Reaction Networks as a Formal Mechanism to Explain Social Phenomena*

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Abstract. Since sociology is seeking mechanisms for explaining social phenomena, we discuss in this paper, whether and how chemical organization theory together with the metaphor of a chemical reaction network can be employed as formal mechanisms to describe social and economic systems. A reaction network is a quite general concept, which allows to model a variety of dynamical systems. Further more, a set of powerful tools can infer potential dynamical properties from the networks structure. Using an economical toy example generated from United Kingdom input-output analytical tables (1995), we demonstrate how chemical organization theory can be applied and can give insight into the structure of the resulting model. Chemical organization theory allows identifying an overlapping hierarchy of important sub-systems in these networks. [1]

1 Introduction

Sociology is seeking mechanisms that explain social phenomena [1]. Mechanisms can be described in various ways, ranging from rich linguistic descriptions to precise mathematical formulas [2]. In general it is desirable to obtain a formal description of a social mechanism. However, there is the danger to loose important details of the social phenomenon during the process of abstraction [3] or to arrive at a more complex model than actually required to explain the designated phenomenon. Therefore it is necessary to posses a rich toolbox, which offers different mechanisms for different levels of abstraction.

Here we discuss one specific but quite powerful metaphor, the chemical reaction network, which can be used to describe a large variety of phenomena from fields of study like economy and sociology. Furthermore, we describe chemical organization theory [4, 5], which allows identifying an overlapping hierarchy of

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important sub-systems in these networks. These sub-systems are candidates for self-sustaining (maybe even autopoietic) systems.

The techniques described here are not only useful to model social systems. In the same way as we build social models, we can use these techniques to build and analyze multi-agent systems (MAS), which is the fundamental philosophy of Socionics [6]

2 Chemical Organization Theory

The basic idea of chemical organization theory is to identify hierarchical structures in terms of chemical organizations, which are closed and self-maintaining sets of elements, e.g., molecules, decisions, communications, or products. These organizations can be visualized using a Hasse-diagram (as shown in Fig. 1, right), which provides a powerful graphical representation of the network's inherent structure.

The networks investigated in this study are equivalent to catalytic flow systems, which are reactions systems where all molecules act only as catalysts and where all molecules decay at a positive rate. Therefore, we require only a simplified version of the chemical organization theory. In particular, we can exclude mass conservation and the complicated concept of mass-maintenance. The required theory can be explained in a quite compact way. In order to explain the theory, we will stick to its terminology. So, we call the elements of a system *molecules* and the relation among elements *reactions*. Molecules and reactions together form a reaction network as exemplified by Fig. 1, left. Let us first define clearly, how the systems look like that we will analyze. We call these systems catalytic algebraic chemistries. The term "algebraic" is used, since a notion of dynamics is missing, and the term "catalytic" is used, since all reactions are assumed to be fully catalytic.

A catalytic algebraic chemistry is a set of molecules together with a set of reaction rules. A reaction rule is just a pair of sets of molecules. A reaction consists of a left hand side and a right hand side. A reaction is interpreted in the following way: The left hand side denotes a set of molecules that are sufficient to produce the molecules on the right hand side. Further more, if the molecules of the left hand side are present in a reactor, then all molecules on the right hand side are produced by this reaction (at least at a low rate). Since we assume a catalytic flow system, the molecules on the left hand side are not used up when the molecules on the right hand side are produced. Molecules vanish only through a general dilution flow, which is equivalent to a spontaneous decay. In the economical systems we analyze here, a molecule like a denotes a product.

2.1 Chemical Organization Theory for Catalytic Flow Systems

In this section, we describe the basic concepts of a simplified version of the chemical organization theory, which is sufficient for the economical and political

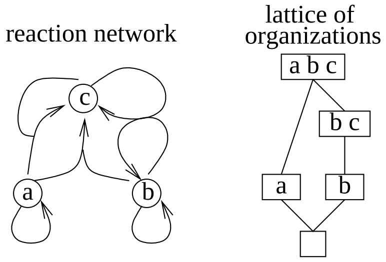

Fig. 1. Example reaction network (left) and its lattice of organizations (right). An arrow denotes a catalytic reaction where all educts are catalysts.

systems investigated here. The simplified version is limited to so called catalytic flow systems, which are reaction systems where all molecules act always as catalysts and all molecules decay spontaneously. Despite of these limiting assumptions, the simplified version of the theory posses already a wide application range, as exemplified by our investigations of the political system and economic networks. Furthermore, various systems in Biology and related disciplines can be treated with the simplified theory, cf., hypercycle, replicator equation, autocatalytic networks.

The reaction system is given as a catalytic algebraic chemistry $(\mathcal{M}, \mathcal{R})$, where $\mathcal{M}$ is a set of molecules and $\mathcal{R}$ is a set of reactions of the form $(A \Rightarrow B) \in \mathcal{R}$, were A and B are sets of molecules, $A, B \in \mathcal{M}$.

The set of reaction rules $\mathcal{R}$ contains all reaction rules of the model. A reaction rule possesses the form $A \Rightarrow B$, where A is the set of molecules on the left hand side and B is the set of molecules on the right hand side. So, the reaction rule $a+b \Rightarrow c$ can be written as $A \Rightarrow B$ with $A = \{a, b\}$ and $B = \{c\}$. Note that here it is sufficient that A and B are sets and not multisets, because we deal solely with catalytic flow systems.

Example (catalytic algebraic chemistry): The pair $(\mathcal{M}, \mathcal{R})$ is a catalytic algebraic chemistry with the set of molecules $\mathcal{M} = \{a, b, c\}$ and the set of reaction rules $\mathcal{R} = \{a+b \Rightarrow c,\ a \Rightarrow a,\ a+c \Rightarrow c,\ b+c \Rightarrow b+c,\ b \Rightarrow b\}$ (Fig. 1). The double arrow $\Rightarrow$ denotes a catalytic reaction, ie. $A \Rightarrow B$ is equivalent to the chemical reaction $A \rightarrow A + B$.

In order to illustrate the meaning of this reaction system, we give an example of a dynamical process that is governed by such a network: Imagine that the process takes place inside a reaction vessel or reactor. Assume that the reactor contains instances of the molecules, such that the concentrations of the molecules are: $[a] = 20$, $[b] = 5$, $[c] = 4$. This concentration vector can be interpreted in the following way: there are 20 units of a, 6 units of b, and 4 units of c present in the reactor. The reactor represents an instance of our reaction system (catalytic algebraic chemistry). Now we can simulate the dynamics by applying the reaction rules to the reactor. E.g., we can apply rule $a+b \Rightarrow c$, which increases the amount of c by one. Note that it does not decrease a nor b, since a and b both act as catalysts (we require that all reactions are fully catalytic). Because we assume here catalytic flow systems, every molecule is effected by a dilution flow, which is equivalent to the fact that every molecule decays spontaneously. This decay can be simply simulated by choosing randomly a molecule and decreasing its number by one. This can be done by randomly choosing a molecule proportional to its concentration, e.g., the probability to choose a is 19/29. Destroying a we arrive at $[a] = 19$, $[b] = 5$, $[c] = 5$. How this update is performed, has to be defined in more detail in order to get a precise description of the dynamics. E.g., we may define a reactor size, i.e. a maximum number of molecules in order to prevent unlimited growth.

The set of all possible subsets is called powerset. Instead of writing $A \subseteq M$ we can write $A \in \mathcal{P}(\mathcal{M})$, where $\mathcal{P}(\mathcal{M})$ denotes the set of all possible sets that contain elements from $\mathcal{M}$.

Example: $\mathcal{P}(\mathcal{M}) = \{\{\}, \{a\}, \{b\}, \{c\}, \{a, b\}, \{a, c\}, \{c, b\}, \{a, b, c\}\}$. The set $\{\}$, which does not contain any element, is called the empty set. $\mathcal{P}()$ is an operator that take a set as input and returns a set of all possible subsets of that set, including the set itself and the empty set.

Let us notice at that point that a set of molecules represents already a large amount of different states our system that we intend to model can be in. So, taking a set of molecule to describe the current state of a system is a strong abstraction. This level of abstraction does not care, how many copies of molecule a are present, nor does it care about the spatial distribution of those copies, and so on. Despite the high level of abstraction, the number of possible sets is still large. The number of possible sets grows exponentially with the number of possible molecules: $|\mathcal{P}(\mathcal{M})| = 2|\mathcal{M}|$, where $|\mathcal{M}|$ denotes the number of elements in the set $\mathcal{M}$. For example for $|\mathcal{M}| = 20$ different molecules there are about 1 million different sets, and for $|\mathcal{M}| = 21$ different molecules there are about 2 million different sets. Some sets are more important than others. Why? Because we can observe some sets more likely than others. The reason for this is that the system becomes stable more likely when these molecules are present. In order to identify and describe these important sets, we introduce specific conditions, properties, or constraints. These constraints will reduce the set of all possible sets, leaving a set of sets that can be regarded as a representation of the systems organizational structure.

2.2 Closed Sets

The first constraint that we introduce is the (algebraic) closure. Given a set of molecules C that is closed, the closure assures that reactions among molecules in C produce only molecules in C. So, a closed set contains all molecules that can be produced by reactions among those molecules.

Definition 1 (closed set). *A set of molecules $C \subseteq M$ is closed, if for all reactions $(A \Rightarrow B) \in R$, with A is a subset of C, B is also a subset of C.*

Example (closed sets): In our example the closed sets are: $\{\}$, $\{a\}$, $\{b\}$, $\{c\}$, $\{a, c\}$, $\{c, b\}$, $\{a, b, c\}$. The set $\{a, b\}$ is not closed, since a and b produce c by the reaction $a + b \Rightarrow c$.

Given a set of molecules A, we can always generate its closure. The closure of A is defined as the smallest closed set that contains A. In order to generate the closure of a set A, we simply add one by one all the molecules produced by reactions among elements from A until we cannot add new molecules anymore. A set A is always contained in its closure. With the following definition we have defined an operator $G_{CL} : \mathcal{P}(\mathcal{M}) \to \mathcal{P}(\mathcal{M})$, which takes a set of molecules as input and returns a closed set of molecules.

Definition 2 (generate closed set). *Given a set of molecules A, we define $G_{CL}(A)$ as the smallest closed set that contains A. We say that A generates the closed set $C = G_{CL}(A)$. We call C the closure of A.*

Example (generate closed set): $G_{CL}(\{a, b\}) = \{a, b, c\}$, because c is produced by reaction $a + b \Rightarrow c$. Further examples are: $G_{CL}(\{a\}) = a$, $G_{CL}(\{\}) = \{\}$. Note that the empty set $\{\}$ is not necessarily always closed. If there is a reaction rule where the left hand side is empty, e.g., $(\Rightarrow c)$ representing an inflow of c, then the empty set is not closed.

The closure implies a union operator and an intersection operator on closed sets. The requirement for a well defined union on closed sets is that the result of the union is closed, too. Imagine that we take two closed sets $\{a\}$ and $\{b\}$ and compute their normal set union $\{a\} \cup \{b\} = \{a, b\}$. Now, $\{a, b\}$ is not closed, because $a + b \Rightarrow c$. So, the normal set union does not fulfil our requirement. Using the generate function, we can easily define a union and an intersection on closed sets. Together with the set of all closed sets, we obtain the lattice of closed sets:

Definition 3 (union and intersection of closed sets). *Given two closed sets A and B, we can define the union and intersection of closed sets by*

$$A \sqcup_{CL} B := G_{CL}(A \cup B), \quad A \sqcap_{CL} B := G_{CL}(A \cap B). \tag{1}$$

The closed set union of two closed sets A and B can be easily calculated by first putting all elements of A and b together and then generating the closed set. Example: Given two closed sets $A = \{a\}$ and $B = \{b\}$, we would like to calculate their closed set union $A \sqcup_{CL} B$. First we compute the normal set union, $A \cup B = \{a, b\}$ and then apply the generate closed set operator G_{CL} to this union, which generates the closed set $\{a, b, c\}$. So, $A \sqcup_{CL} B = G_{CL}(\{a\} \cup \{b\}) = G_{CL}(\{a, b\}) = \{a, b, c\}$.

The set of all closed sets $\mathcal{O}_{CL}$ form a lattice: $\langle \mathcal{O}_{CL}, \sqcup_{CL}, \sqcap_{CL} \rangle$, which is a common algebraic structure (a poset in which any two elements have a greatest lower bound and a least upper bound). The property of closure is important, because the closed set represents the largest possible set that can be reached from a given set of molecules. Furthermore a set that is closed cannot generate new molecules and is in that sense more stable than a set that is not closed.

It is not important here to go into detail what an (algebraic) lattice is. It is sufficient to know the following: A lattice is a mathematical concept. It is defined by a set (here the set of all closed sets), and two operators that map a pair of elements to an element (here the closed set union and intersection, which map two closed sets to a set). When the lattice is not too big, we can draw it nicely as a Hasse diagram (Fig. 1, right). The biggest element is at the top (here the largest closed set, which is always the set containing all possible molecules) and the smallest element is at the bottom (here the smallest closed set). We can also read from the Hasse diagram, how the union and intersection work. A union of two sets leads to the smallest set that is above both sets. An intersection leads to the largest set below the two sets. As can be seen in the Hasse diagram, union and intersection are somehow symmetric. The Hasse diagram implies also a partial order, i.e. a set is smaller than another set, if it is below it.

In summary, given a reaction system by a set of molecules and a set of reaction rules, we can now find all closed sets and display the lattice of closed sets as a Hasse diagram, which provides already information concerning the structure of the reaction system. The set of closed sets is nearly always smaller than the set of all sets. In our example we lost just one set ({ a, b}) by introducing the constraint of closure. Nevertheless, in other systems we usually reduce the number of sets by a much higher rate.

2.3 Self-maintaining Sets

In the same way as we have introduced the closure, we will now introduce the constraint of self-maintenance, and later the organization, which is a closed and self-maintaining set. Note that the definition of self-maintenance holds only for catalytic flow systems. For more general reaction systems, which are not considered in this paper, the definition is more complex. Given a set of molecules C that is self-maintaining, the constraint of self-maintenance assures that every molecule of C is produced by at least one reaction among molecules in C. So, a self-maintaining set can produce all molecules inside. It is not necessarily closed.

Definition 4 (self-maintaining set). *A set of molecules $C \subseteq M$ is self-maintaining, if for all molecules $a \in C$, there exists a reaction $(A \Rightarrow B) \in R$, with $A \subseteq C$ and $a \in B$.*

Example (self-maintaining sets): In our example the self-maintaining sets are: $\{\}$, $\{a\}$, $\{b\}$, $\{a, b\}$, $\{b, c\}$, $\{a, b, c\}$. Note that the set $\{a, b\}$ is self-maintaining but not closed, since a and b produce a, b, and c.

Given a set of molecules A, we can always generate a self-maintaining set that is contained in A. The self-maintaining set generated by A is defined as the biggest self-maintaining set contained in A. In order to generate the self-maintaining set from A, we simply remove one by one all the molecules not produced by reactions among elements from A until we cannot remove molecules anymore. The self-maintaining set generated by A is always contained in A. The self-maintaining set generated by A is be equal to A, iff A is self-maintaining.

Definition 5. *(self-maintaining set) Given a set of molecules A, we define $G_{SM}(A)$ as the biggest self-maintaining set contained in A. We say that A generates the self-maintaining set $C = G_{SM}(A)$.*

With this definition we have defined another operator of the form $G_{SM} : \mathcal{P}(\mathcal{M}) \rightarrow \mathcal{P}(\mathcal{M})$, which takes a set of molecules as input and returns the associated self-maintaining set. Example (generate self-maintaining set): $G_{SM}(\{c\}) = \{\}$, because there is no reaction that can produce c by using only c. Further examples are: $G_{SM}(\{a\}) = a$, $G_{SM}(\{a, c\}) = \{a\}$. Note that the empty set $\{\}$ is always self-maintaining. The operator G_{SM} implies a union operator and an intersection operator on self-maintaining sets in the same way as the closure did.

Definition 6 (union and intersection of self-maintaining sets). *Given two self-maintaining sets A and B. The self-maintaining set generated by their union and intersection are defined as:*

$$A \sqcup_{SM} B := G_{SM}(A \cup B), \quad A \sqcup_{SM} B := GSM(A \cap B). \tag{2}$$

So, the self-maintaining set intersection of two self-maintaining sets A and B can be easily calculated by first taking only those elements that appear in A and B together and then generating the self-maintaining set by removing the molecules that are not produced anymore. Example: $A = \{a, c\}$ and $B = \{b, c\}$ are self-maintaining sets of molecules. The intersection is $A \cap B = \{c\}$, which generates the self-maintaining set $\{\}$. So, $A \sqcap_{SM} B = G_{SM}(\{a, c\} \cap \{b, c\}) = G_{SM}(\{c\}) = \{\}$.

Again, the set of all self-maintaining sets $\mathcal{O}_{SM}$ together with the self-maintaining set union $\sqcup_{SM}$, and the self-maintaining set intersection $\sqcap_{SM}$ form an algebraic lattice. We can now display the set of all self-maintaining sets by a Hasse diagram.

2.4 Chemical Organizations as Closed and Self-maintaining Sets

Now we put both constraints together in order to define the central concept of chemical organization theory: an organization. Note that the term "organization" has been chosen for historical reasons. It is a technical term denoting a mathematical object and should not be confused with the term found in economics or the social sciences; in particular there is no relation to Luhmann's concept of an organization. A chemical organization is more related to the concept of an autopoietic system.

Definition 7 (organization). *An organization is a closed and self-maintaining set of molecules.*

Given an organization $O \subseteq \mathcal{M}$, we know that every molecule of O is produced by at least one reaction among molecules in O and all possible products that can appear by reactions among molecules of O are also contained in O. Example (organization): In our example the organization are: $\{\}$, $\{a\}$, $\{b\}$, $\{b, c\}$, $\{a, b, c\}$.

Given a set of molecules A, we can always generate an organization. Here, we define this organization as the largest organization that can be reached from the set A. In order to generate this organization, we first generate the closure of A, and then generate the self-maintaining set of this closure. So, in order to generate an organization from a set A, we simply add one by one all the molecules produced by reactions among elements from A until we cannot add new molecules anymore. Then we remove one by one all the molecules not produced by reactions among elements from A until we cannot remove molecules anymore. The generated organization is unique, which follows directly from the uniqueness of the closure and generate self-maintaining set operator.

Definition 8 (generate organization). *Given a set of molecules A, we define* $G(A)$ *as the biggest organization that can be reached from A. Formally,* $G(A) := G_{SM}(GCL(A))$*. We say that A generates the organization* $O = G(A)$*.*

Example (generate organization): $G(\{a, b\}) = \{a, b, c\}$, because there is no reaction that can produce b by using only b. Further examples are: $G(\{c\}) = \{\}$, $G(\{a\}) = a$, $G(\{a, c\}) = \{a\}$. As before, the operator Gimplies a union operator and an intersection operator on organizations in the same way as the closure did.

Definition 9 (union and intersection of organizations). *Given two organizations A and B. The organization union and intersection is defined as the organization generated by their set union and intersection, respectively:*

$$A \sqcup B := G(A \cup B), \quad A \sqcap B := G(A \cap B). \tag{3}$$

Example: $A = \{a\}$ and $B = \{b\}$ are organizations. $A \sqcup B = \{a, b, c\}$. $A \sqcap B = \{\}$.

The set of all organizations $\mathcal{O}$ (of a catalytic algebraic chemistry) together with the organization union $\sqcup$, and the organization intersection $\sqcap$ form an algebraic lattice $\langle \mathcal{O}, \sqcup, \sqcap \rangle$.

We can now display the set of all organization by a Hasse diagram, which we may call the organizational structure of the reaction system (Fig. 1, right). An organization represents an important combination of molecular species, namely those that are likely to be observed in a reaction vessel on the long run. A set of molecules that is not closed or not self-maintaining would not exist for long, because new molecules can appear or some molecules would vanish, respectively.

2.5 Dynamics

So far we have analyzed the reaction system statically. This means that time has not played any role in our analysis. However, the result of the static analysis has strong implications for the potential dynamics of the reaction system. One such implication is expressed by a theorem that relates fixed points (stationary states) to organizations, and by doing so, underlines the relevancy of organizations. The theorem says that, given the dynamics of the reaction system by a continuous ordinary differential equation (ODE) of a form that is commonly used to describe the dynamics of reaction systems and that obeys the rules given by the reaction system, then every fixed point of this ODE is an instance of an organization. This implies that we can only have a stationary state with exactly those

		Product									
	Product	1 Agriculture	2 Forestry	3 Fishing	4 Coal extraction	5 Oil and gas extraction	6 Metal ores extraction	7 Other mining and quarrying	8 Meat processing	9 Fish and fruit processing	10 Oils and fats processing
1	Agriculture	2 684	-	-	-	-	0	-	2 928	768	627
2	Forestry	0	16	-	-	-	-	-	-	-	-
3	Fishing	0	-	16	-	-	-	-	2	251	1
4	Coal extraction	0	-	-	140	-	0	0	1	0	10
5	Oil and gas extraction	-	-	-	-	928	-	-	-	-	-
6	Metal ores extraction	0	-	-	-	-	-	-	-	-	-
7	Other mining and quarry	1	-	0	0	-	0	104	2	1	0
8	Meat processing	9	-	0	1	10	0	1	2 001	44	3
9	Fish and fruit processing	10	0	3	0	7	0	1	34	512	2
10	Oils and fats	1	-	0	0	1	0	0	57	53	253

Fig. 2. Upper left section of a 138x138 table of an product vs. product IO-model, 1995, UK. Unit: basic pricesin Mio. GBP. For example an entry can be interpreted in the following way: *Meat processing* buys for 2928 Mio GBP *Agriculture* products, but no *Forestry* products, 2 Mio GBP *Fishing* products, etc. Here, "0" denotes that the entry is below 1 Mio GBP. Source: [7]

molecules that form an organization. It is not possible to find a stationary state with a combination of molecules that are not an organization. And this implies further that only organizations are candidates for autopoietic systems. However, an organization is not necessarily an autopoietic system, since a stationary state is not necessarily stable. In an instable stationary state the system can reside for ever, as in a stable stationary state, but a tiny perturbation would cause the system to move away from this state towards a different (stable) attractor.

3 Application to Economical Systems

In this section we sketch how a reaction network model can be derived for an economical system and how chemical organization theory can be applied to such models. Note that this section is preliminary and should only illustrate how the theory might be applied. The data we used is not sufficient to draw any conclusion concerning a real economical system. However, the toy model we generate demonstrates that our theory can uncover interesting "hidden" structures that are not obvious when looking at the network.

3.1 Deriving a Toy Model from an Input/Output Table

We exemplify our approach by investigating an input-output model of UK's industry in 1995 [7]. The model consists of 138 products and a 138×138 IO table that describes which product is used to produce which product. Each product is an aggregate of a large amount of elementary concrete products of a specific class. Furthermore, some products represent also institutions that consume products. When we say "product" in the following, we refer to one of these 138 product aggregates. Figure 2 shows the upper left 10×10 section of the 138×138 IO table. The flow from one product to another product is measured in Mio GBP basic costs. The full table is available from Ref. [7].

Before we derive a reaction from the IO Table we have to specify our assumptions: We assume that a positive entry (> 0) at position (x, y) in the IO table means that product x is used to make product y, because there is a flow of money from y to x. Furthermore we assume, the higher the entry the more important is x to make y. An important question at that point remains: is x required to make y, is x sufficient to make y, or even both? Since the table does not provide information to decide these questions, we have to make some further preliminary assumptions at that point. These assumptions can be relaxed later, when additional information is available. The name of a product surely provides a hint concerning the required products to produce it. But taking just the product's name to infer which kind of input is sufficient to make that product appears too speculative to us, since we omit this information here.

There are two fundamental ways, how to derive reaction rules from the table. Let us assume that x_1, x_2, …, x_n denote all products that receive money from y. This means that x_1, x_2, …, x_n are somehow used for making product y. The two methods differ in whether we assume that all products x_1, x_2, …, x_n are required to make y, or whether a single product is sufficient. Note that given only the IO table as data, it does not make much sense to consider an intermediate case, e.g., where some x_i are required to make y, because we do not have information which one to take.

AND-Method: The AND-Method assumes that all products $x_1, x_2, \ldots, x_n$ are required and sufficient to make y. Or in other words, if one of the products x_1, x_2, …, x_n is missing, product y can not be made, if there is no other rule. Therefore we define for product y a reaction rule of the form

$$x_1 + x_2 + \cdots + x_n \Rightarrow y. \tag{4}$$

Dynamically, this rule is interpreted in the following way: if product x_1, x_2, …, x_n are produced, then y will be also produced sooner or later. Here is an example of a reaction rule derived using the AND-method and a threshold of 5 Mio GBP:

Agriculture + Meat Processing + Fish and fruit processing + Oils and fats ⇒ Meat Processing

Note that every entry of the IO-table below the threshold is set to zero and thus the respective product relationship is not considered. After applying the threshold, four products are left that receive money from Meat processing.

OR-Method: The OR-method assumes that each single product from x_1, $x_2, \ldots, x_n$ is sufficient to make y. This assumption implies reaction rules of the form: $x_1 \Rightarrow y$, $x_1 \Rightarrow y$, …, $x_n \Rightarrow y$. For the previous example we obtain instead of one single rule the following four rules, which can be interpreted that one of the four products is sufficient to create instances of Meat processing:

Agriculture ⇒ Meat processing, Meat Processing ⇒ Meat processing, Fish and fruit processing ⇒ Meat processing, Oils and fats ⇒ Meat processing.

As said before, the pure IO table does not allow to decide which combination of products is necessary and sufficient to produce a product. Looking at the names of the products in the previous example, we can already see that neither the OR-method nor the AND-method are fully satisfying. So, for a more detailed

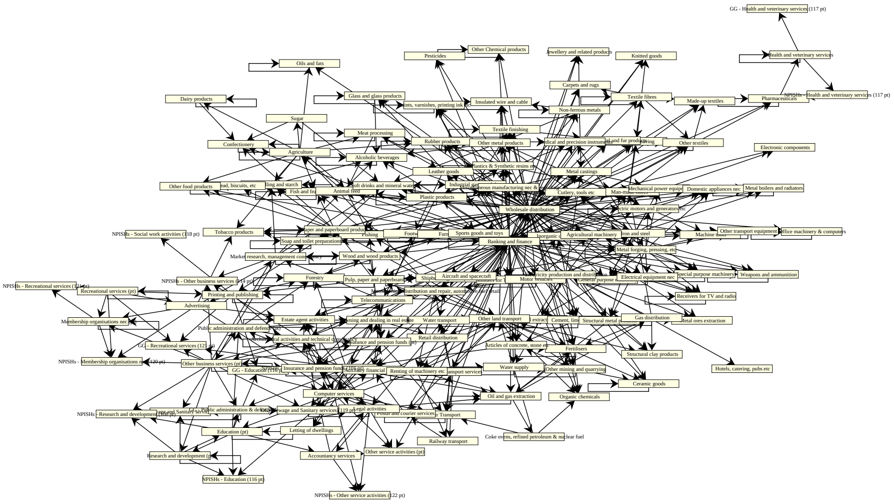

Fig. 3. Illustration of a network derived from an 138x138 product vs. product IO model of UK's industry, 1995. An edge represents a flow of currency, which must be above 6% of the total amount of currency (sum of a column in Fig. 2). In this figure we assume that if there is an edge from x to y, then x is required to produce y. (optimized 2-D embedding using LEDA graphwin class).

investigation that aims at elucidating the structure of a particular industrial IO system more detailed data will be required.

In this work we take the AND-method for deriving reaction rules, since we believe it is more realistic than using the OR-method. Especially for more complex products, such as cars, a combination of products is surely required to make them. The OR-method would lead to a network where nearly everything can be made from everything in a couple of steps – provided that the threshold is small, thus leading to a network without a structure that can be detected by the chemical organization theory.

Using the AND-method means that all inputs of a product are assumed to be required and sufficient to make it. So there is one rule for each product. The left hand side of this rule contains all inputs that are above a certain threshold. For the analysis we used a relative threshold of 6%, which means that an input is considered, if and only if it is higher than 6% of the sum of all inputs of this product. For the purpose of demonstration this threshold is reasonable, but when our method should be applied for concrete analysis, we recommend to carefully study the impact of the threshold. For example, assume the following extreme case: a product requires 100 other products, each contributing 1% to the total input; the result will be no rule at all, or a rule that has no products on the left hand side, which means that the product requires nothing to be produced.

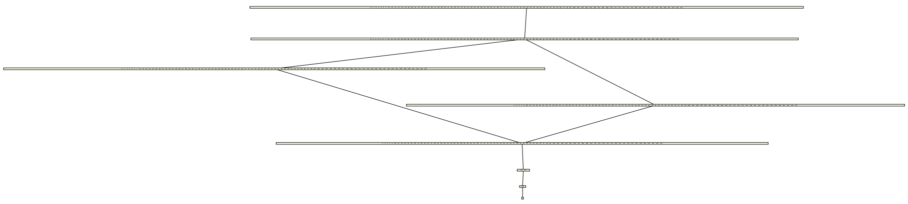

Fig. 4. Fraction of the lattice of organization of the network shown in Fig. 3 (UK industry, 1995). The diagram shows all organizations contained in the top most organization, which consists of 90 products. The width of an organization corresponds to the number of products inside.

Figure 3 gives an impression of the derived reaction network. The figure illustrates that it is quite difficult, if not impossible, to identify structures on the basis of this visualization, which is already optimized to some extent. In order to elucidate the structure hidden in this network, we will apply chemical organization theory, which will be introduced in the next section.

3.2 Preliminary Results

Applying the theory, several thousand organizations are found. Figure 4 shows a small fraction from the lattice of organization. The smallest organization (Fig. 5) with more than 3 products contains already 80 products, including *forestry* (2) but not *agriculture* (1) (Fig. 6). Figure 5 shows the reaction network of this organization. It is already less complicated compared to the full system. Since it is closed and self-maintaining, it makes sense to investigate the relations within such a sub-system first.

Having identified an interesting organization, we can continue with our analysis by asking, which kinds of products are required for the organization, or which kind of product can we remove so that the remaining set still generates the original organization. Using the terminology of our theory, we can look for the internal generators. For example, an industry that has only inputs is not required. Removing all nodes that have only incoming edges we would arrive at a smaller internal generator. In Fig. 5 we can see that removing the product *jewellery and related products* would result in a set of size 79 that still generates the original organization. As opposed to this, the product *forestry* is necessary. If we remove *forestry* from the organization, the remaining set of size 79 generates an organization containing only three products.

Looking more closely at the reaction network (Fig. 6) we can see, why *forestry* is important for that organization: *Forestry* is required for *Wood and wood products*, which is required for *Pulp, paper and paperboard*, which is required for *Paper and paperboard products*, which is finally required for *Printing and publishing.* The product *Printing and publishing* is required for many other products, among which are important products like *Advertising* and also *Forestry* itself. Therefore,

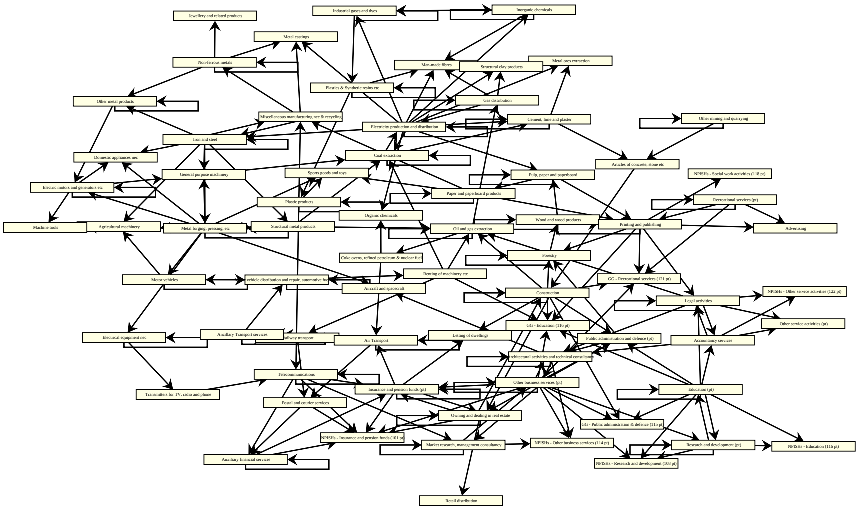

Fig. 5. Reaction network of an organization that consists of 80 products (IO-model, UK, 1995). For the sake of clarity, two central products (Banking and finance and Wholesale distribution) are removed, because they are connected with many other products.

if we remove *Forestry*, we remove the support for many products, so that the resulting set of products is not self-maintaining any more and would generate an organization containing only three products.

4 Discussion

The results presented here are preliminary. Although we have used real world data, the derived reaction network is unrealistic, because our assumptions for deriving the network were oversimplifying. The aim of this paper is to illustrate the method and to demonstrate that the method can extract information from complex networks, which would be hard or impossible to get otherwise.

In the context of our theory, there are couple if interesting open questions: What kind of products are required for an organization? How do the generators of an organization look like? How do the smallest internal generators of an organization look like? This may characterize the potential stability of the system.

Furthermore we may map real data to the set of organizations. Assume that we have data on the time evolution of the size of the different products (industries) over time. We can now measure whether and with what intensity an organization is present in a certain state. This provides a new way to project a

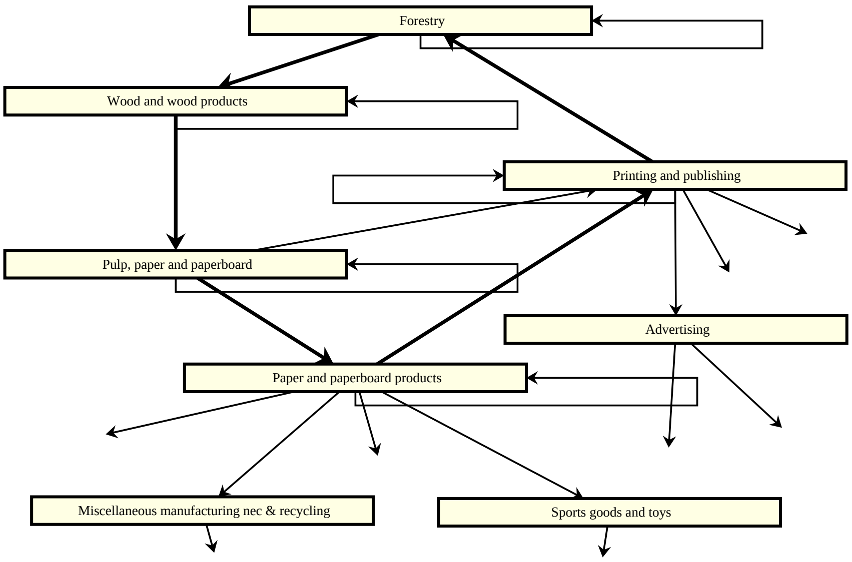

Fig. 6. Illustration of the role of Forestry (fraction of the network shown in Fig. 5). The figure depicts a set of products that is self-maintaining(ie. all products are produced within the network) but not closed, since other products are produced, which are not depicted.

high dimensional system to a system (e.g., a set of small organizations), which may give further insights into the structure of the network.

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