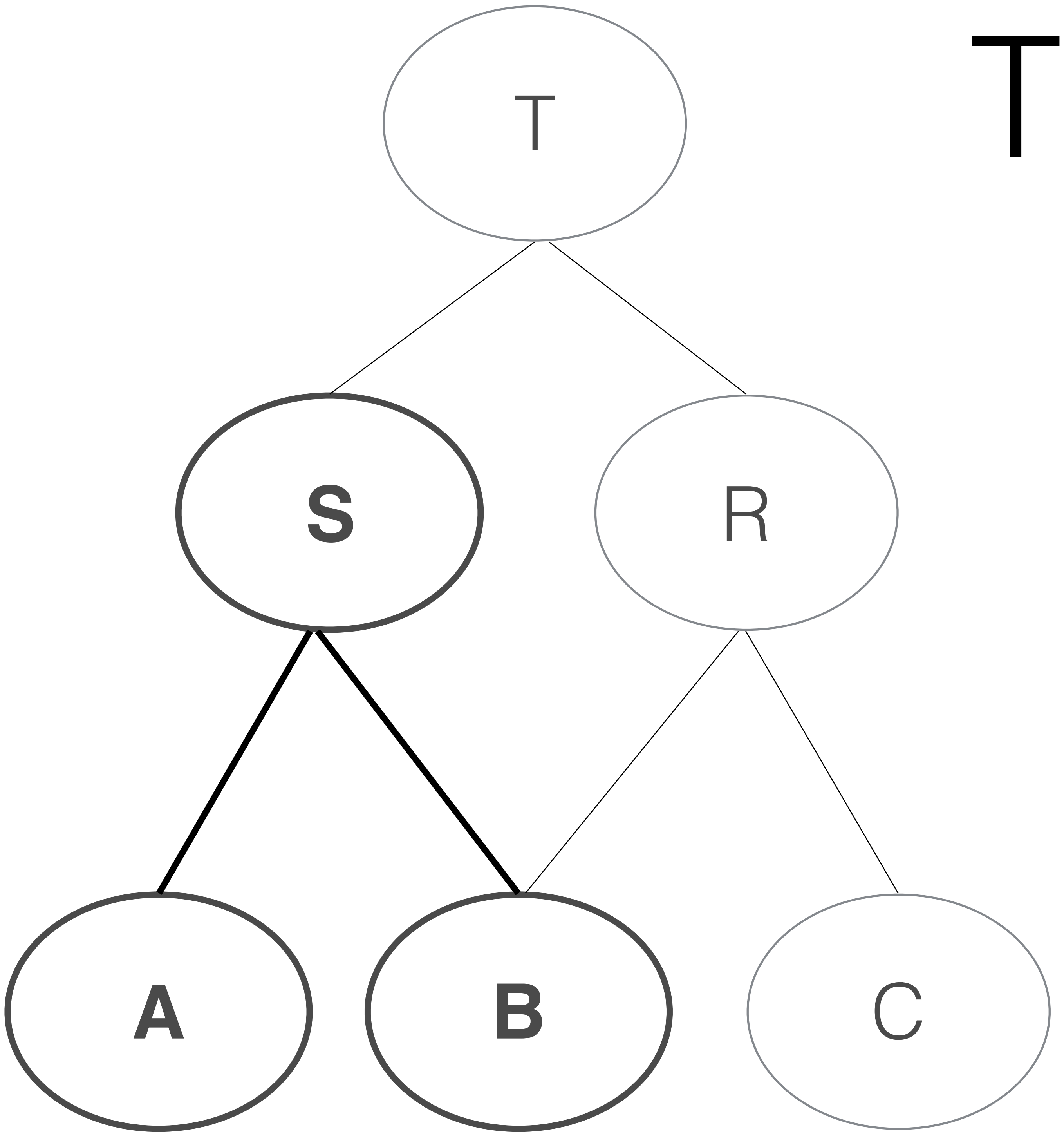

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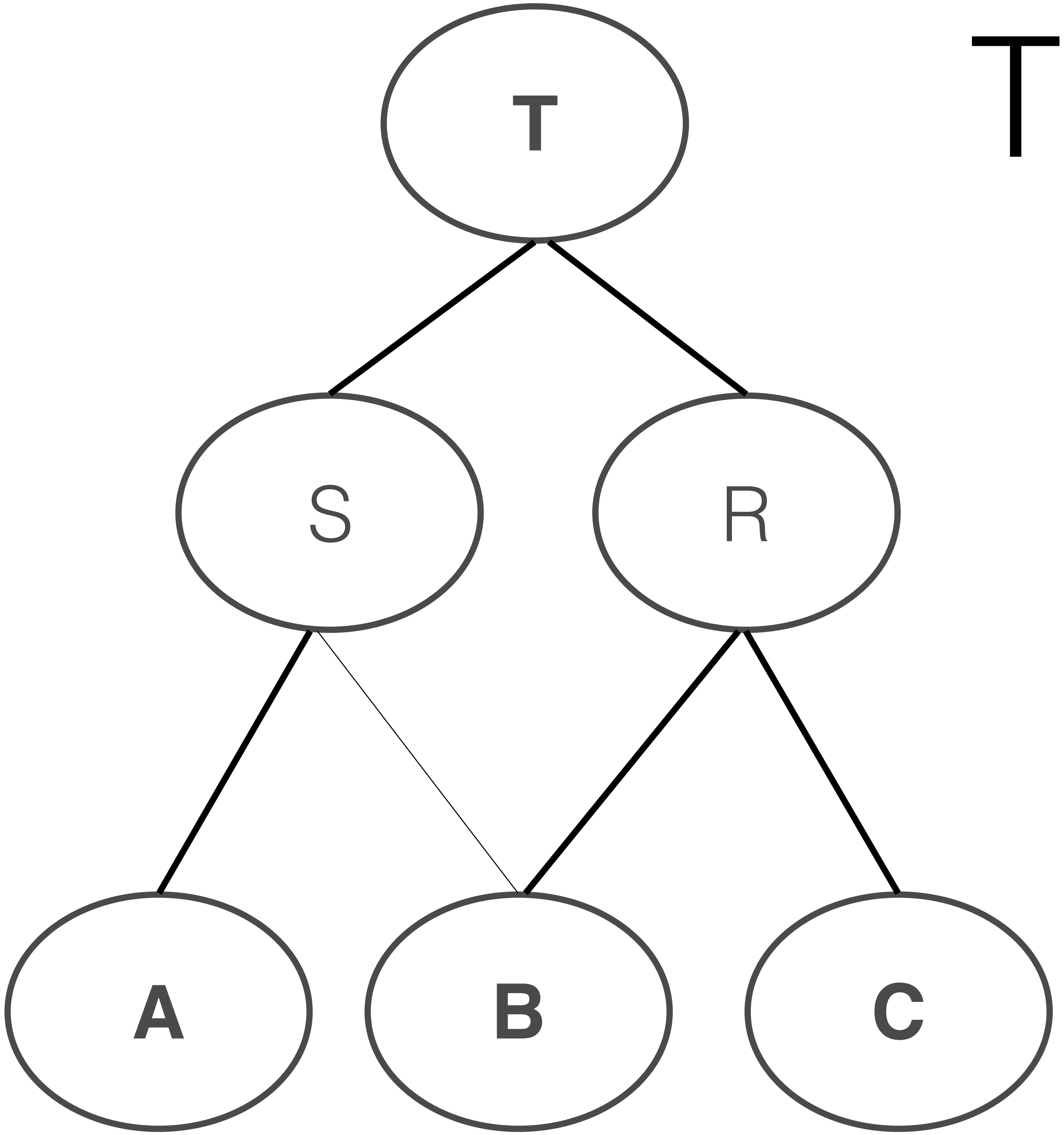

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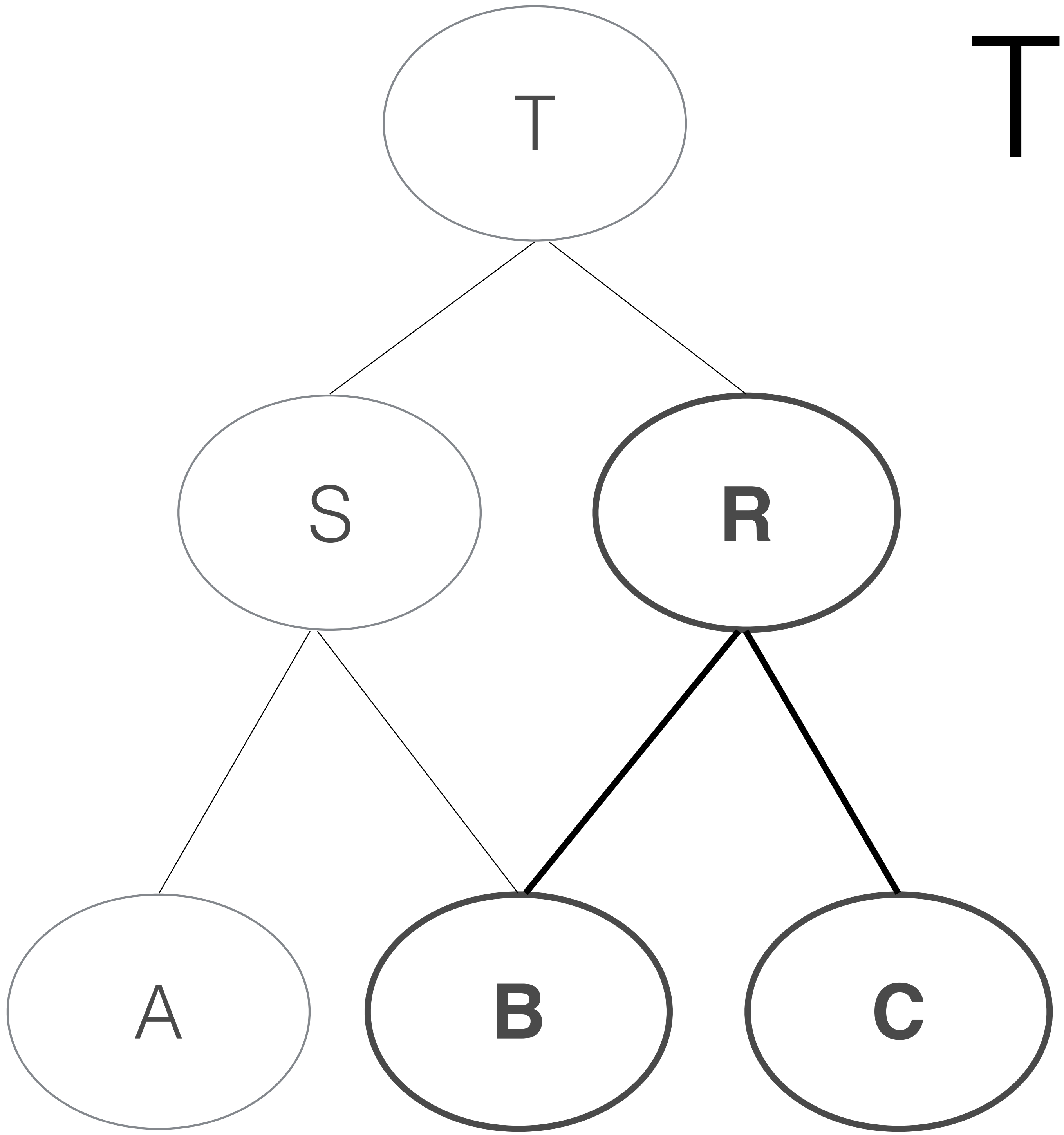

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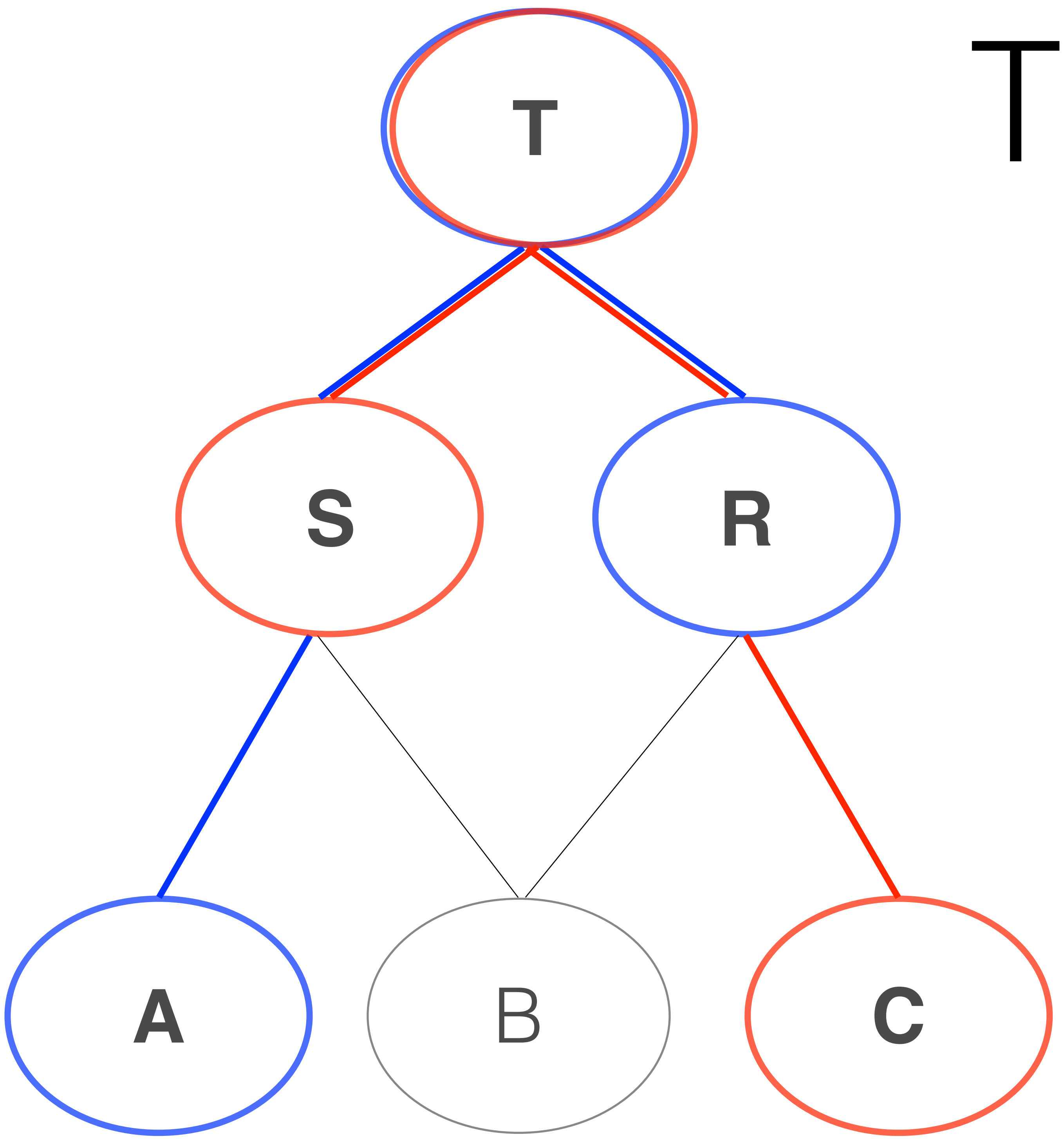

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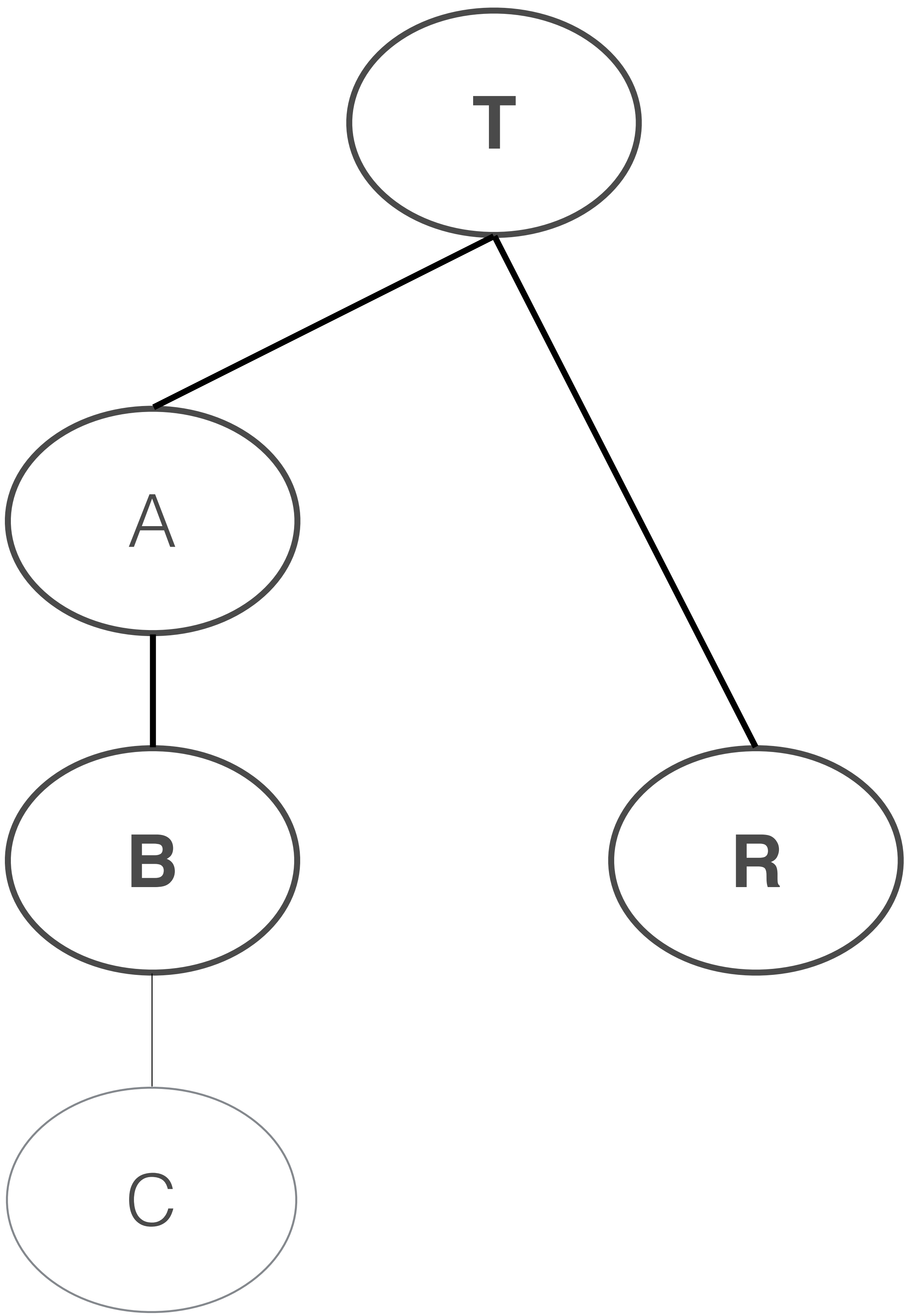
Theorem 2



In a lattice:

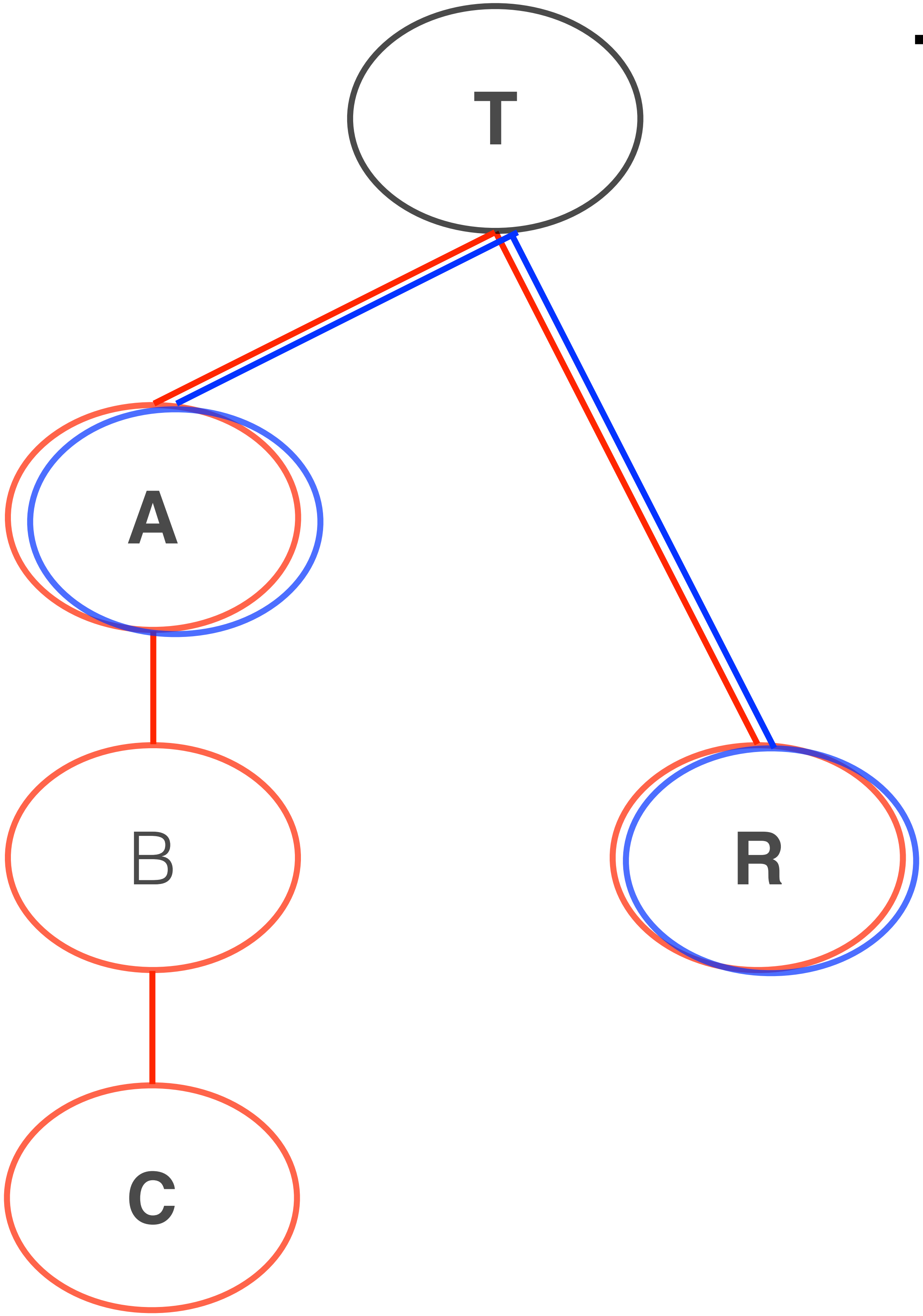
A, B, C, R are Organisations
A < B < C

We want to find T = B U R

If A U R = C U R

Then B U R = A U R = C U R

Theorem 2



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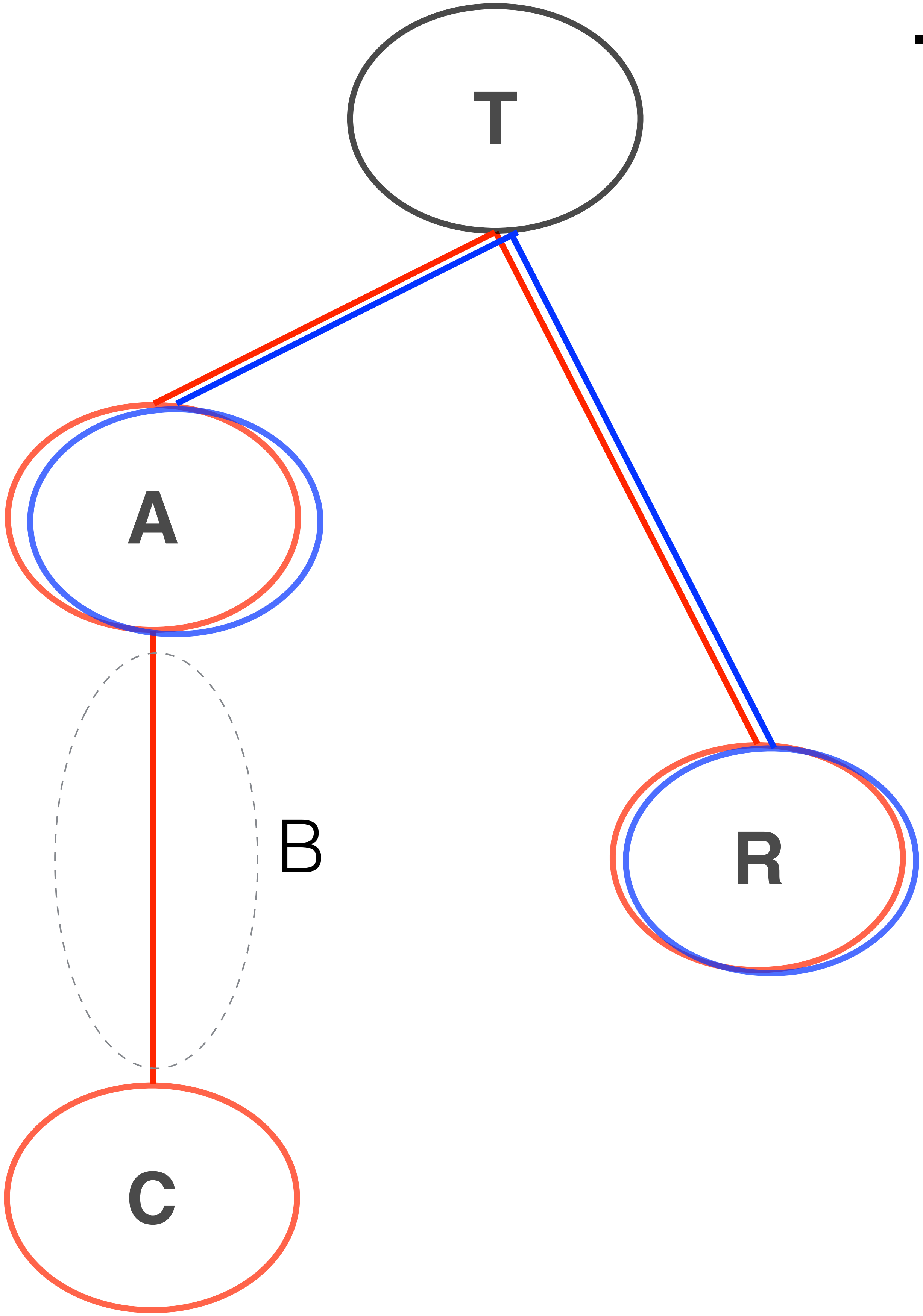
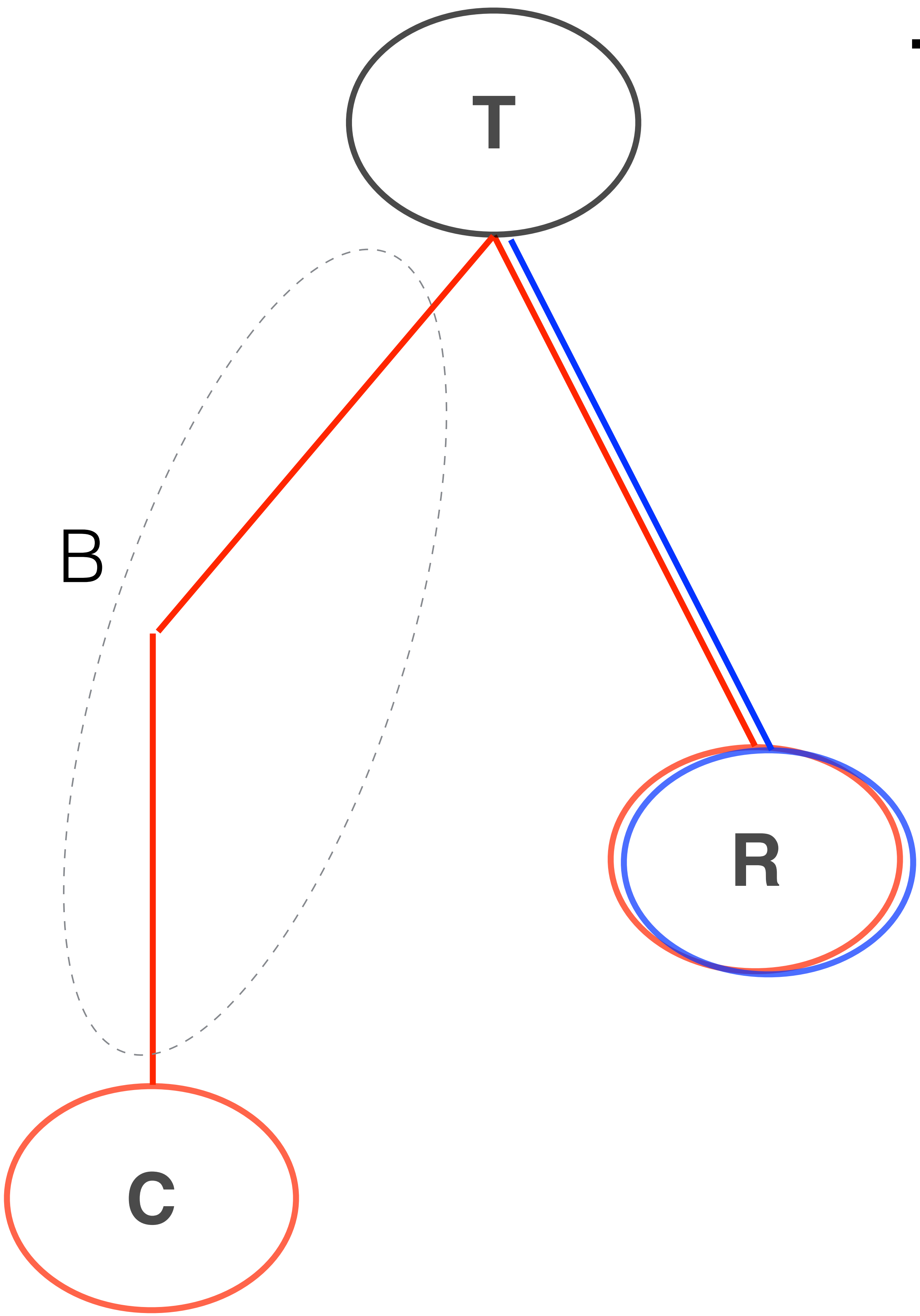


If A U R = C U R

Anything in between just goes there.

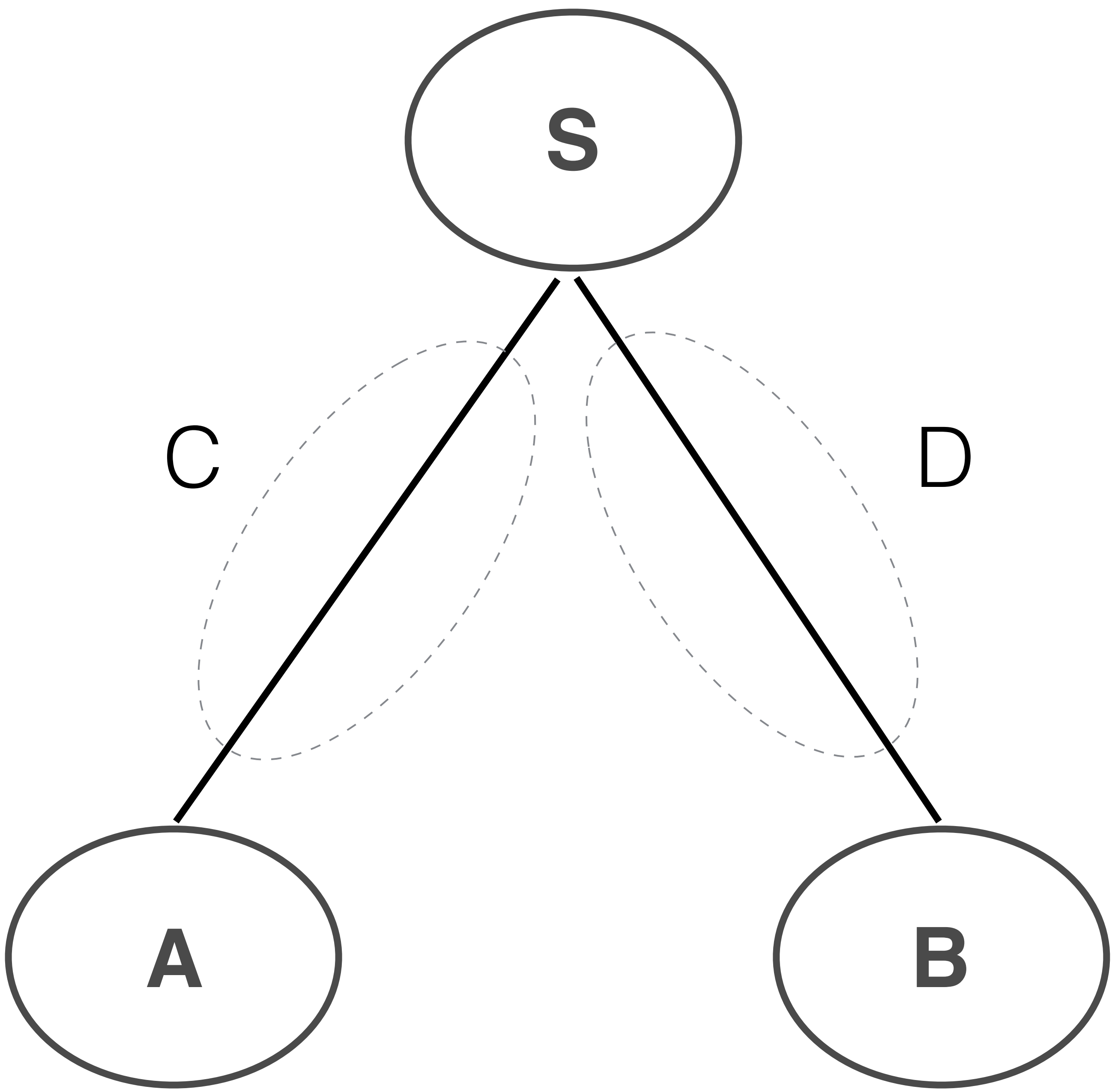
Theorem 2



But T U R = T = C U R

Thus

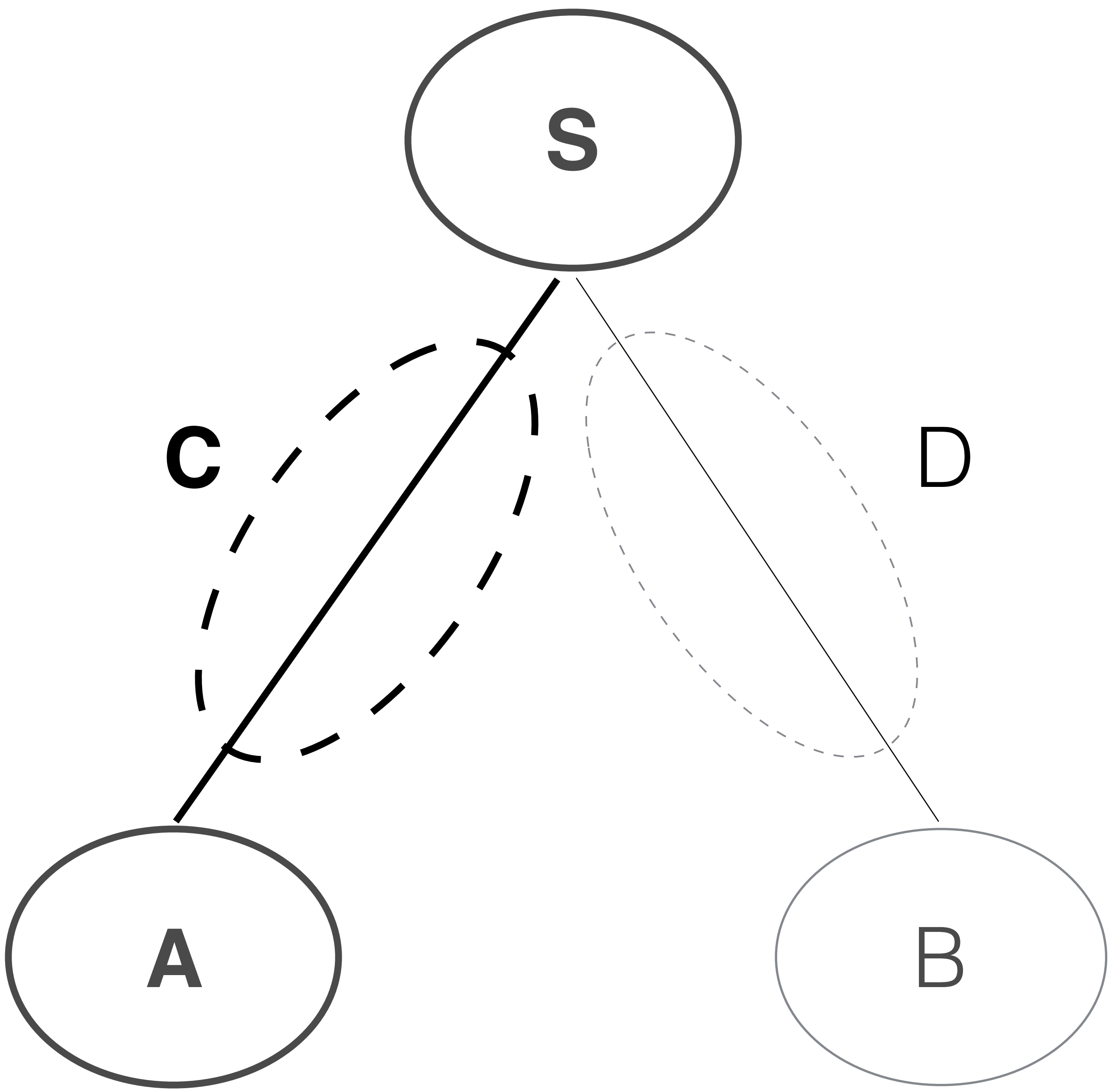
Theorem 3



If A U B = S;
if C, A ≤ C ≤ S;
if D, B ≤ D ≤ S;

then:
C U D = S.

Theorem 3



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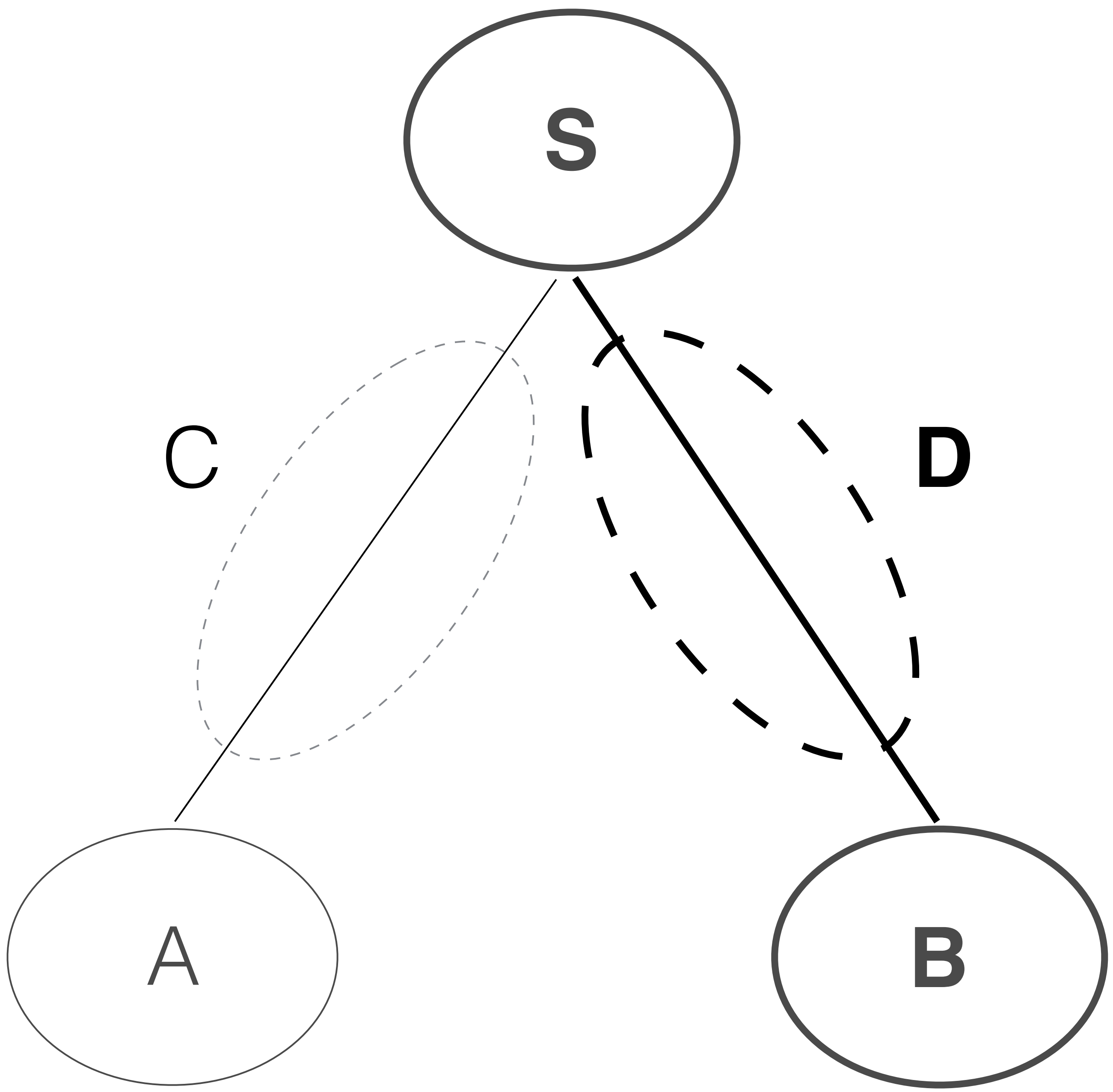

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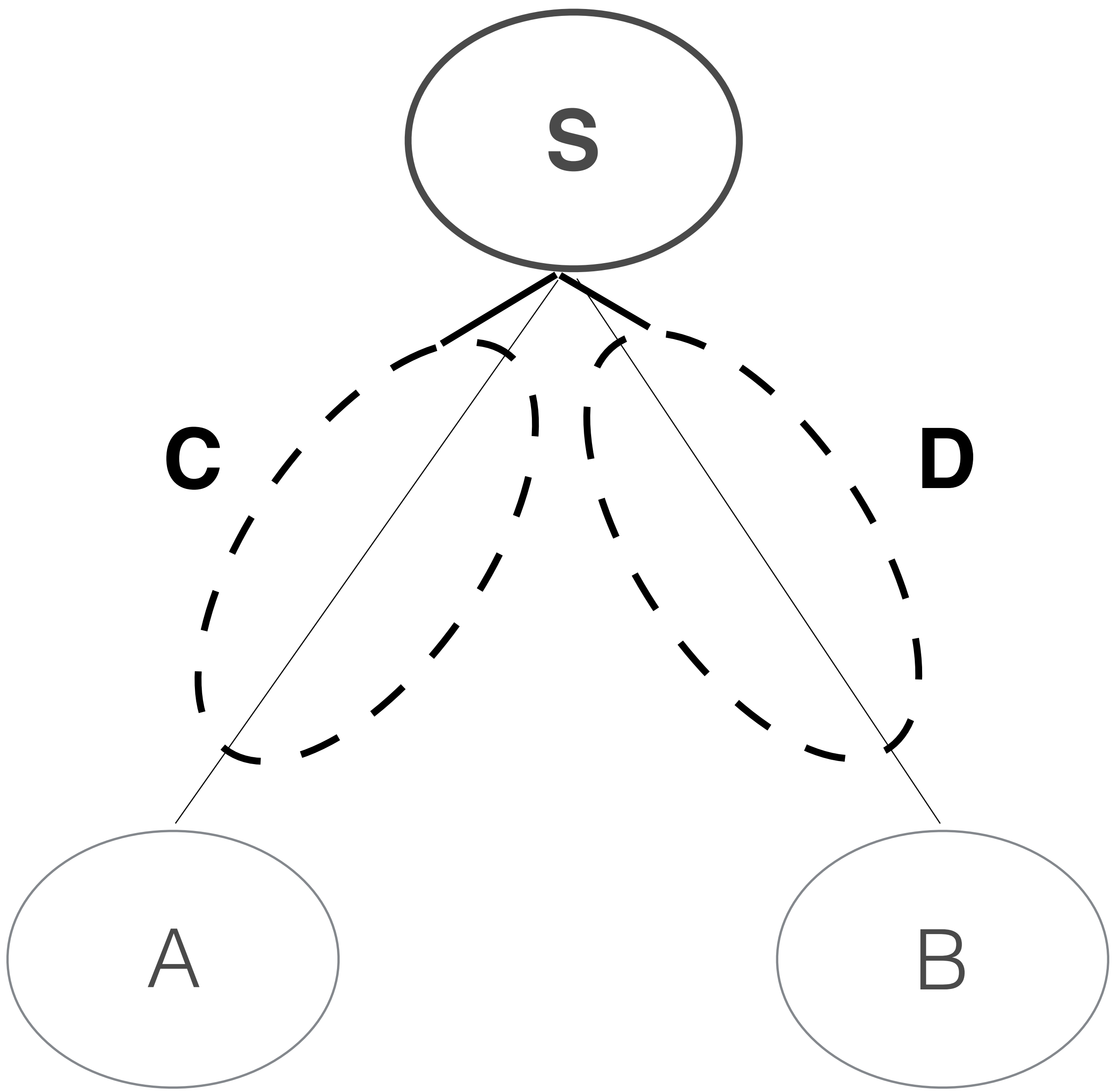
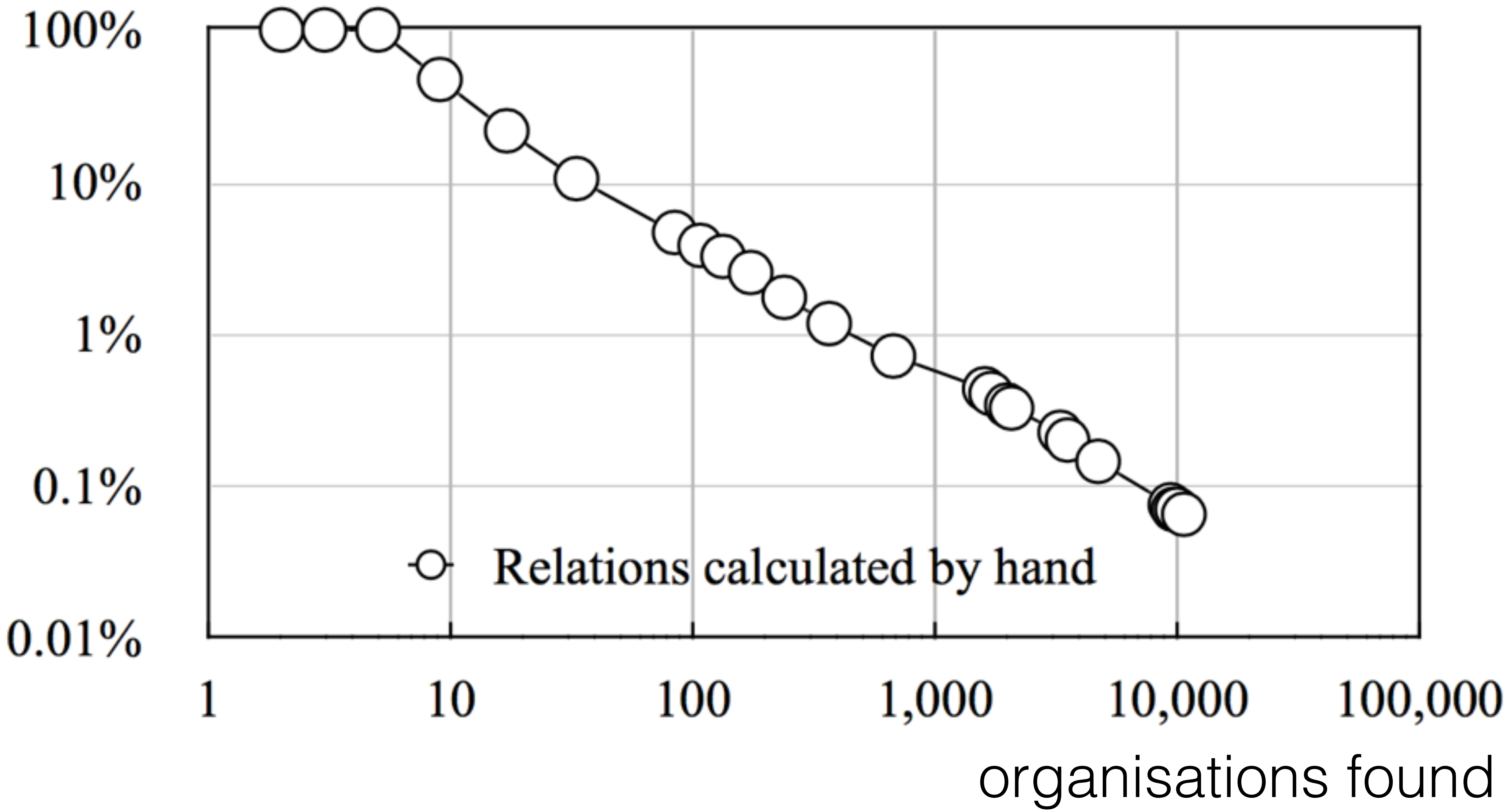
Theorem 3



If A U B = S;
if C, A ≤ C ≤ S;
if D, B ≤ D ≤ S;

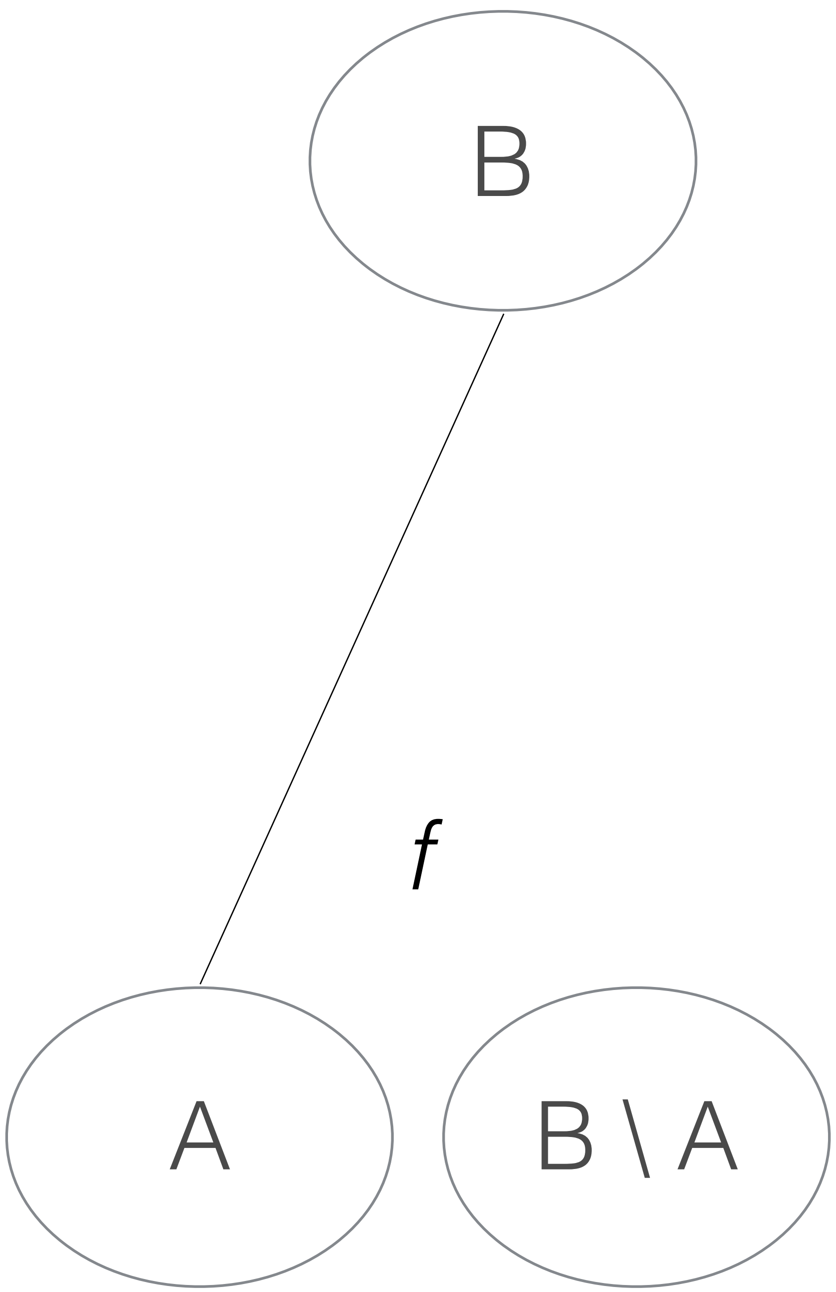
then:
C U D = S.

How many Union and Intersections are Calculated vs Demonstrated



Problem

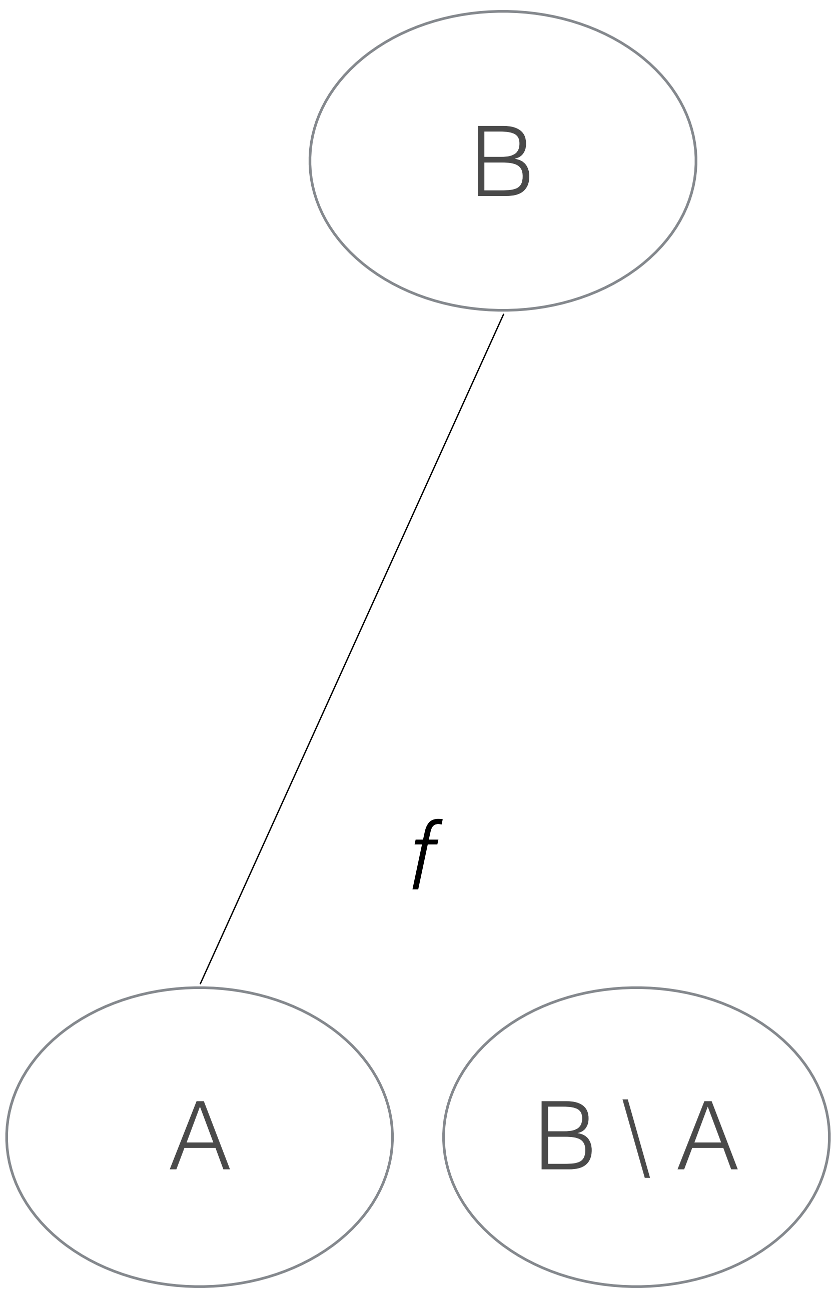
what molecules to ignore

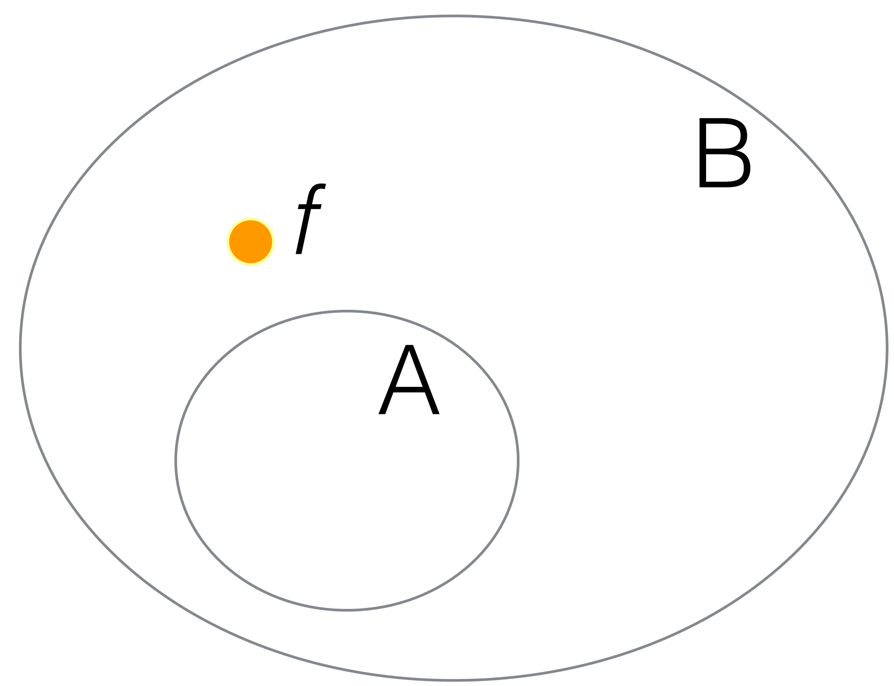


what subsets of
molecules to ignore

Problem

what molecules to ignore





what subsets of
molecules to ignore

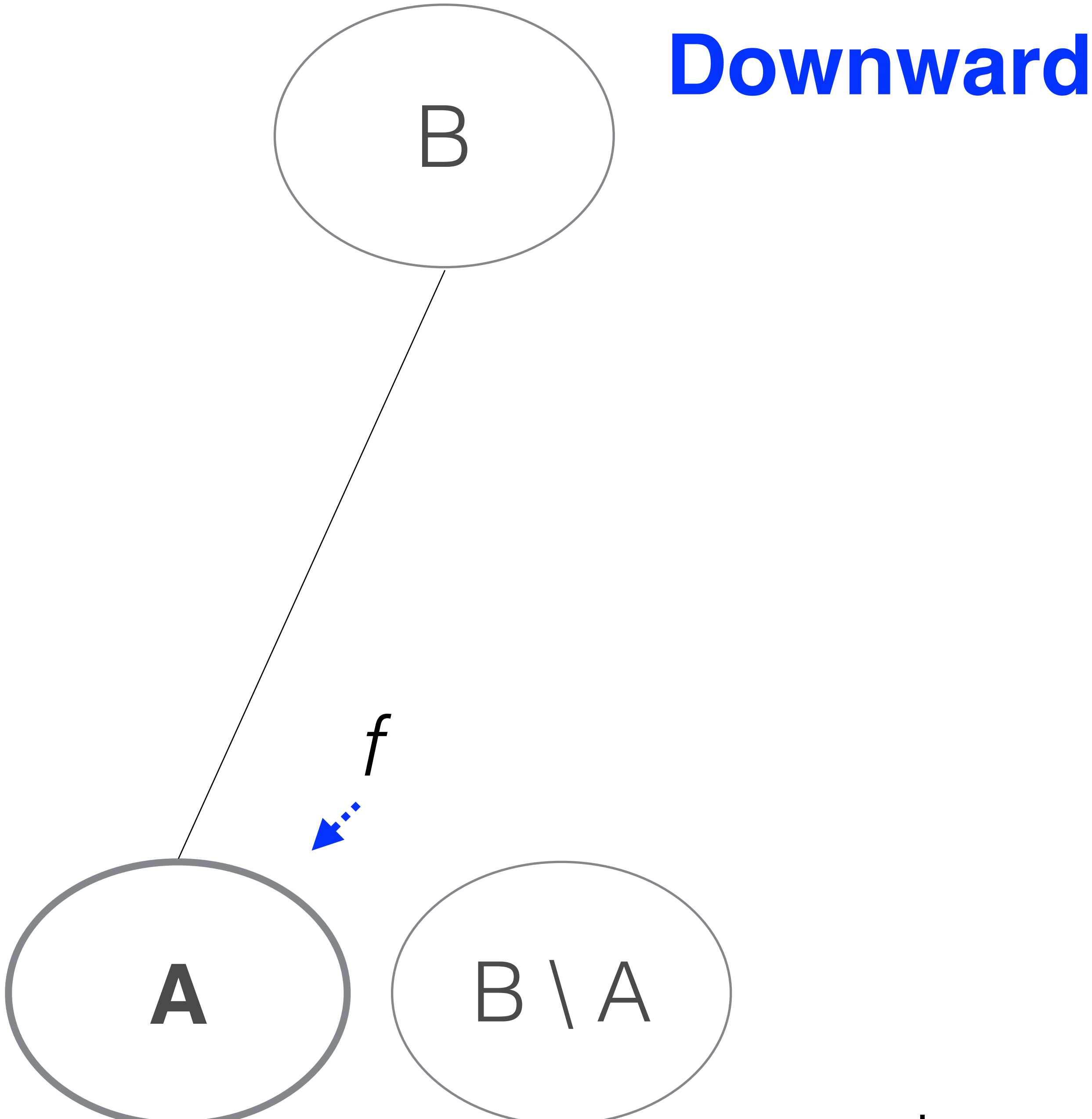
4 options

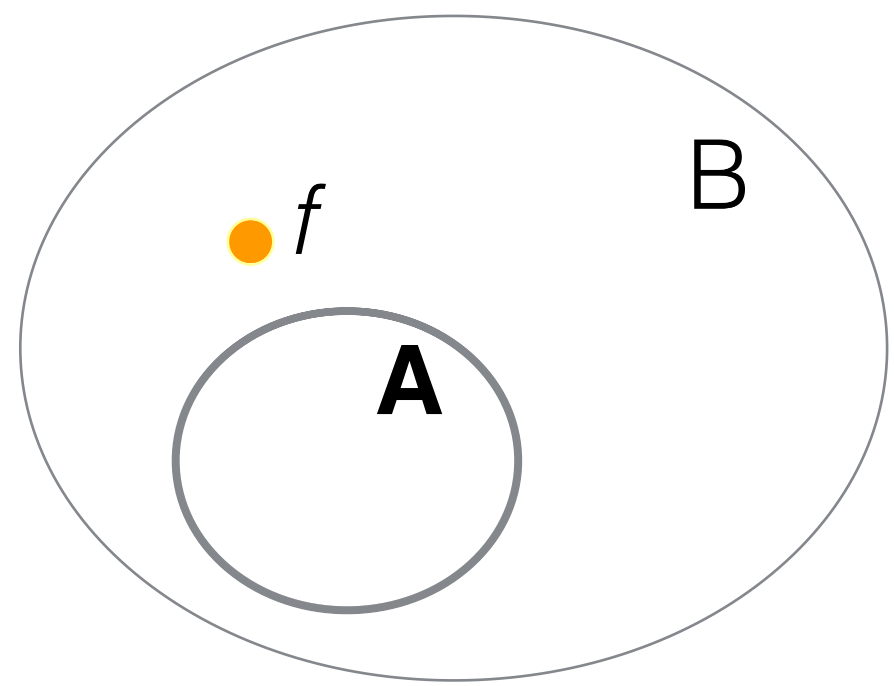
Af —> B > A

Af —> C with B > C > A, f ∈ C

Af —> D with B > D > A, f ∉ D

Af —> A





what subsets of
molecules to ignore

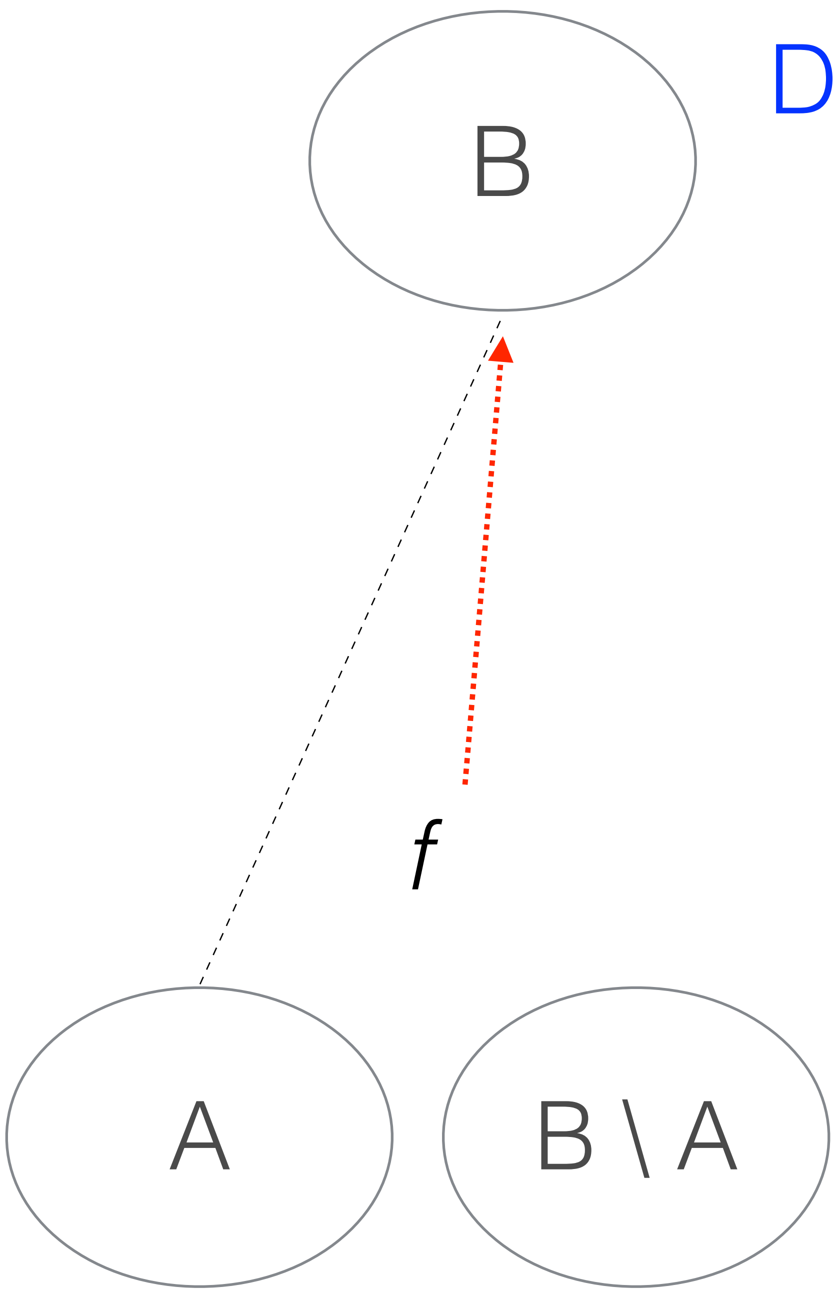
4 options

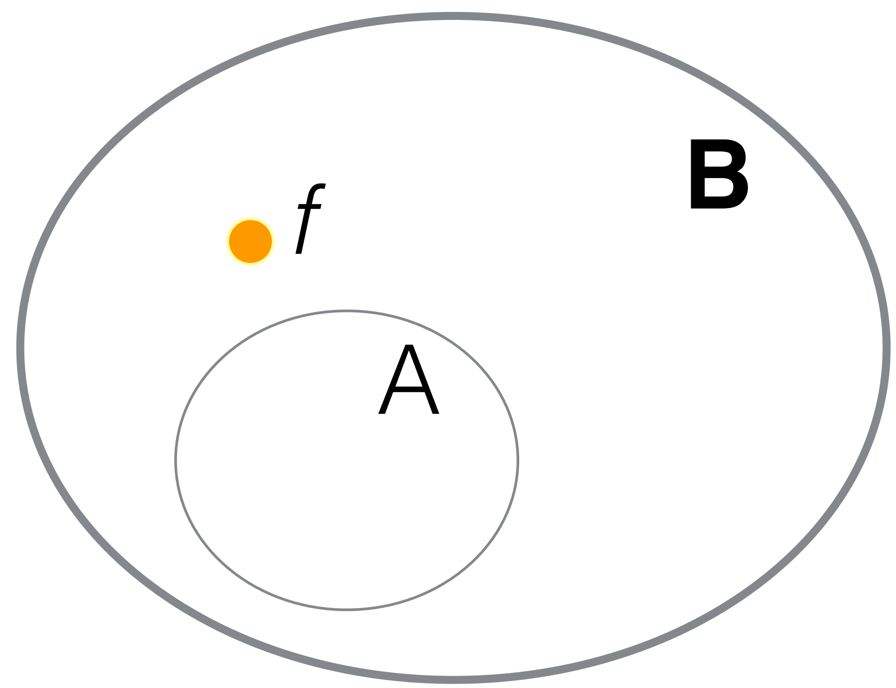
Upward **Af —> B > A**

Af —> C with B > C > A, f $\in$ C

Af —> D with B > D > A, f $\notin$ D

Downward Af —> A





what subsets of
molecules to ignore

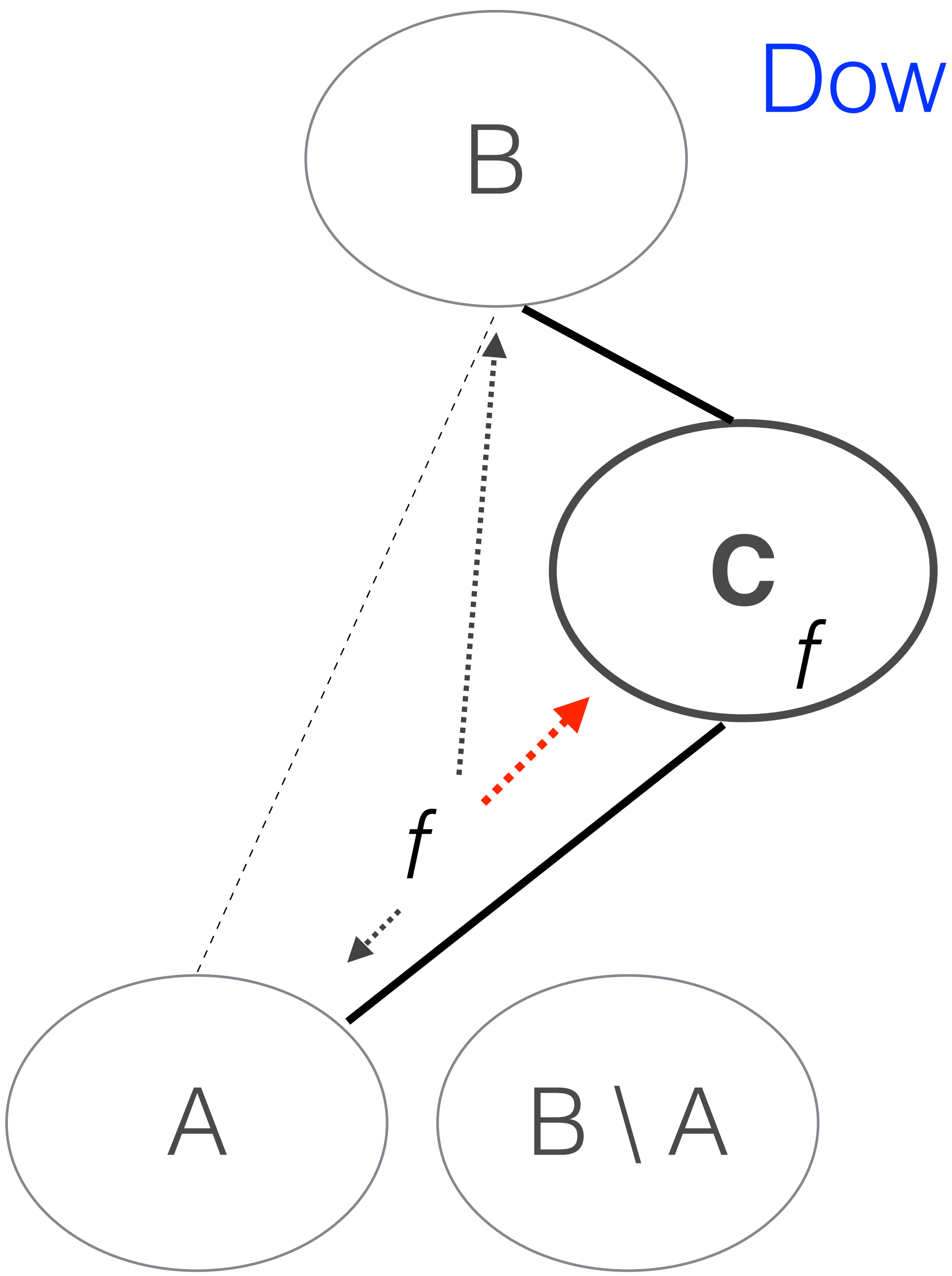
4 options

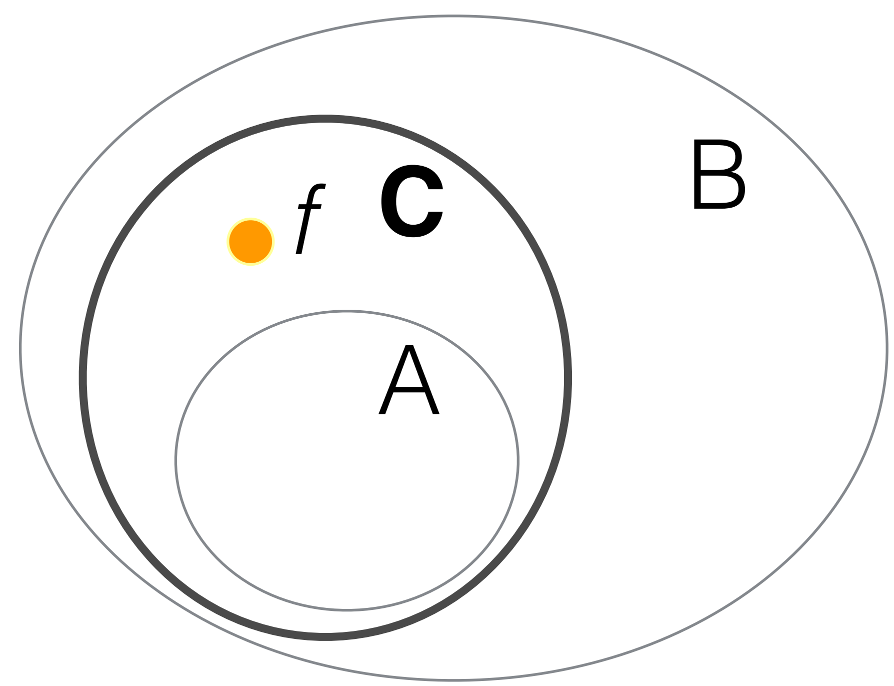
Upward Af —> B > A

Upward **Af —> C with B > C > A, f ∈ C**

Af —> D with B > D > A, f ∉ D

Downward Af —> A

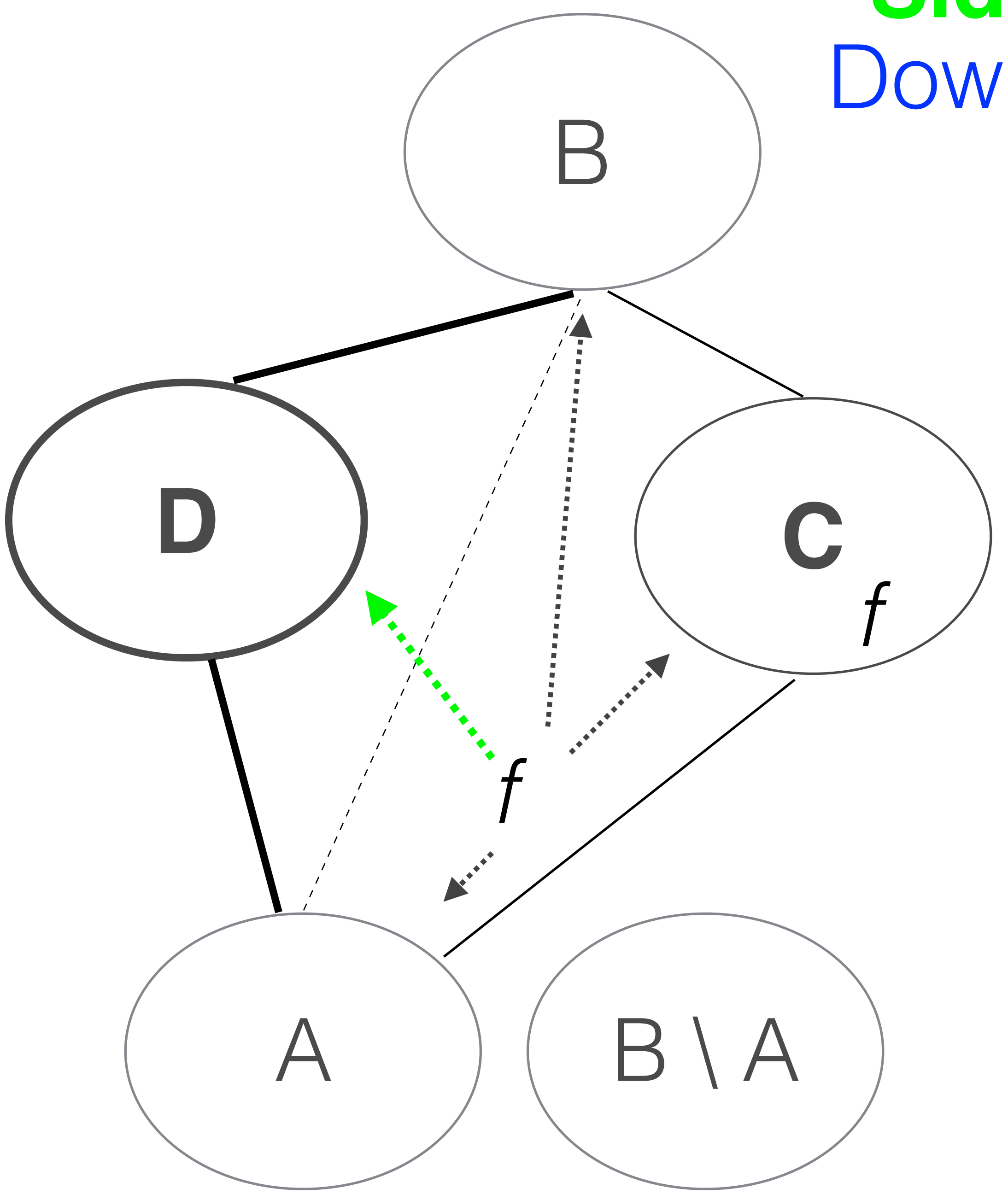


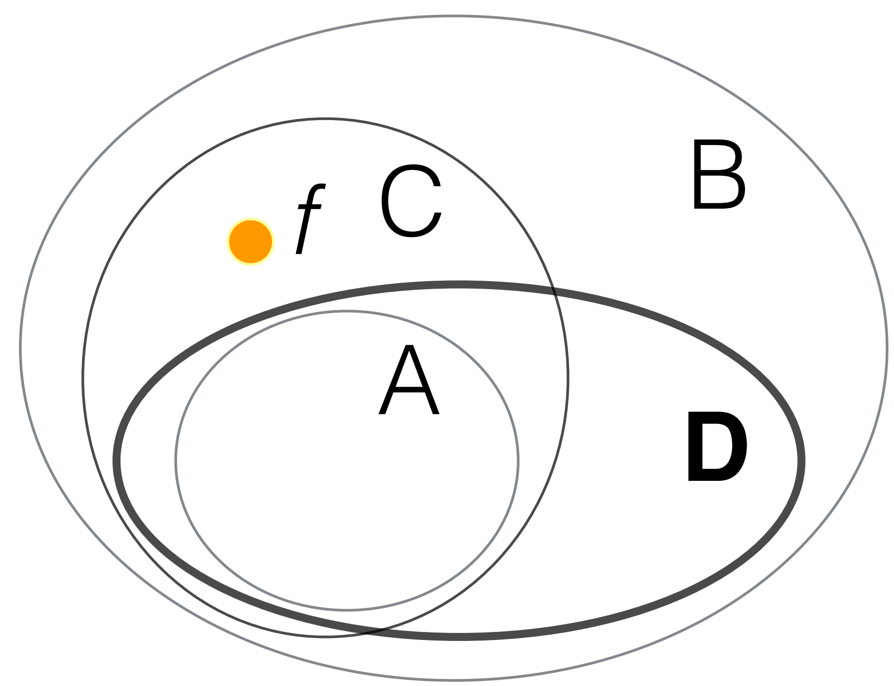


what subsets of
molecules to ignore

4 options

Upward Af —> B > A
Upward Af —> C with B > C > A, f ∈ C
Sideward Af —> D with B > D > A, f ∉ D
Downward Af —> A





what subsets of
molecules to ignore

Applying the Lattice
one molecule at a time

- Start with a set of organisations.
- Calculate all the union and intersections and add them;
- Until you cannot add anything anymore;
    - Now you have a sub-lattice
- Take an Org, add ***ONE*** molecule to find a new Organisation

- Go from sub lattice to sub lattice

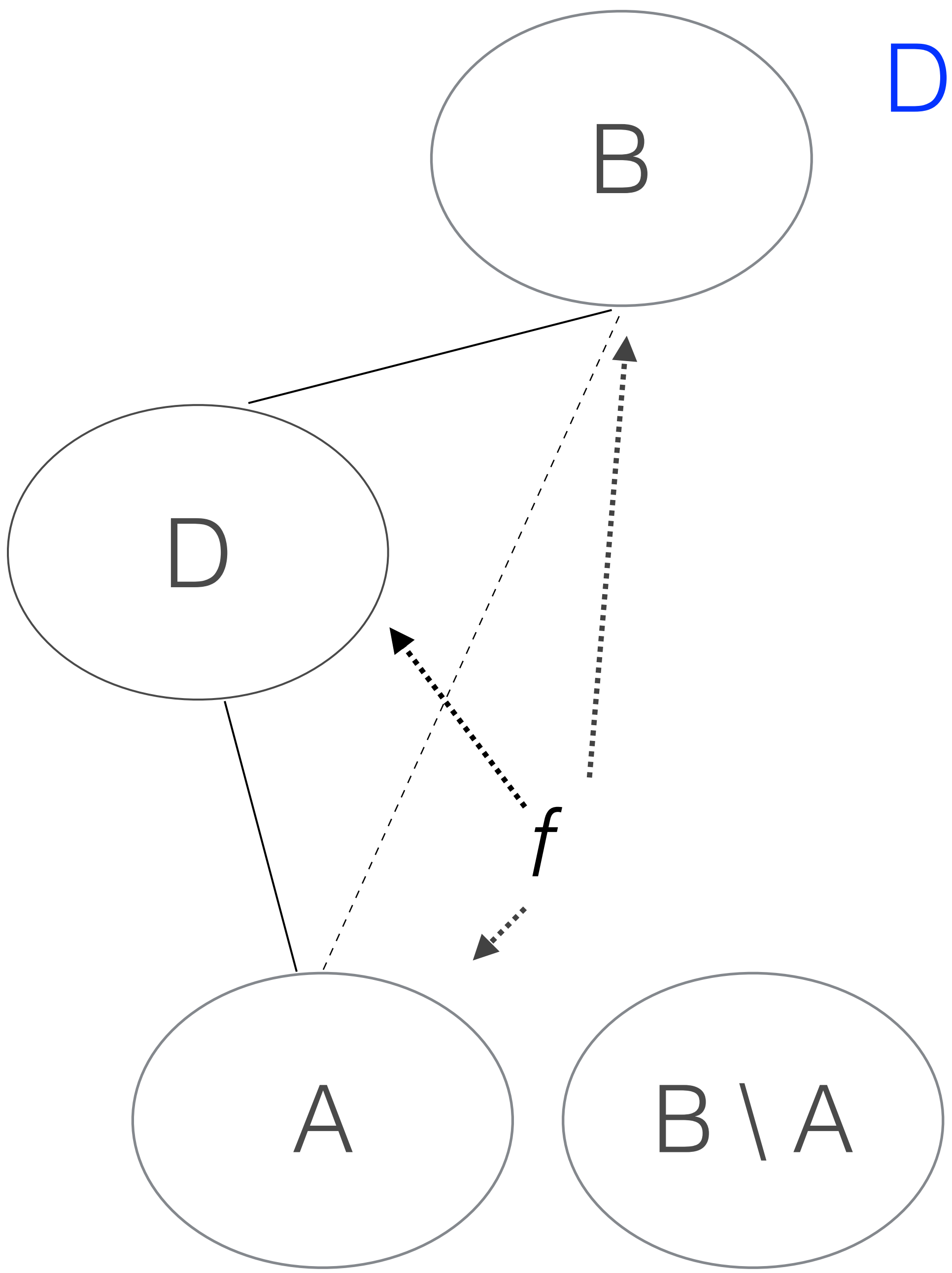
- …until you have found all the organisations.

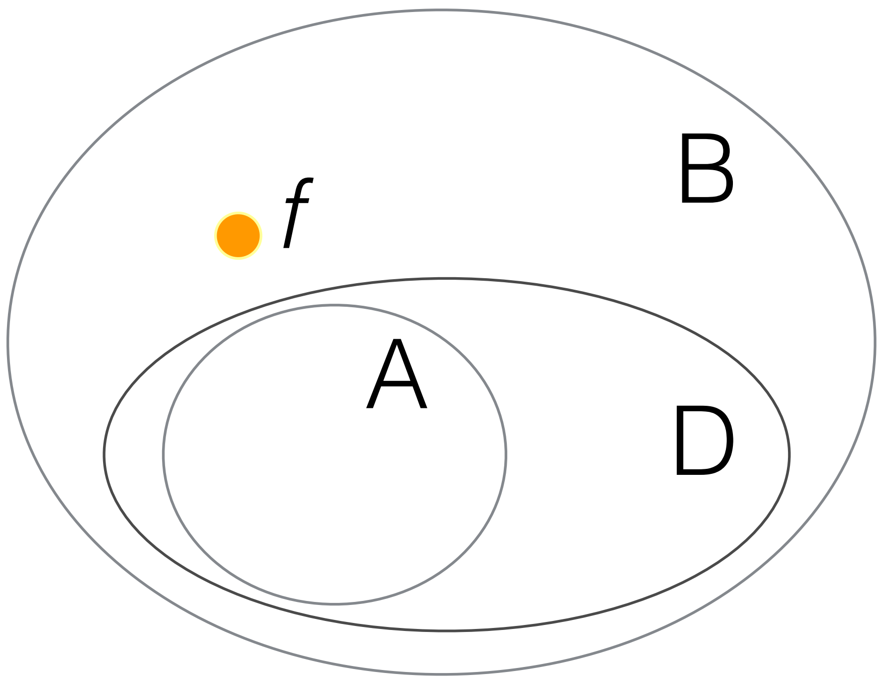
~~4~~ 3 options

Upward Af —> B > A

Sideward Af —> D with B > D > A, f ∉ D

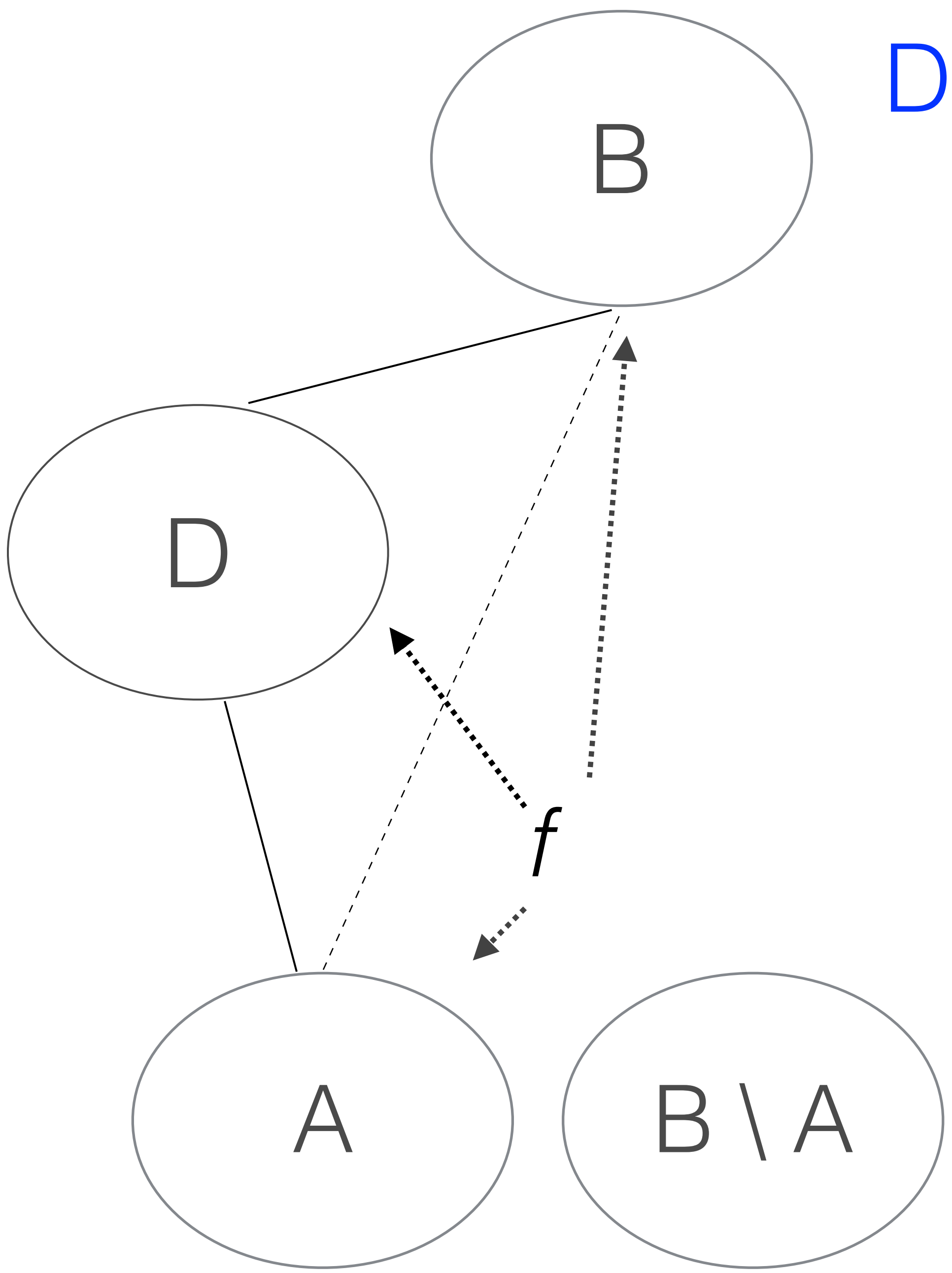
Downward Af —> A





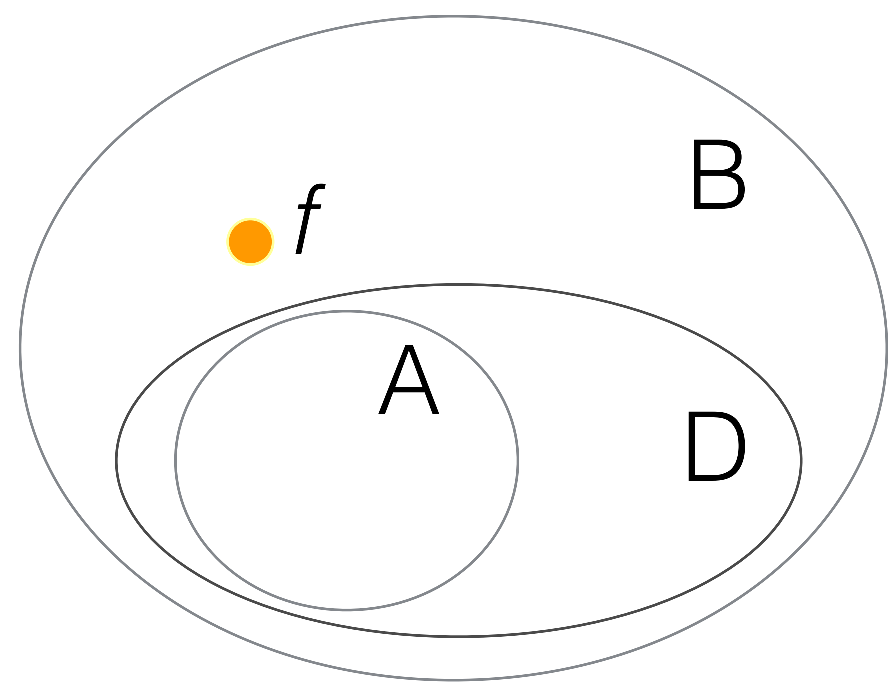
what subsets of molecules to ignore

We don't need to study the sidewards



Sideward Af —> D with B > D > A, f ∉ D

Downward Df —> D

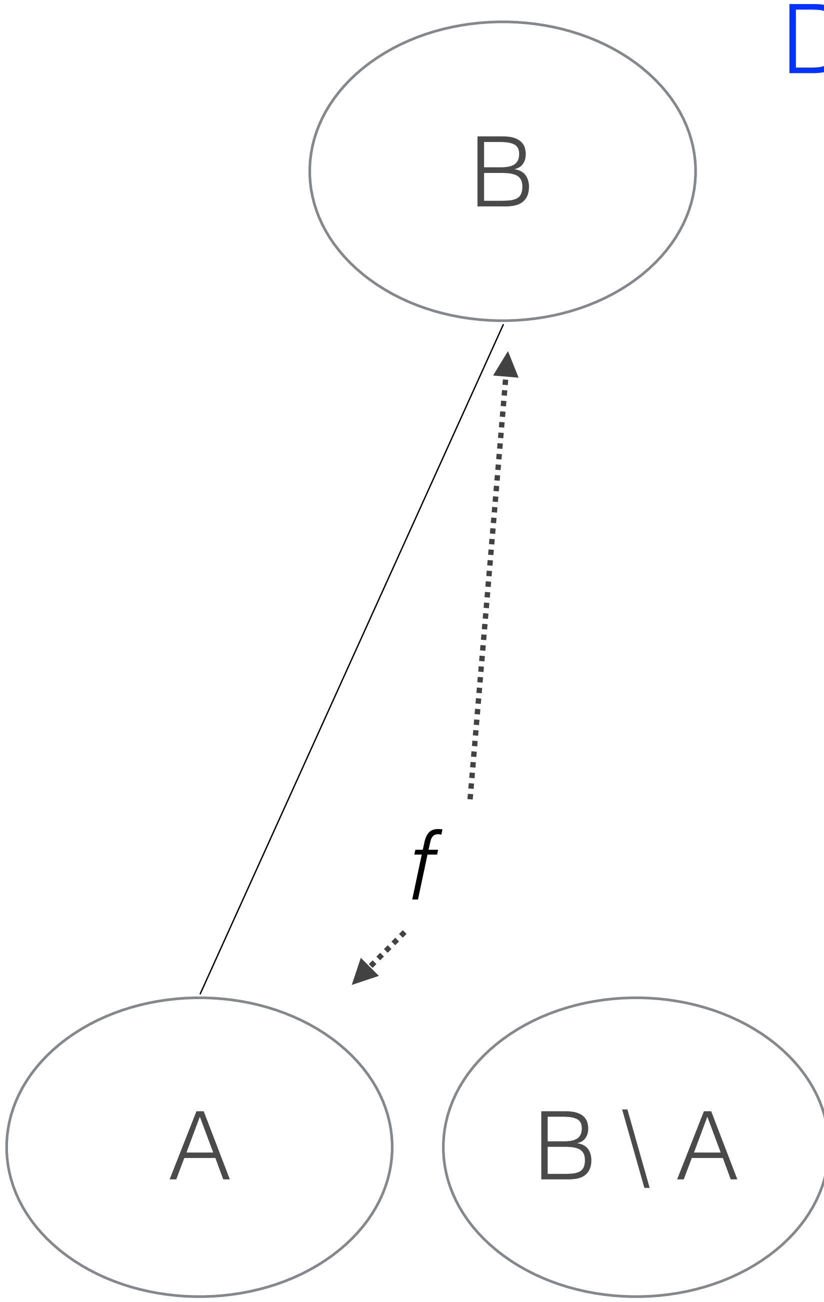


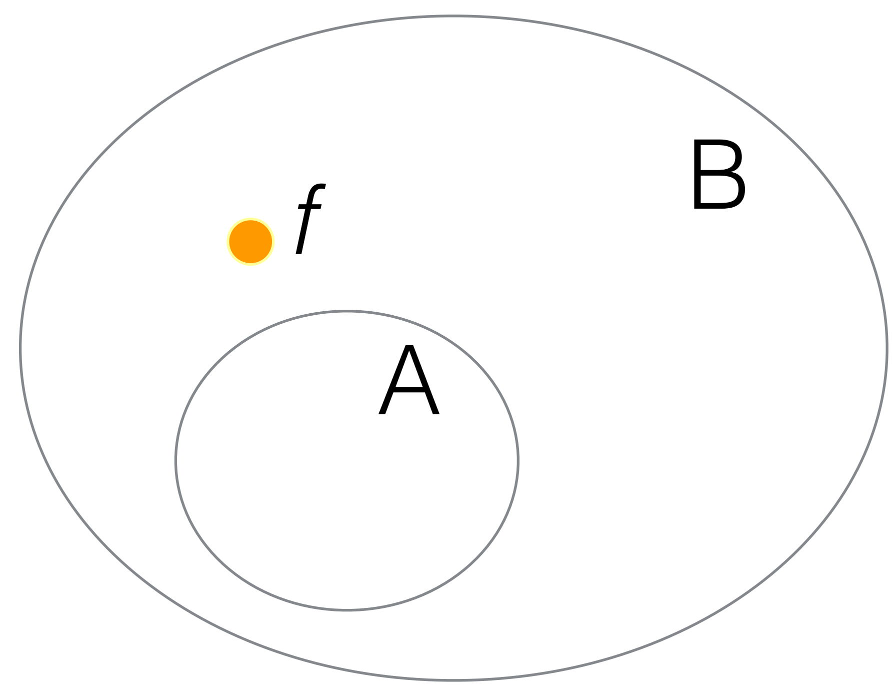
A sideward molecule of an organisation is always a downward molecule of another organisation

~~4~~ ~~3~~ 2 options

Upward Af —> B > A

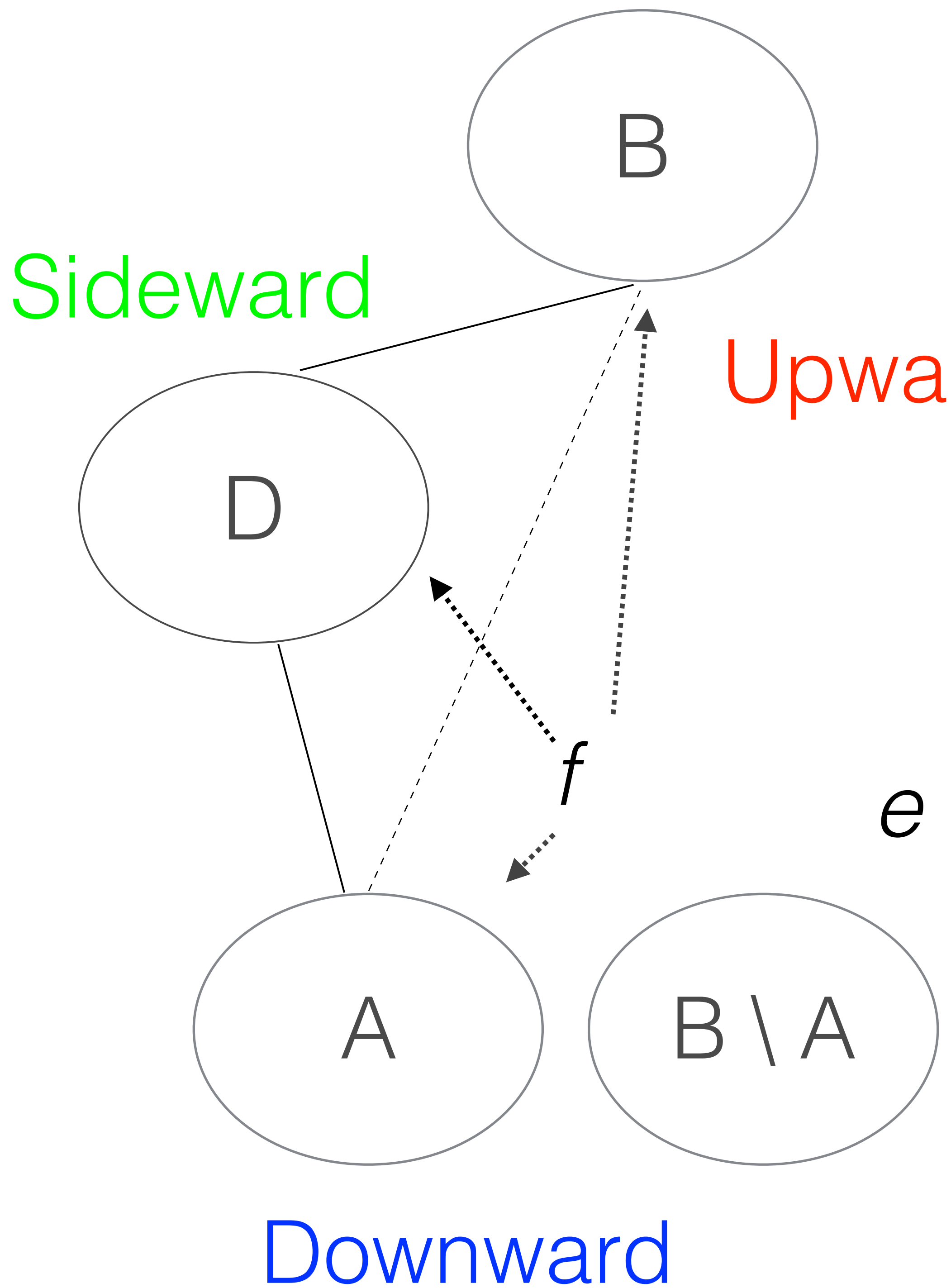
Downward Af —> A





what subsets of molecules to ignore

Taking 2 molecules at a time



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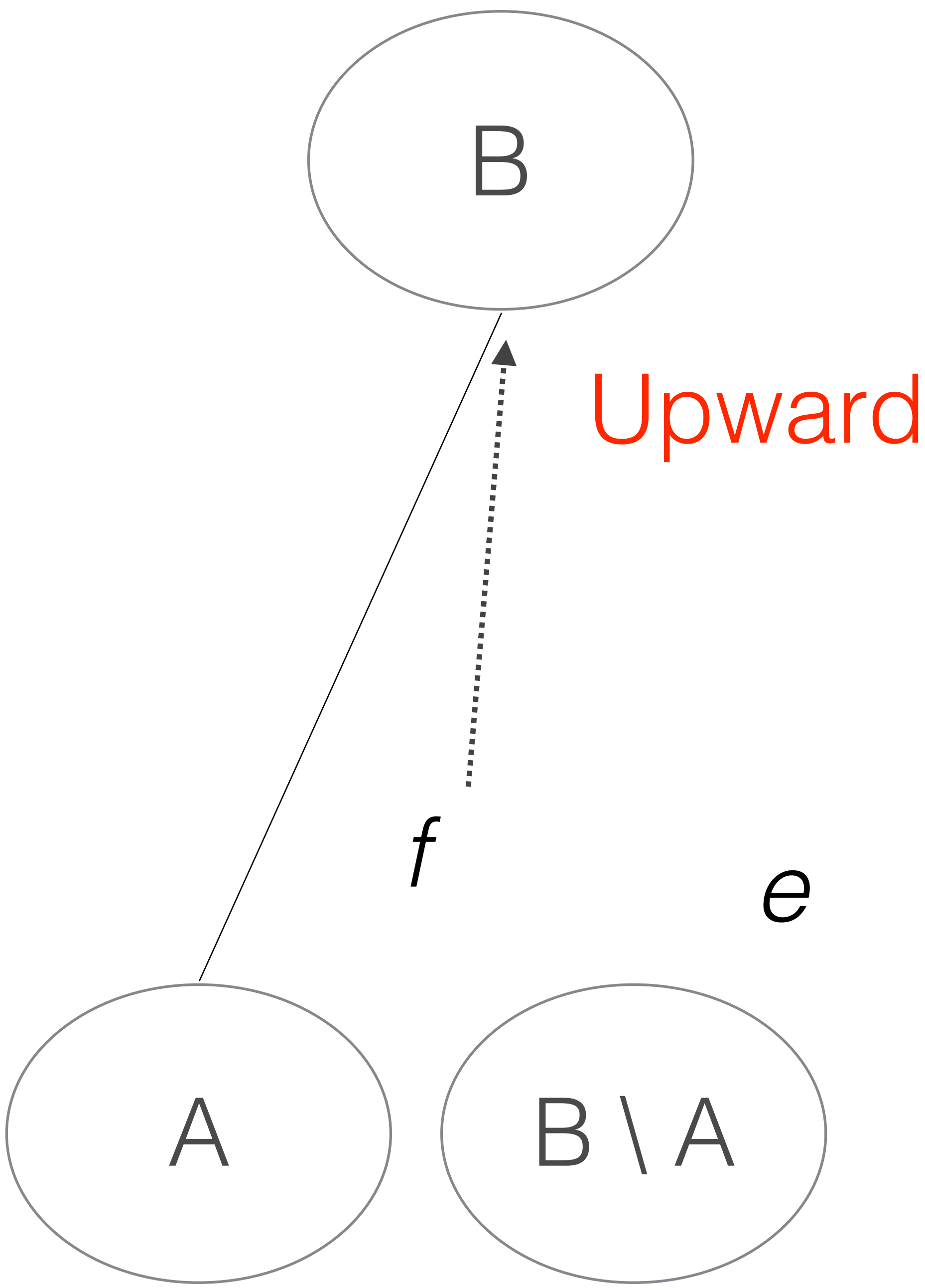
<tr><th colspan="2" rowspan="2">cases</th><th colspan="2">e goes</th></tr>
<tr><th>up</th><th>down</th></tr>
<tr><th rowspan="2">f goes</th><th>up</th><td>1</td><td>2</td></tr>
<tr><th>down</th><td>2</td><td>3</td></tr>
</table>

what subsets of
molecules to ignore

Case 1, 2: If one molecule goes upward



cases		**e goes**	
		up	down
f goes	up	**1**	**2**
	down	**2**	3

We need to calculate
$G_O(A \cup f \cup e) = G_{SM}(G_C(A \cup f \cup e))$

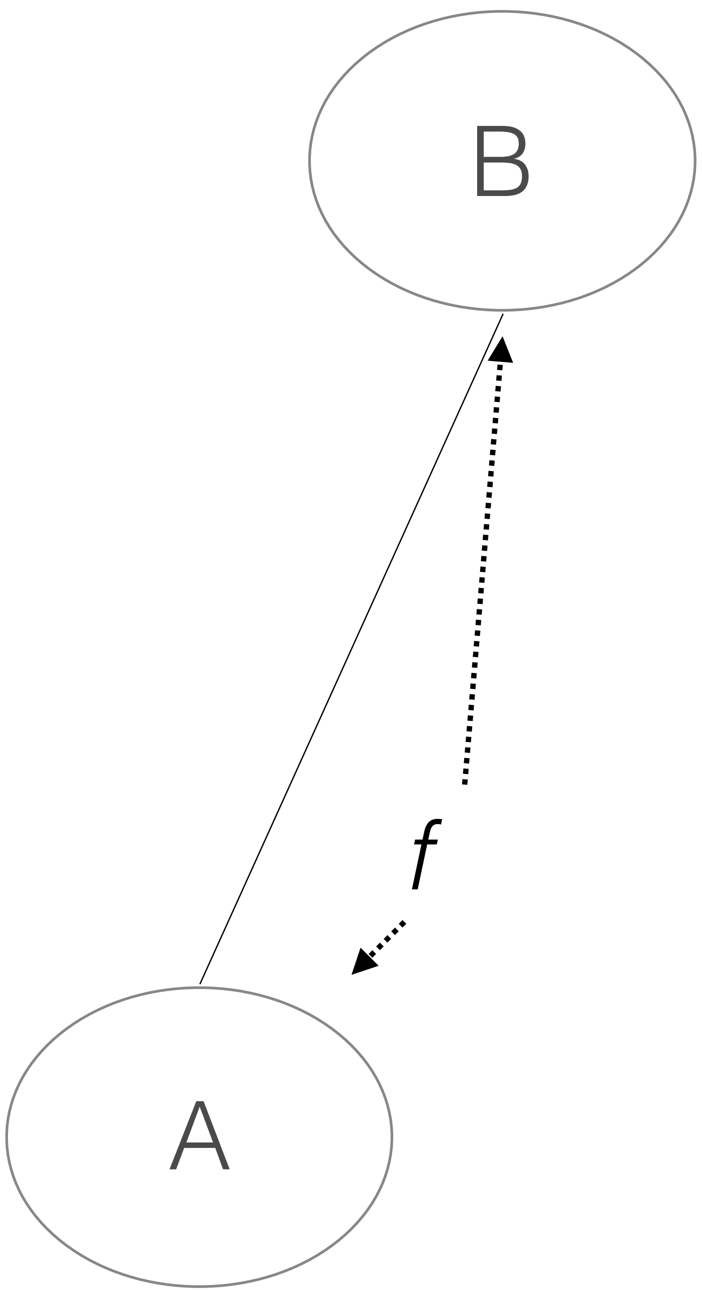
We know that
$A \cup f \leq G_O(A \cup f) = B \leq G_C(A \cup f)$;
thus $G_O(A \cup f) = G_C(A \cup f)$

$G_O(A \cup f \cup e) =$
$= G_{SM}(G_C(A \cup f \cup e)) =$
$= G_{SM}(G_C(G_C(A \cup f) \cup e)) =$
$= G_{SM}(G_C(G_O(A \cup f) \cup e)) =$
$= G_O(B \cup e)$

Which is something we obtained before.
So cases 1, 2, will not lead to anything new. We don't need to calculate them

Problem

what molecules to ignore



cases		e goes	
		up	down
f goes	up		
	down		

what sets of molecules to ignore?
Any subset where at least a subset of molecules of it goes upward

Solved

Theorem: No Organisation Left Behind

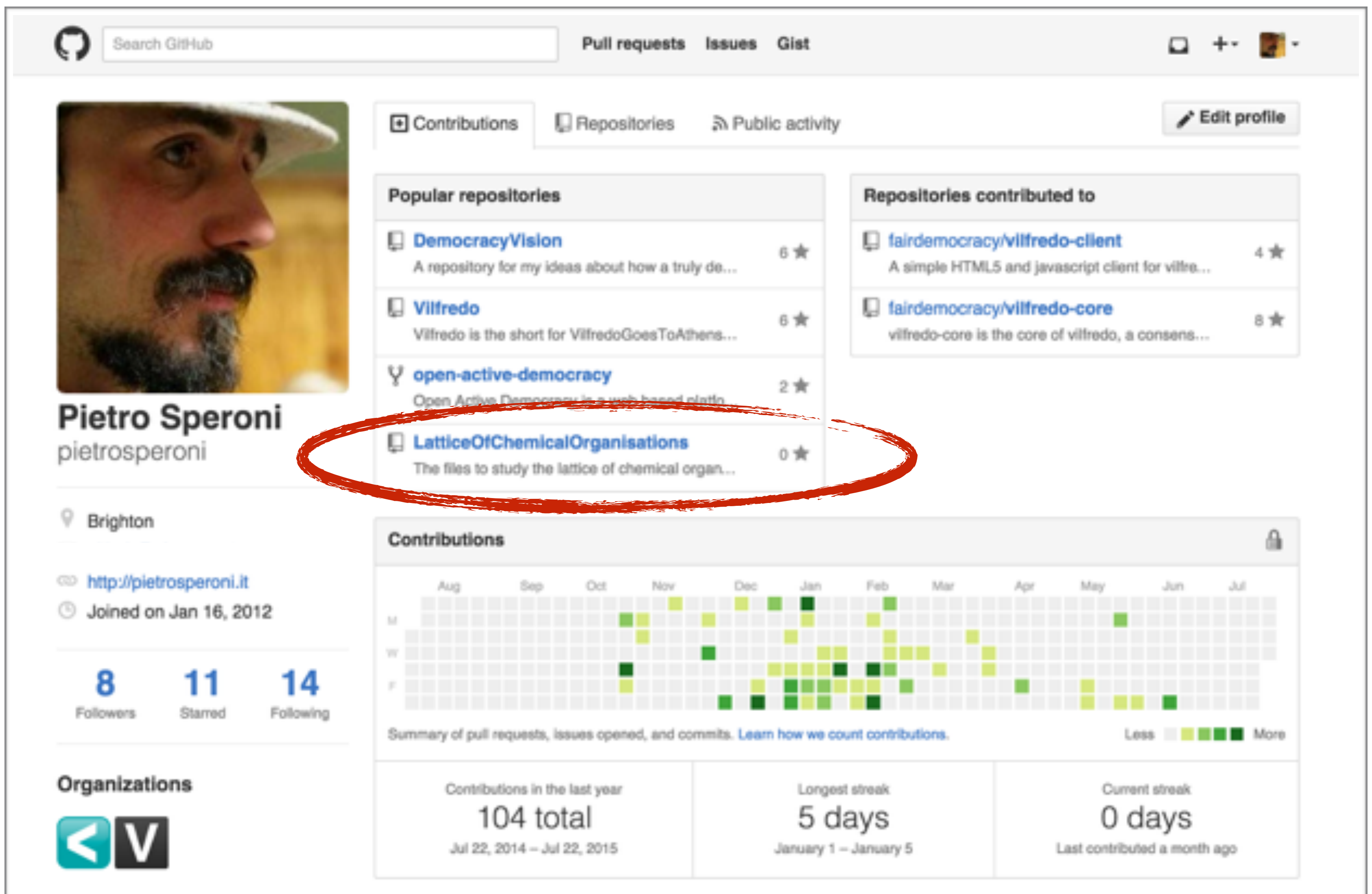
Take away message

If something has a mathematical property:
use it

Note:

The code is available on git hub

https://github.com/pietrosperoni/LatticeOfChemicalOrganisations/tree/Public



https://github.com/pietrosperoni

Thank You

pietrosperoni.it