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Octavian Iordache

# Implementing Polytope Projects for Smart Systems

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*...understanding arise from discrimination,*
*that is, through analysis (dissolution)*
*followed by synthesis, as stated in symbolical*
*terms by the alchemical dictum:*
*"solve et coagula" (dissolve and coagulate).*

*Carl Gustav Jung*
*Aion: Researches into the Phenomenology*
*of the Self*
*Princeton University Press, 1969*

# Preface

The first industrial revolution was the mechanization of production using water and steam power. Innovations related to coal powered engines, steam, cotton, steel, and railways helped to give us the first industrial revolution of mass production and mechanization. It was followed by the second industrial revolution which introduced mass production mainly with the help of electric power. This revolutionary step was triggered by the introduction of electricity, heavy and mechanical engineering, and synthetic chemistry.

This was followed by the third revolution, the use of electronics and information technology to further automate production. The third industrial revolution was triggered by innovations in electronics and computers, petrochemicals, materials for electronics, and aerospace.

The fourth industrial revolution entails the fusion of digital with the physical industrial production in cyber-physical systems. It is characterized by a synthesis of technologies that is suppressing the lines between the physical, biological, and digital levels. A host of new technologies is driving a wave of innovation that takes us into the new stage of industrial revolution. This concerns internet, nanotechnology, bioscience, electronics, photonics, advanced materials, and renewable energies. Changes to our own techno-economic system started in the mid-1980s, but we had to wait the turn of the century to witness their impact on our production methods.

The smart systems containing multifunctional parts that can perform sensing, controlling, and actuating represent a major topic for the fourth industrial revolution in engineering. Smart systems should be envisaged giving that the third industrial revolution devices, tools, methodologies, or organizations based on electronics and information technology for automation reached or will reach soon their limits. This means that external administration and control by computers is impossible or will cost much more than the embedded hardware and software infrastructure. The fact that external administrators get more and more overstrained by industrial development tasks have led to the new request for smart systems and structures in engineering. Industrial smartness was emphasized by recent initiatives as

"Industry 4.0", "Smart Manufacturing Leadership Coalition" (SMLC), "Advanced Manufacturing Partnership", and "Industrial Internet Consortium" (IIC). These are charting a course for investing in and furthering the development of the emerging technologies and outlining the key features of the fourth industrial revolution.

Designed to face ever-growing complexity challenges, polytope projects are based on a general reference architecture inspired and shared by the functional organization of organisms and enterprises such as informational and cognitive systems, the scientific and engineering methodology, and the operational structure of existing self-evolvable systems. In order to reflect different aspects, physical, technological, scientific, and so on, the reference architecture assigns the polytopic character in the way we are looking for necessary messages into multipart objects that can be seen from many different perspectives, at several conditioning levels alternatively involved in increasing and decreasing hierarchical order.

Being comprehensive physical and virtual architectures that guide the investigation, fabrication, and operation of smart systems, the polytope projects represent potential sources of prosperity and power for the next decades. Implementing a polytope project onto different systems, such as physical, biological, technological, scientific, and economical, is an important and useful instrument in creating significantly new capabilities and structures.

Dedicated to the realization of polytope projects for smart industrial systems, this book is divided into nine chapters. The book begins with the presentation of polytope projects for cyber-physical and smart systems in Chap. 1. Chapter 2 focuses on chemical engineering process synthesis. Flow-sheet trees and cyclic schemes for separation, and smart configurations for multi-component separations are discussed. Smart drug delivery systems, periodicity features, and networks of chemical reactions are presented in Chap. 3. Conditioned random walks and restricted random evolutions are studied in Chap. 4. Applications refer to placements, packing, advanced materials, folding, and polymers. Chapter 5 examines self-assembly and self-configuring at different scales from molecular to macro systems. Significant case studies concern computing in biochemical systems and self-reconfiguring robots. Smart chemical engineering devices and technologies are the subject of Chap. 6. Modular microreactor systems and timed automata are presented as polytope projects. Chapter 7 focuses on inferential engineering designs, concept-knowledge theories, relational concept analysis, and model-driven architectures. Industrial systems are focused in Chap. 8. Smart manufacturing, Industry 4.0, reference architectures, and models for new product development and testing are presented here. Chapter 9 summarizes the methodology of implementing polytope projects, highlights the connection with other research and development directions, and evaluates the perspectives of polytope projects.

Appendices introduce dual graded graphs and Hopf algebras.

The book presents in detail significant case studies: flexible flow-sheeting of separation operations, drug delivery systems and chronotherapy, smart materials, structuring and assembling at different scales, modular chemical microreactors, smart technologies and devices, programmable devices, inferential engineering designs, smart manufacturing systems, reference architectural models, verification

and validation models for engineering, and so on. Despite the fact that a majority of case studies are related to chemical or to materials science engineering, the presented methodology aims to be general and equally applicable to other fields of engineering or science.

The first motivation of the book was to show that cyber-physical systems, smart systems and structures, and Industry 4.0 concepts could be implemented not only for software, electronics, and mechanical engineering but also for chemical processes engineering. Another significant objective is to develop systemic or combinatorial mathematical models of smart systems to offer predictive capabilities at different levels and scales. The new developed systemic models will complement the conventional detailed models based on natural sciences.

Introducing a groundbreaking field of most important practical and theoretical interest and a key area for the next revolutionary step for industries, the book will be useful to engineers, researchers, and entrepreneurs working in chemical, biochemical, pharmaceutical industries, materials science or systems chemistry and to students in different domains of production engineering and applied mathematics.

Montreal, Canada Octavian Iordache
October 2016

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# Abbreviations

| | |
|---|---|
| CPS | Cyber-Physical Systems |
| DDS | Drug Delivery Systems |
| DGG | Dual Graded Graphs |
| DPT | Dual Process Theory |
| FCA | Formal Concept Analysis |
| IDT | Inferential Design Theory |
| IIC | Industrial Internet Consortium |
| IT | Information Technology |
| OMG | Object Management Group |
| PSA | Pressure Swing Adsorption |
| RAMI 4.0 | Reference Architecture Model Industry 4.0 |
| RCA | Relational Concept Analysis |
| SGAM | Smart Grid Architecture Model |
| SMB | Simulated Moving Bed |
| SMLC | Smart Manufacturing Leadership Coalition |

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# Chapter 1
# Introduction

## 1.1 Polytope Projects

### *1.1.1 Levels and Emergence*

Complex systems exhibit hierarchical self-organization in levels under selective constraints. Self-organization will occur when individual independent parts in a complex system interact in a jointly cooperative manner that is also individually appropriate, such as to generate a higher level organization. Complex systems can be observed at different levels of investigation. For example we can study an industrial installation at the level of molecules, of different phases as gas-liquid-solid, or at the level of devices interactions.

Modern ontological theories of levels for reality have been developed by Hartmann (1940, 1952), and by Poli (2001).

Hartmann considers four basic levels of reality and associated objects: material or inanimate, biological or animate, cognitive or psychological, and intelligent or spiritual and emphasizes the finite number of sublevels to be taken into account at any basic level.

Poli delineates at least three ontological strata of the real world: the material, the psychological and the social stratum.

Figure 1.1 shows the Hartmann's four levels of the real world. Hartmann ranked these four levels in the hierarchy: material < biological < cognitive < intelligent and studied the emergence of new levels in the hierarchy.

A property is considered as emergent if it shows novelty that cannot be explained from the properties and interactions of the lower level entities. The challenge is to explain from were the novelty comes.

Following the hierarchy of levels shown in Fig. 1.1, the hierarchy of emergence types is resulting. There are four levels of emergence, each level corresponding to a reality level. On the basic level there are atoms and molecules. On the next level there is the emergence of life, on the next level the emergence of conscious states



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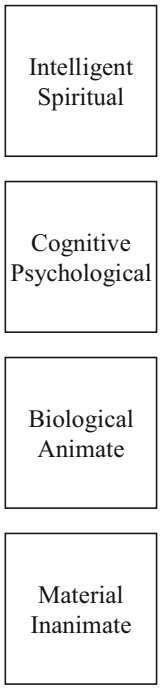


**Fig. 1.1** Four levels of reality: hierarchical framework

and then, the emergence of product of human mind, such as technologies and scientific theories have to be considered (Hartmann 1940; Popper 1987).

The existence of material systems allowed the 1st order emergence of biosystems, followed by the 2nd order emergence of cognitive systems, and this in turn by the 3rd order emergence of intelligent systems. There is a qualitative difference between the levels.

Cariani (1992) distinguishes physical emergence, from biological emergence, psychological emergence and social emergence. Physical emergence is related to the appearance of new physical structures, as for instance the Bénard cells in fluids thermal convection (Nicolis and Prigogine 1977). Biological emergence is related to the increase in morphological complexity and to the appearance of new functions in biological evolution. The immune system is an example. The cognitive that is psychological emergence is correlated to the appearance of new ideas and explanations (Piaget 1971). Another type of emergence is the one encountered in social evolution, which corresponds to the appearance of social structures and cultural or technological innovations.

This approach requires clarifying the relation between higher levels and lower levels in ontological hierarchy. The study refers to the micro-macro, local to global or the two-ways mechanism of emergences and also to the concept of downward causation called also immergence (Pattee 2000). An emergent feature is supposed to have some kind of causal power on lower level entities. Downward form of causality, operates from upper to lower level, and complements the upward

causation. Lower entities exercise an upward causation on the emergent features. New properties that were not seen in the parts of a system emerge only when the system as a whole exhibit downward causation.

This implies a two-levels and two-way causal relation. As illustrative example we may consider several component transport processes organizing in a flexible device or installation. The component transport processes affect how the device or installation evolve, upward, and the development of the device or installation affect the behavior and the interaction of the component processes, downward.

As an operational approach, the emergence was regarded as a dynamic, non-linear process that leads to novel properties, structures, patterns at the macro-level or global level of a system from the interaction of the part at the micro-level or local level. Such novelty cannot be understood by reductionism but may be studied by looking at each of the parts in the context of the system as a whole. Detecting and breaking complexity frontier allows in fact exploiting properties of emergence, as non-linearity of interactions and coherence. Due to non-linear reinforcement, local interactions may result in a larger effect in the form of a novelty at the macro-level.

Some studies associate the emergence to predictability and to complexity decrease. A feature use to be considered emergent if it can provide better predictability on the system behavior, compared to the lower level entities. The predictability needs an information theoretic approach and this involves sensors, actuators or observers. The measure of the emergence the system provides should be an intrinsic property of the whole system including the sensors and the actuators.

Entropy and algorithmic complexity, entropy production, production of entropy production, represents appropriate candidates for such quantifiable aspects of complexity and emergence (Iordache 2012).

### *1.1.2 Integrative Closure*

Integrative closure hypothesis appears as a natural consequence of mutual restrictedness or exclusiveness of the new levels relative to the previous ones, and of the finite number of levels to be considered (Iordache 2010).

The starting idea for integrative closure was to reassess and completes the interrelation between the four basic ontological levels in the study of nature: material, biological, cognitive or psychological and intelligent or logical (Hartmann 1952).

It was acknowledged that the hierarchical structures cannot serve as unique model for multi-level knowledge organization. Facing complexity the task of knowledge integration remains pertinent. Integrative closure is a strategy allowing confronting complexity.

Figure 1.2 shows the four levels of reality and their integrative closure hypothesis.

The four basic levels are denoted: S (or K0), K1, K2 and K3.

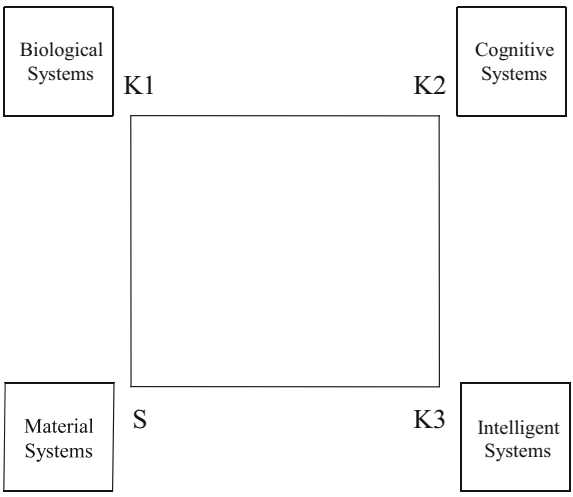


**Fig. 1.2** Four levels of reality: integrative closure

Figure 1.2 is a presentation of the integrative closure hypothesis as a connected version of Hartmann's four levels ontological hierarchy shown in Fig. 1.1.

The integrative closure aims to make ends meets, for the four levels or realms, emphasizing the hypothetical interconnection between the material realm, S and intelligent realm, K3. The closed system is supposed to cross the gap between these farthest levels. This gap crossing corresponds to the cyber-physical systems. The cyber part is associated to K3 while the physical part is associated to S.

Integrative closure looks to the four level-level interactions steps to facilitate the study and to take into account the necessary ingredients, as shown by the evolvable systems in nature and technology.

Hartman's hierarchical structure was closed and replaced by a network or a cycle. It is generally acknowledged that both hierarchical trees and cycles are necessary for evolvability. It is the timing of cycling/de-cycling and the mix of hierarchies and cycles that matters for evolution.

Integrative closure hypothesis is looking for structural analogies and a common methodology for different domains as bio-inspired systems, knowledge organization, problem solving or technological developments.

Centered, four realms frameworks, resulting by integrative closure have been presented as the architecture shared by autonomous systems (Iordache 2010, 2011).

### *1.1.3 Self-integrative Closure*

The growth in complexity is not only about differentiation but also about integration and coordination.

The pursuit of evolvability towards further step of self-evolvability for systems imposed the study of polytopic architecture associated to the general framework as

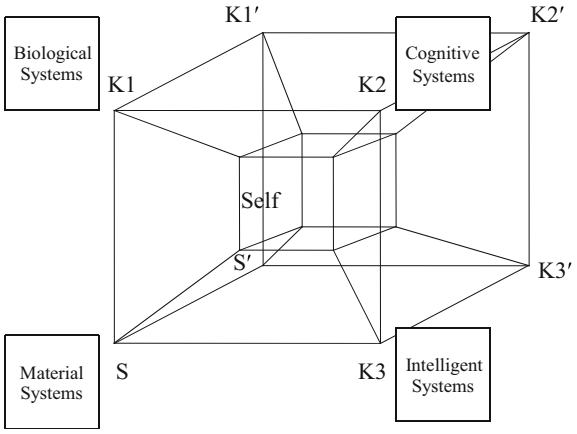


**Fig. 1.3** Self-integrative closure

shown in Fig. 1.3. Figure 1.3 illustrates the concept of self-integrative closure with specific reference to the Hartmann's four levels of the real world.

The basic levels are S, K1, K2 and K3 represented on the front face of the outer cube and S′, K1′, K2′ and K3′ represented on the back face of the outer cube of the polytope.

Following Hartmann ontology, for the polytope shown in Fig. 1.3 we could identify:

- S-Material Systems
- K1-Biological Systems
- K2-Cognitive Systems
- K3-Intelligent Systems

For technological and engineering systems we refer to a hierarchy of artificial systems inspired by the four level of Hartman's ontology as for instance:

- S-Materials or Smart Materials, Evolving or Living Technologies
- K1-Bio-Inspired or Bio-Mimetic Systems, Artificial Life
- K2-Cognitive-Inspired Systems, Neural Computer, Artificial Brain
- K3-Artifacts, Artificial Intelligent System, Cyber-Physical Systems

It should be emphasized that the objects of engineering are natural systems and artifacts or artificial systems and that the reality levels as biological, cognitive and intelligent may serve for inspiration purposes.

For instance, evolutionary computation studies and evolvable devices may be inspired by biological principles but do not attempt to model or to mimic detailed data or processes from real genomes. Bio-inspired artificial design is not constrained by high fidelity to the original natural complex system. Examples include genetic algorithms calculus inspired by evolution and genetics, artificial neural networks and artificial neural codes inspired by cognition studies but not restricted to this.

To re-apply the engineering understanding in developing new ways of study or explanations of biological, cognitive or intelligence of relevance for real world systems, may be considered as a long-term objective only.

The swinging between the two faces of the outer cube in polytope as shown in Fig. 1.3 is mediated by the inner cube identified as the Self.

This reference framework was labeled as self-integrative closure (Iordache 2012, 2013).

Modifications of the direct sequence S, K1, K2, K3 during reverse processing K3′, K2′ K1′ and S′ may happen.

Emergency from the direct sequence is replaced by de-emergency in the reverse sequence. During these complementary processes of emergency, de-emergency, and re-emergency the differences allowing and accompanying self-evolvability may be generated.

Designed to face higher complexity challenges, the implementable polytope projects are based on this general reference architecture of existing self-evolvable systems.

Some concepts and theories that could be correlated to polytope projects have been identified.

Illustrative examples are the polystochastic models (Iordache 1987, 2009, 2010, 2013) the hyperstructures (Baas 2006, 2009, 2015a, b) and the meta-meta-modeling architectures (Crawley et al. 1997; Alvarez et al. 2001; Mellor 2004; OMG 2008).

### *1.1.4 Polystochastic Models*

Complexity studies are focused more on processes than on things. In that sense Whitehead's process philosophy with it emphasize on process over substances may be considered as a precursory for modern complexity science (Whitehead 1978).

Complying with Leibniz's relational world philosophy, the reality is considered as the totality of interactions not things.

To direct on processes combination at higher levels of conditioning was the initial objective of the polystochastic modeling in chemical engineering (Iordache 1987, 2010).

To account for complexity it was necessary to consider conditioned processes resulting in a kind of compound process, that is a process of processes or in other words a meta-process. Since a collection of inter-related events is understood to be a process, a conditioned process is a process of processes since the conditioning is a process too.

In a simplified form, the first models describing adaptability considered only two levels or two spaces, the space of states, S and the space of conditions, K and their interaction. The adaptive or learning system was presented with a series of conditions $k \in K$, on each of which it changes states $s \in S$, allowing sequential adaptability (Iosifescu and Grigorescu 1990). After that, the level of conditions K

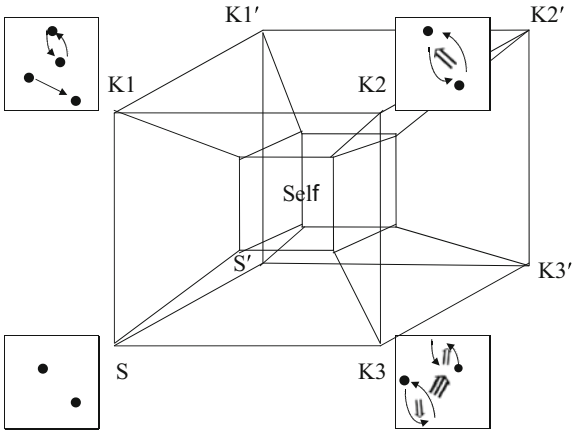


**Fig. 1.4** Polystochastic models

was replaced by multiple levels by involving conditions K1, meta-conditions K2 and meta-meta conditions K3. A meta-condition is a condition of conditions.

Figure 1.4 illustrates the basic cognitive frame for self-evolvability in which the states S interact in a specific way with K1, K2, and K3.

The notations from Fig. 1.4 are:

- S-states,
- K1-processes
- K2-process of processes (meta-processes)
- K3- process of processes of processes (meta-meta-processes)

The traditional objects of study were the states, S denoted here by dots.

Then the interest shifted from states to processes denoted here as arrows between dots →.

In the next step of modeling the conditioned processes have been introduced. These imply the study of processes of processes or meta-processes. We make use of double arrows: "⇒" to describe these in Fig. 1.4. Then process of processes of processes or meta-meta-processes has been accounted for. We make use of triple arrows "⋙" to describe these.

Studies of self-evolvable systems show that if there is a process there is a counter-process too. The same is valid for meta-processes and for meta-meta processes. Assembly and disassembly, composition and decomposition, construction and deconstruction coexist. Implementing polytope projects may start from the direct sequence S → K1 → K2 → K3 and balance this by the reverse sequence: K3′ → K2′ → K1′ → S′. This reverses the arrows direction in K1, K2 and K3.

Variation of the direct sequence during reverse processing may happen.

Conditioning from the direct sequence is replaced by de-conditioning in the reverse sequence. It is during these dual processes of conditioning, de-conditioning and re-conditioning that the differences allowing self-evolvability are generated.

The polystochastic models unifying methodology was present since the very first papers (Iordache 1987) and becomes more explicit and more developed in the later ones (Iordache 2010, 2012, 2013).

### *1.1.5 Hyperstructures*

Notable theoretical perspectives more or less close to the polytope projects approach are the hyperstructures (Baas 2006, 2009, 2015a, b; Baas et al. 2015) and the memory evolutive systems (Ehresmann and Vanbremeersch 2007). These research directions develop, in different ways, the idea of iterative constructions of systems of systems over systems and so on. The systems of different layers of reality show specific properties.

Baas et al. (2004) compare two different approaches to the modeling of complex natural systems, in particular of their hierarchical organization with higher-order structures and their emergence processes. These approaches are the hyperstructures and the memory evolutive systems, MES. The hyperstructures are structural while memory evolutive systems based on category theory, take dynamics more into account. The dynamical organization and mechanisms developed for memory evolutive systems rely on general ideas that might be disengaged from the categorical setting and extended to the general frame of hyperstructures.

Figure 1.5 illustrates the schematic formation of a hyperstructure (Baas 2015a, b).

We can consider the development of the hyperstructure as a process starting from basic objects the circles representing the 0-dimensional, 0D objects. The next level corresponds to lines 1D representing the objects with properties. The next level corresponds to polygons 2D representing the so-called 1-bonds. The next level that may be represented in 3D corresponds to 1-bonds with properties. The 4D level would correspond to the so-called 2-bonds and describe interactions between 1-bonds with properties structures.

A polytope for hyperstructures is shown in Fig. 1.6.

Structuring or construction and restructuring or reconstruction coexists.

Implementing polytope project may start from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

We associated $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ to $0D \rightarrow 1D \rightarrow 2D \rightarrow 3D$ in the hyperstructure.

For the polytope shown in Fig. 1.6 we can identify:

- S-Basic Objects
- K1-Objects with Properties
- K2-1-Bonds
- K3-1-Bonds with Properties
- Self-2-Bonds

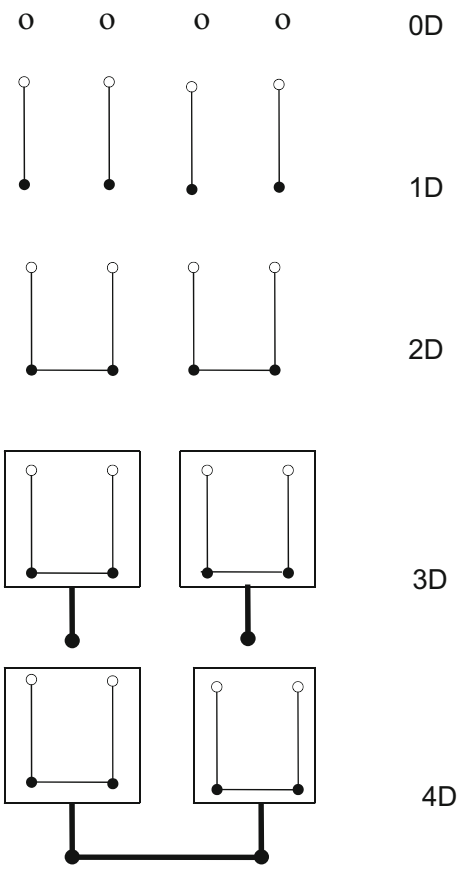


**Fig. 1.5** Hyperstructure formation

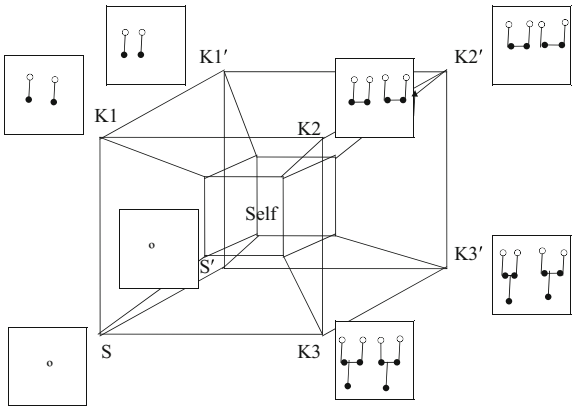


**Fig. 1.6** Polytope for hyperstructures

Self is associated to the 4D, 2-bonds. Self controls the interactions between the two faces of the polytope representing the direct and reverse sequences.

Overlapping and modifications may come about and the front face and back face of the polytope are not necessarily identical.

Bonding from the direct sequence is replaced by de-bonding in the reverse sequence. It is during these direct and reverse processes of bonding, de-bonding, and re-bonding that the self-evolvability become possible.

### *1.1.6 Meta-Meta-Modeling Architectures*

Since the complex systems are structured in levels of realms, associated to multiple scales it is expected that the modeling methods will adopt a similar hierarchical or network architecture.

The four level structures were proposed by the object management group, OMG to describe informational systems. OMG is an organisation for the standardization in the object oriented field of the software development in which many of the leading software production companies participate (OMG 2008).

For OMG applications in statistics the 0-level refers to data, the 1-level to Models that is models of data, the 2-level to methodologies that is to Meta-Models and the 3-level to methodologies that define methodologies that is to Meta-Meta-Models. Additionally a lower level layer representing physical reality may join the OMG architecture at the 0-level.

The four levels will be denoted by K3, K2, K1, and K0 or S, respectively.

K3 is the 3-level, the so-called Meta-Meta-Models level. One model at level K3 is necessary to define all the K2 level models. The OMG standard for the K3 model, also called Meta Object Facility, MOF, is able to define itself (Crawley et al. 1997; Mellor 2004). MOF is a common framework that is used to define other modeling frameworks within the OMG. K3-model is the language used by MOF to build Meta-Models, called also K2-models. Examples of the 2-level, K2-models are the Universal Modeling Language, UML and the relational models. UML has been accepted as a standard notation for modeling object-oriented software systems. Correspondently, at the 1-level, K1, there are UML models and relational models relevant to a specific subject. K1 is based on user concepts. The 0-level denoted K0 or S contains user runtime data or objects. It may be used to describe the real world also.

Different Meta-Meta-Model architectures have been considered as for instance that shown in Fig. 1.7

For the polytope shown in Fig. 1.7 we can identify:

- S-Data
- K1-Models
- K2-Meta-Models
- K3-Meta-Meta-Models

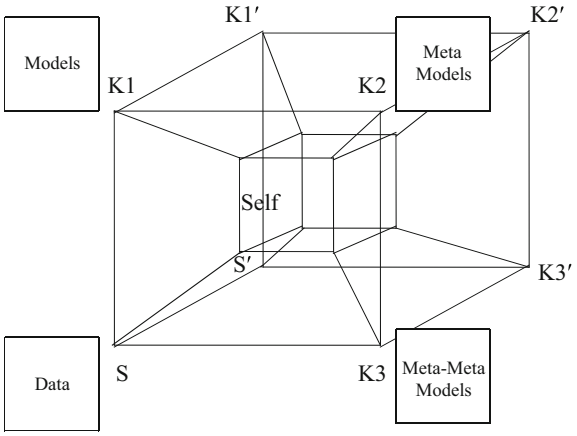


**Fig. 1.7** Meta-meta models

The top and bottom levels in architectures are different. In the hierarchical Meta-Meta-Model architecture every element should be an instance of exactly one element of a model in the immediate next level.

For example, the level K3 could describe elements from the UML Meta-Model K2 but not elements from the user models K1.More flexibility is allowed by the centered architectures.

Implementing the polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

Adjustment of the direct sequence during reverse processing may arise.

Modeling from the direct sequence is replaced by de-modeling in the reverse sequence.

It is during these direct and reverse processes of modeling, de-modeling, and re-modeling that the variations letting self-evolvability are generated.

### *1.1.7 Polytopes and n-Levels Systems*

The presented polytope frame refers mainly to n-levels of conditioning with n = 3 (Iordache 2013).

Figure 1.8 illustrates the polytope for 3-levels systems.

Here S, K1, K2 and K3 are associated to the 0, 1, 2 and 3-levels.

The polytope outlines that complementing the construction or direct way $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ we need to look at the dual way $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

Notice that for some case studies S and S′ were denoted by K0 and K0′.

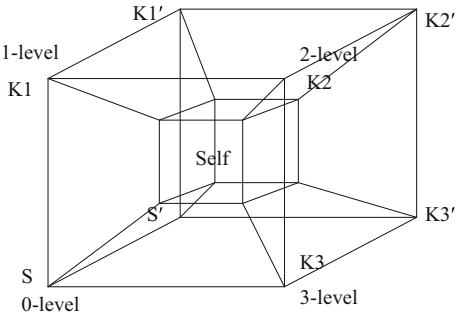


**Fig. 1.8** Polytope for 3-levels systems

For the polytope shown in Fig. 1.8 we can identify:

- S-0-level
- K1-1-level
- K2-2-level
- K3-3-level

The dialogue between the direct way and the reverse way is critical since the boundaries where new information could be created consist of coexisting tendencies of unification and diversification. The central Self describes the interaction of the two ways in duality relation. These ways have been also referred as forward way, from S to K3, and backward way, from K3′ to S′. The Self is associated to 4D and may be considered as a 4-level construction.

Mathematical instruments useful to describe composition and decomposition rules, that is the direct and reverse sequence in the polytope have been the dual graded graphs (Fomin 1994, Appendix A) and the Hopf algebras (Joni and Rota 1979; Hivert 2005; Blasiak 2010, Appendix B).

The concept of Hopf algebras occurs in a natural way in the field of combinatorial constructions and deconstructions.

Joni and Rota (1979) made the key observation that many discrete structures give rise to Hopf algebras whose product encode the assembly or composition and coproducts encode the disassembly or decomposition of these structures.

Figure 1.8 illustrates the reversing of the trend of increasing levels, that is, the front face of the polytope by connecting to the Self, and mapping it to the back face of the polytope and the corresponding decreasing order of levels.

This polytope architecture was proposed as reference architecture, for understanding and framing a large variety of problems, for designing, building and testing potentially self-evolvable systems (Iordache 2012, 2013).

Further ontological analysis of the complex systems may require construction of several sub-levels for each level of the general polytopic architecture represented by hypercube.

Figure 1.9 illustrates the polytope for n-levels and sub-levels.

For the example shown in Fig. 1.9 the basic levels S, K1, K2 and K3 are represented by polytopes isomorphic to the polytope initially shown in Fig. 1.8.

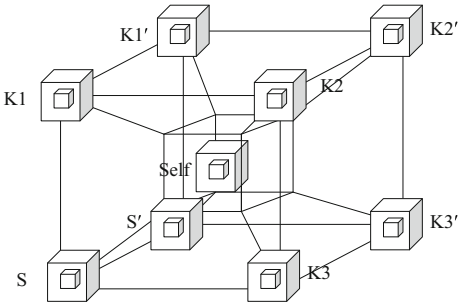


**Fig. 1.9** Polytope for n-levels and sub-levels

The splitting in sub-levels parallels and in some sense recapitulates the initial configuring of reality in the four levels S, K1, K2, and K3.

Since there is no fixed limit for growing complexity, higher dimensional polytopes as for instance 5-cubes and others polytopes may be considered as reference architecture instead of the 4-cube. The process could be repeated for higher n, but it becomes increasingly difficult to represent these multidimensional architectures in a 2-D drawing.

The initial frame offers a generic, 4-cube or hypercube, relational model whose elements are configured as self-similar structures. This means that it can be re-scaled from the smallest to the largest or reversely without modifying it formally.

This has the advantage that it is a configuration that is shareable across different domains.

The self-similarity allows parallel processing with similar software. In this nested architecture, the transformation between the representation of any model at one meta-level and its representation in the meta-level below can be described by information preserving one-to-one mapping. This mapping provides the basis for a powerful area of functionality that any potential meta-modeling tool should look to exploit.

We can consider the development of the hypercube as a process starting from dots 0D, to lines 1D, to squares 2D, to cubes 3D, to hypercubes 4D and so on.

The polytope shown in Fig. 1.9 is a hypercube of hypercubes since each corner is 4D hypercube.

The form of the reference architecture may follow closely the cognition process, and this in turn the function of the associated designs for devices or computers.

## 1.2 Smart Systems

### *1.2.1 Smart Materials and Structures*

The label smart, and interchangeably used–intelligent, is employed in many different contexts, because its meaning with regards to objects is yet not certainly

defined. Smart, in some contexts, refers to an independent device or technology, which usually consists of a sensor, an actuator, and a microcomputer. The term smart is also commonly used to characterize an object that was enhanced by implementation of additional features, which introduce multiplatform communication and increase its computational abilities. The so-called intelligence of such device or technology can be revealed by cooperation in a network of other devices or technologies, which have the ability to check the system state updates and decide whether to act on them or not. Such a network is called a smart network. One refers also to smart objects, as items having the ability to store, link related data as well as may offer access to data for a human or machine consumer.

In the case of factories, smart is sometimes used as a synonym of automated and refers to factories with systems for monitoring and controlling appliances. The monitoring function should not be limited to turning devices, on and off. Devices included in a smart factory should be able to operate autonomously according to the predefined patterns or user requirements. The smart factory is a factory whose level of integration has reached a depth that self-organization function in production and in all enables the concerned business processes production. The virtual image of the factory enables intelligent decisions. The goal is to increase efficiency, effectiveness, flexibility and versatility (Zuehlke 2008).

Smart materials are referred as materials that are capable of sensing the environment and actively responding to it in a controlled way (Fox and Kemp 2009).

A smart material is one which reacts to its environment all by itself. The change is inherent to the material and not a result of embedded electronics. The reaction may exhibit itself as a change in volume, a change in color or a change in viscosity and this may occur in response to a change in temperature, stress, electrical current, or magnetic field. In many cases this reaction is reversible, a common example being the coating on glasses which reacts to the level of light, turning the ordinary glasses into sunglasses when you go outside and back again when you return inside. This coating is made from a smart material which is described as being photo-chromic.

There are many groups of smart materials, each exhibiting particular properties which can be harnessed in a variety of high-tech and everyday applications. These include shape memory alloys, piezoelectric materials, magneto-rheological and electro-rheological materials, magnetostrictive materials and chromic materials which change their color in reaction to various stimuli.

The distinction between a smart material and a smart structure was underlined (Varadhan 2005; Wadhawan 2005).

A smart structure incorporates some form of actuator and sensor, which may be made from smart materials, with control hardware and software to form a system which reacts to its environment. Such a structure might be an engineering device which continuously alters its profile during processing to give the optimum shape for the operating conditions at the time.

Conventional smart structures are defined as miniaturized devices that incorporate functions of sensing, control and actuation (Akhras 2000; Gessner 2007).

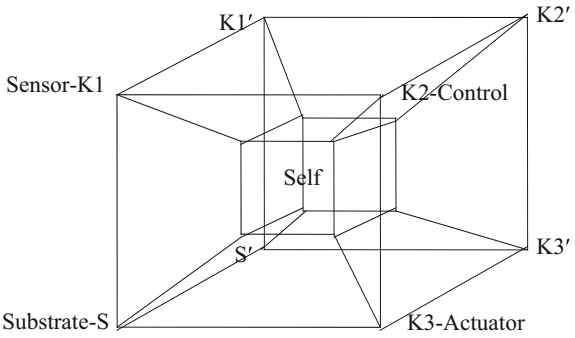


**Fig. 1.10** Smart structures

These may be associated to the polytopic architecture as follows:

- S-Substrate
- K1-Sensors
- K2-Control
- K3-Actuator

Figure 1.10 illustrates the smart structures.

The basic five components of a smart structure have been described as follows:

- Data Acquisition (tactile sensing): the aim of this component is to collect the required raw data needed for an appropriate sensing and monitoring of the structure.
- Data Transmission (sensory nerves): the purpose of this part is to forward the raw data to the local and/or central command and control units.
- Command and Control (brain): the role of this unit is to manage and control the whole system by analyzing the data, reaching the appropriate conclusion, and determining the actions required.
- Data Instructions (motor nerves): the function of this part is to transmit the decisions and the associated instructions back to the members of the structure.
- Action Devices (muscles): the purpose of this part is to take action by triggering the controlling devices/units.

Obviously the smart structure is a bio-inspired system.

Implementing polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

For example, the sensing or actuating process gets de-sensing or de-actuating followed by re-sensing or re-actuating process and so on.

During these complementary processes a difference allowing self-evolvability is generated.

For the polytope shown in Fig. 1.10 one could identify the levels in the reverse sequence as for instance:

- K3′-De-actuating
- K2′-Un-control

- K1′-De-sensing
- S′-New substrate

Implementing a polytope project onto conventional smart systems is estimated to be an important and useful tool in creating new capabilities and structures, a mechanism of novelty and innovation.

The novelty may appear, at the boundary of distinctive tendencies represented by direct and reverse sequence. The interface between tendencies is where the most interesting events take place.

### *1.2.2 Cyber-Physical Systems*

Cyber-physical systems-smart systems that have cyber technologies, both hardware and software, deeply embedded in and interacting with physical components, sensing and changing the state of the real world-represent a core opportunity area and source of competitive advantage for the innovation economy in this century. Examples of cyber-physical systems (CPS)-based initiatives include smart transportation systems, smart medical devices and technologies, smart buildings, next-generation air transportation systems, and the Smart Grid (Baheti and Gill 2011; Fang et al. 2012).

For CPS the real (physical) objects and processes associated with information processing (virtual) objects and processes are anytime interconnected information networks. Optionally a CPS may have human-machine interfaces and provides the ability to dynamically adjust the system (Yuan et al. 2015).

The term cyber-physical systems (CPS) characterizes the new generation of systems with integrated computational and physical capabilities that can interact with humans through many new modalities. The ability to interact with, and expand the capabilities of, the physical world through computation, communication, and control is a key enabler for future technology developments. Opportunities and research challenges include the design and development of next-generation devices, cars, airplanes, hybrid gas-electric vehicles, fully autonomous urban driving or factories, and prostheses that allow brain signals to control physical objects (Strang and Anderl 2014; Lee et al. 2015).

Over the years, systems and control researchers have pioneered the development of effective system science and engineering methods and tools, such as time and frequency domain methods, state space analysis, system identification, filtering, prediction, optimization, robust control, and stochastic control. At the same time, computer science engineers have made major breakthroughs in new programming languages, real-time computing techniques, visualization methods, compiler designs, embedded systems architectures and systems software, and innovative approaches to ensure computer system reliability, cyber security, and fault tolerance. Engineers have also developed a variety of modeling formalisms and verification tools. Cyber-physical systems research aims to integrate knowledge and

engineering principles across the computational and engineering disciplines (networking, control, software, human interaction, learning theory, as well as electrical, mechanical, chemical, biomedical, material science, metallurgical and other) to develop new CPS science and supporting technology.

In industrial practice, many engineering systems have been conceived by decoupling the control system design from the hardware and software implementation details. After the control system is designed and verified by extensive simulation, unstructured tuning methods have been used to address modeling uncertainty and random disturbances. The integration of various subsystems, while keeping the system functional and operational, has been time-consuming and costly. For example, in the chemical industry, a reactor control system relies on system components manufactured by different companies with their own software and hardware. The challenge for original equipment manufacturers that provide parts to a supply chain is to hold down costs by developing components that can be integrated into different reactors.

The increasing complexity of components and the use of more advanced technologies for sensors and actuators, wireless communication, and multi-core processors pose a major challenge for building next-generation device control systems. Both the supplier and integrator need new systems science that enables reliable and cost-effective integration of independently developed system components. In particular, theory and tools are needed for developing cost-effective methods to:

- Design, analyze, and verify components at various levels of abstraction, including the system and software architecture levels, subject to constraints from other levels
- Analyze and understand interactions between the device control systems and other subsystems
- Ensure safety, stability, and performance while minimizing device cost

To confront such challenge the cyber-physical (CPS) systems have been introduced.

The CPS allows the fusion of computation and a physical process. Typically, a CPS is composed of physical process monitored and controlled by a cyber system, which is a networked system of distributed sensing, communication, and computational devices.

In a CPS, heterogeneous embedded systems monitor and control a physical process, usually via feedback loops where the physical process affects computation and vice versa. Emerging CPS devices are characterized by large-scale system sizes, heterogeneity of resources, uncertain system dynamics, and extensive physical interactions.

Unlike traditional embedded systems aiming to optimize computation in highly constrained environments using limited resources, the emphasis of CPS research tends to be more on tight coupling between the computing and physical parts. Embedded systems can be considered CPS when they sense or influence dynamic physical environments.

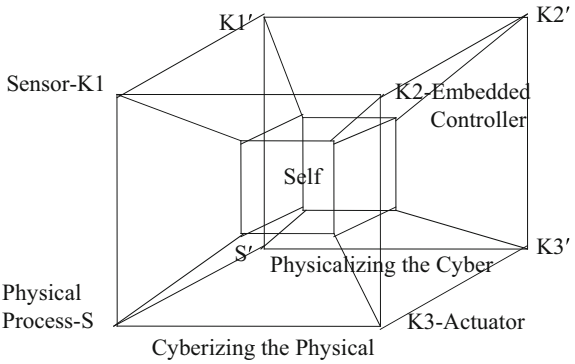


**Fig. 1.11** Cyber-physical systems

CPS may be considered as the next computing revolution and has been identified as a new key area of research and engineering. CPS applications include high-confidence control and safety, advanced automatic systems, energy conservation, environmental control, instrumentation, critical infrastructure control, defense systems, distributed robotics, industrial control systems, smart structures, cellular communication, and autonomic computing systems.

CPS design is an interdisciplinary research area of computer architecture, software, network, physical systems, control, and other engineering disciplines. This emerging area enables new opportunities and poses additional research challenges including CPS decomposition and interoperability, robustness safety and security, control of hybrid systems, real-time embedded system abstractions, architecture development, and model-based development.

Typically, a CPS is configured as a closed-loop feedback control system.

Figure 1.11 illustrates a basic CPS architecture, where sensors, actuators, and controllers can be a network of elements.

These may be associated to the polytopic architecture as follows:

- S-Physical Process
- K1-Sensors
- K2-Embedded Control
- K3-Actuator

Embedded controllers are computational systems incorporating a set of components such as processors, memory, storage, and input and output devices. This infrastructure is abstracted to layers in order to simplify the development flow. System abstraction layers include hardware, operating system, software, and data. Modern components are characterized by the complexity of functions and interactions, with data traversing through different abstraction layers.

Implementing polytope project for cyber-physical systems starts from the direct sequence S → K1 → K2 → K3 and complements this by the reverse sequence: K3′ → K2′ → K1′ → S′. For the polytope shown in Fig. 1.11 one could identify for instance:

- K3′-De-actuating
- K2′-Un-control
- K1′-De-sensing
- S′-New physical system

This means to put together the cyberizing of the physical and the physicalizing of the cyber (see Fig. 1.11). The two complementary approaches have been identified and studied by Lee (2007, 2010). Cyberizing the physical, from K3 to S, means to endow physical subsystems with cyber-like abstractions and interfaces. Physicalizing the cyber, from S′ to K3′, means to endow software and network components with abstractions and interfaces that represent their dynamics in time.

Implementing a polytope project onto existing cyber-physical systems is likely to be an important and useful instrument for innovation able to create significantly new capabilities and structures.

### *1.2.3 Intelligent Technical Systems*

Industry 4.0 is a holistic automation, business information, and manufacturing execution architecture to improve industry with the integration of all aspects of production and commerce across company boundaries for greater efficiency. The concepts of industry 4.0 are in harmony with worldwide digitalizing initiatives, including smart factories, Industrial Internet, smart manufacturing, and advanced manufacturing (Kagermann et al. 2013).

The first industrial revolution in the late 18th century used coal powered steam engines, which flourished the textile industry and other mechanization systems; the second industrial revolution in the final third of the 19th and beginning of the 20th centuries introduced electrically-powered mass production, creating steel industry, and telegraph and railroad systems.

The invention of transistors in 1947 led the dawn of the digital age and information technology, thus the third industrial revolution has offered remarkable applications of computers and electronic devices since the 1970s.

The third industrial revolution propelled the global economic development and the manufacturing advancement by utilizing information and automation technology, making the beginning and the continued progress of the digital era. Smart electronics has been proliferating and relentlessly moving toward a higher level of connectivity and mobility (Schwab 2016; Hwang 2016).

The genesis of the term, fourth industrial revolution, also dubbed Industry 4.0, was rooted in governmental high-tech strategy in 2011. Industry 4.0 will leverage the internet, digital technologies and quantum sciences to drive further into autonomous, intelligent cyber-physical systems.

As industry 4.0 is evolving, it is fitting to define it as the get-together assembly of cyber-physical systems, cloud technology, internet of things and internet of services, and its integration and interaction with humans in real-time to maximize

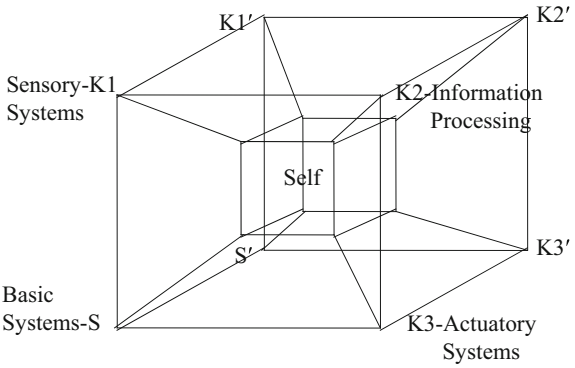


**Fig. 1.12** Intelligent technical systems

value creation. Through the fusion of the physical and the virtual world, interoperability, advanced artificial intelligence and autonomy will be integral parts of the new industrial era. In this era, interesting technological developments are underway or will be pursued in both commercial sectors and military around the world (Lee et al. 2015; Hermann et al. 2016; Hwang 2016).

Terms as intelligent or smart technical systems are naturally related to the fourth industrial revolution considered to be driven by the internet, particularly the incorporation of the real and the virtual worlds. This means the fusion of digital with the industrial production and use.

Intelligent technical systems may be considered as preliminary implementations of the industry 4.0 concepts (Dumitrescu et al. 2013; Gausemeier et al. 2014).

Figure 1.12 illustrates the structure of an intelligent technical system.

It shows:

- S-Basic System
- K1-Sensory Systems
- K2-Information Processing Systems
- K3-Actuatory Systems

Primarily, the course of information processing is the driving force for the change from mechatronics to intelligent technical systems. This technological concept is established on the basic structure of mechatronic systems that is shown in Fig. 1.12. Mechatronic systems are distinguished by the functional and spatial integration of sensors, actuators, information processing and a basic system. Also of significance is the relationship to the human and the environment in which the mechatronic system operates. In general, mechatronic systems can also be composed of subsystems which themselves are mechatronic systems.

The basic system is commonly a mechanical structure. Generally, any desired physical system is conceivable as a basic system. The relevant physical values of the basic system or its environment are measured using sensors in order to monitor and then to improve the system behavior. The sensors supply the input variables for information processing, which, in most cases, takes place digitally, that is discretely in terms of value and time. The information processing unit determines the

necessary changes of the basic system using the measurement data as well as the user specifications (human-machine interface) and also available information from other processing units (communication system). The information processing unit consists of control functions. The behavior adaptation of the basic system is caused by actuators.

The relationships between the basic system, sensors, information processing and actuators are represented as flows. In principle, three types of flows can be distinguished: information flows, energy flows and material flows. As already mentioned, within the field of intelligent technical systems the focus lies on the information flow.

Smart manufacturing systems describe the evolution of the manufacturing environment where the integration of information, technology and human innovation drive a better, faster and more efficient production system operating at the highest level of quality and output. It has been called the fourth industrial revolution—where real world meets virtual plant. Smart manufacturing system is an operating model where machines talk to one another and share data at every point. It is the use of intelligence at a fully-integrated level to allow companies to connect the customers' needs to supply chain to the production equipment to the operators to putting the product in the consumer's hands-a full circle of data exchange (Bryner 2012; Davis et al. 2012).

Implementing polytope project for technical systems starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$.

This should be complemented by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

For the polytope shown in Fig. 1.12 one could identify for instance:

- K3′- De-actuating
- K2′-Information Reprocessing
- K1′ -De-sensing
- S′-New Basic System

The direct sequence does not quite grasp the essence of creativity imposed by self-evolvability request. We expect that innovation and creativity appear, at the boundary of distinctive tendencies. These are the most valuable, diverse and productive elements in a system. Direct sequences should have dialogical interactions with reverse sequences and it is the mix and equilibrium of both that counts. Polytope projects may be viewed as potential creators of novelty and mechanisms of innovation.

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# Chapter 2
# Processes Synthesis

## 2.1 Flow-Sheets Generation

### *2.1.1 Separation Sequences*

Many problems in chemical engineering are concerned with composition or combination and decomposition or separation. The unit operations are the basic steps for chemical technologies. Technologies involve several unit operations structured in schemes or flow-sheets to obtain the desired products.

Separation operations transform a mixture of substances into distinct products. Mixing operations perform in reverse direction. Separation and mixing should be compatible.

To allow separation, the components should differ in some properties, such as particle size, density, electric charge, solubility, volatility, substrate affinity, reactivity and so on.

For instance, filtration separates particles of different sizes, distillation separates mixtures of liquids with different boiling points that is with different volatilities, chromatography separates dissolved substances by different interactivity with a sorbent, electrophoresis separates molecules based on their different interaction with a gel under an electric potential and so on.

Depending on the unrefined mix, different processes can be in use to separate the components. The processes of separation are described by separation schemes or flow-sheets.

The separation sequence synthesis problem consists in designing an installation that can extract the specified products from the specified feed.

Complex separations have multi-levels architectures and this may be observed, described and designed at different levels of investigation. We can describe a chemical fabrication at the molecular level, at the configuration level of devices and their interactions, or at the level of interactions between installations or between plants.



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For design, at the molecular level there exist developed packages of models based on mass and heat transfer, fluid mechanics differential equations and balance equations. The package includes large data base of constants, parameters and software.

Contrary to the situation at the molecular level, at the configuration level there is a need for innovative methods and models to generate and select separation schemes (Yeomans and Grossmann 1999; Avami et al. 2012). A significant objective is to develop systemic or combinatorial mathematical models of engineering systems to offer predictive capabilities at different levels and scales. The systemic models will complement the conventional detailed models based on natural sciences.

Conceptual design of multi-component separation sequences leads to large number of process alternatives even when the scope of the design is limited to one type of units.

Flow-sheet generation and analysis is the preliminary stage of process design, in which the building blocks of the process are chosen, their interconnections are specified, and the results evaluated. Separation device are often the largest and heaviest items of process equipment in a production system. Consequently, it is of interest to improve its design. Most studies identify four approaches for solving the combinatorial problem of synthesis of separation sequences, namely: evolutionary, algorithmic, heuristic and artificial intelligence methods.

In evolutionary methods a processing system is devised, analyzed and changed in one or more ways so as to improve it. Evolutionary strategy includes the following steps: generate an initial process, define the evolutionary rules, and determine the evolutionary strategy.

Algorithmic methods transform the synthesis step into large-scale optimization problems and different optimization strategies developed in the field of dynamic programming are used to solve it. Because of the large combinatorial nature of the problem, for complex flow-sheets it is unsuitable to investigate thoroughly all possible sequences. Consequently, simple heuristic and qualitative rules are used to generate or to select initial sequences which are likely to be nearly optimal and which need a more detailed investigation. Most of the proposed heuristics were classified into some groups including: composition heuristics, separation-factor heuristics, separation-technique heuristics (Gomez and Seader 1985; Garg et al. 1991; Westerberg 2004).

### *2.1.2 Configurations as Dual Graded Graphs*

The task of separating multi-component mixtures into streams enriched in the respective constituents is commonly carried out in conventional separation columns arranged in series or parallel. Due to restrictions for energy and cost, current research aims at alternative column arrangements that offer energy savings (Christiansen et al. 1997; Halvorsen and Skogestad 2011).

The schemes represented by separation trees are fundamental in chemical engineering and they have been extensively studied.

A simple column performs a separation of a single feed into two products. The simplest case is the separation of a ternary mixture with components ordered by the property allowing separation.

One of the most common operations for restructuring a separation tree is described by the rotation operation shown in Fig. 2.1. It refers to the rotation of the edge (x, y). Here R denotes right rotation and L denotes left rotation.

For separation columns the rotations correspond to the transition between indirect split and direct split (Fidkowski and Krolikowski 1987). Denote by 1, 2 and 3 the components to be separated.

Using brackets we may describe the indirect split by (12)3 and the direct split by 1(23).

The interpretation is indirect split for L and direct split for R. In the indirect sequence for distillation, the first split delivers the heaviest component 3 as bottoms from the first column, followed by the 1 and 2 separations in the second column.

In the direct sequence for distillation the components are separated in the order of volatilities, firstly 1 then 2 and 3 as overhead products.

In the case of four-component mixture 1234, there are five possible sequences each of three columns (Thompson and King 1972).

Figure 2.2 shows the sequences alternatives for separation of four component mixtures.

The five-component mixture can be separated following 14 sequences.

A separation scheme may be considered as a succession of direct and indirect splits or in other words a succession of L and R steps. We may generate the separation schemes based on the trees associated to dual graded graphs (Fomin 1992, Fomin 1994; Nzeutchap 2006; Iordache 2012, 2013, Appendix A).

As example we will consider the planar binary trees, PBT shown in Fig. 2.3

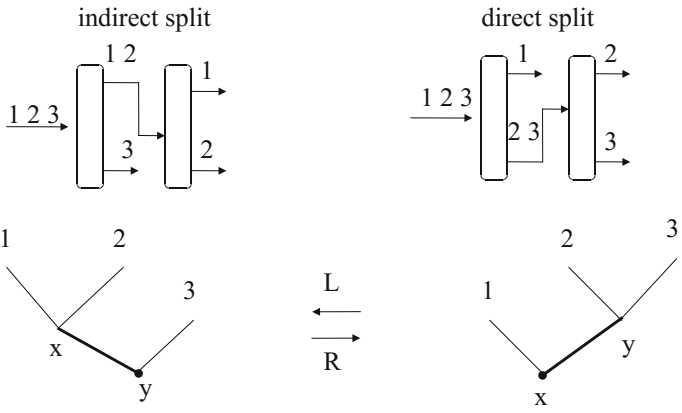


**Fig. 2.1** Rotation operation

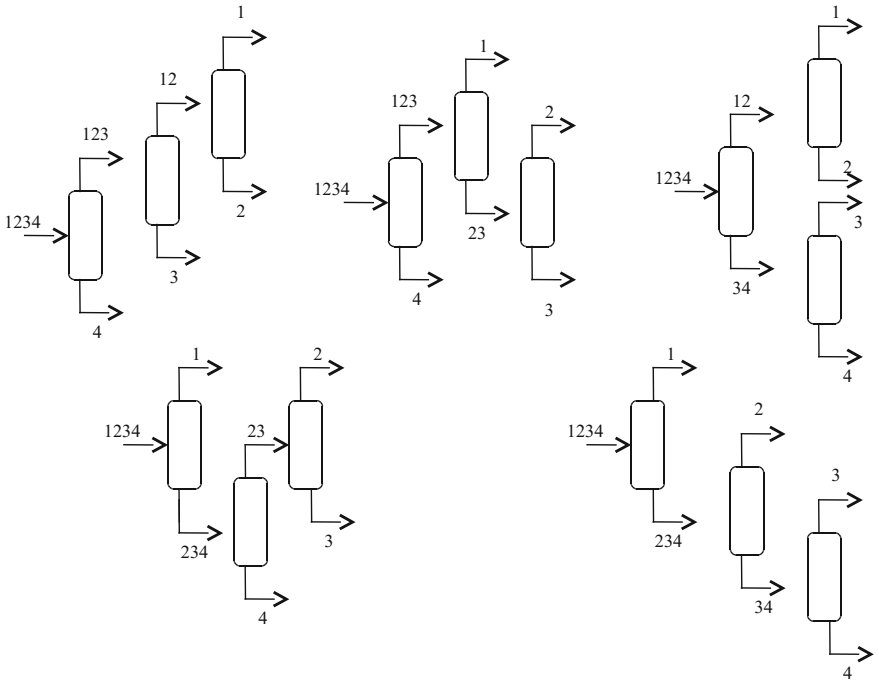


**Fig. 2.2** Sequences for separation of four component mixtures

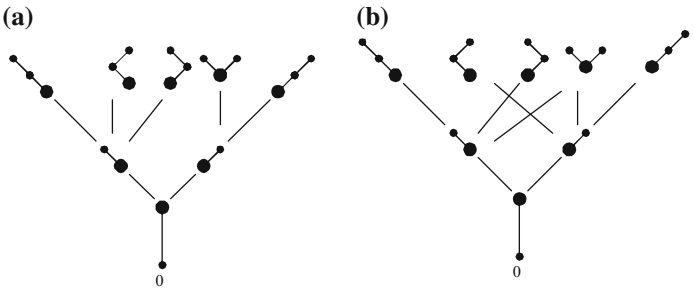


**Fig. 2.3** Planar binary trees

The physical interpretation of L and R portions of such trees may be separation in the light phase for L and separation in the residue phase for R.

The binary tree shown in Fig. 2.3a corresponds to the upward hierarchical separation scheme while the dual tree shown Fig. 2.3b corresponds to the downward dual integration schemes.

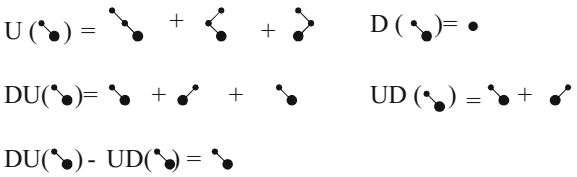


**Fig. 2.4** Commutation relation for planar binary trees

Upward direction corresponds to adding new separation devices in the hierarchical separation scheme. Downward direction is associated to recirculation, recombination and integration.

Figure 2.3a shows the U-graph while Fig. 2.3b shows the D-graph associated to PBT.

Here U denotes the up operator generating the U-graph while D denotes the down operator generating the D-graph (Fomin 1994, Appendix A).

Figure 2.4 illustrates the successive applications of U and D operators.

Observe that the Heisenberg commutation relation: DU-UD = I is verified and the two trees are 1-dual (Stanley 1988, 1990; Fomin 1994).

### *2.1.3 Integration Schemes*

Distillation systems are key installations in petrochemical plants.

The main disadvantage of the distillation is its high-energy requirement.

Several techniques are used to overcome this problem like integration of the distillation schemes with the overall process (Skogestad 1997).

One interesting direction of improving the heat integration for separations is to make the system as compact as possible, to couple the separation U stages to combination D ones.

We consider the coupling of both directions U and D, where U refers to the scheme from Fig. 2.3a and D to the scheme from Fig. 2.3b.

The difference between a tree structure and a poset or lattice structure is outlined by the DGG approach. In the U-graph tree each schemas can be realized in a unique way while in the poset structure of the D-graphs several ways of realization are possible. This multiplicity ensures the flexibility of the dual schemas.

The two directions should be coupled taking into account that the thermal effect of a separation may be compensated by the thermal effect of integration.

Figure 2.5 illustrates the duality of PBT separation and recirculation. The black dots "•"correspond to different vertices in the U-tree or D-tree that is to variants of separations.

Figure 2.5 outlines the relation between different configurations of columns.

The trees of direct way S → K1 → K2 → K3 show the progress of separation.

Implementing polytope project starts from the direct sequence S → K1 → K2 → K3 and should complement this by the reverse sequence:

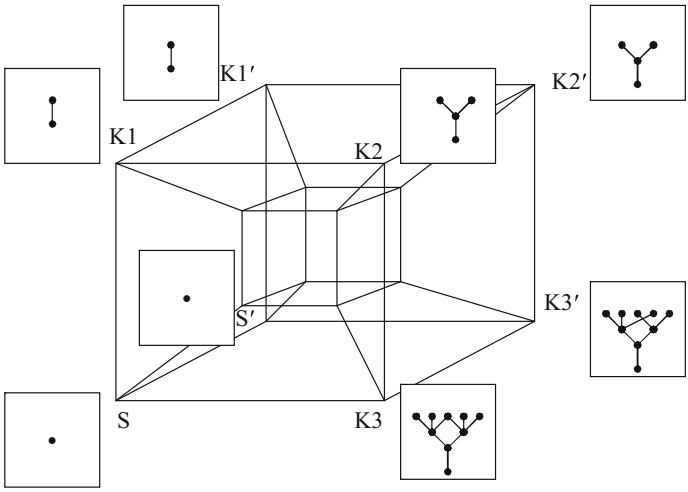


**Fig. 2.5** Polytope for planar binary tree configurations

$K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$. The planar binary tree of reverse way $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$ corresponds to recirculation.

A level in the polytope shown in Fig. 2.5 is a new step on a trajectory in the U-tree or D-trees.

It is the specific coupling of both schemes, up U and down D, which allows process improvement as new separations, heat integration, reverse flow or periodic functioning schemes.

The inner cube of the polytope shown in Fig. 2.5 allows the interactions and triggers the switching between the two schemes in duality. It is the switch from the divergent trend of increasing levels, that is, the front face of the polytope connected to the inner cube, toward the back face of the polytope and the corresponding convergent trend of decreasing levels.

The duality of operations is involved by separation of mixtures via cyclic operations (Sorensen and Prenzler 1997). The regular operations, inverted operation and cyclic operations with a side withdrawal have been studied by Demicoli and Stichlmair (2003).

Self-separations for components have been studied in reactive distillation technologies (Doherty and Malone 2001; Sundmacher and Kienle 2003).

The DGG model based configurations should be compared with numerous heat integration sequences of columns studied in chemical engineering literature (Skogestad 1997; Reid 2000; Ji and Bagajewicz 2002; Repke and Klein 2005).

Progressive distillation is an innovative use of duality separation integration for crude oil distillation schemes.

Two major orientations are typical for distillation, the indirect and the direct sequence.

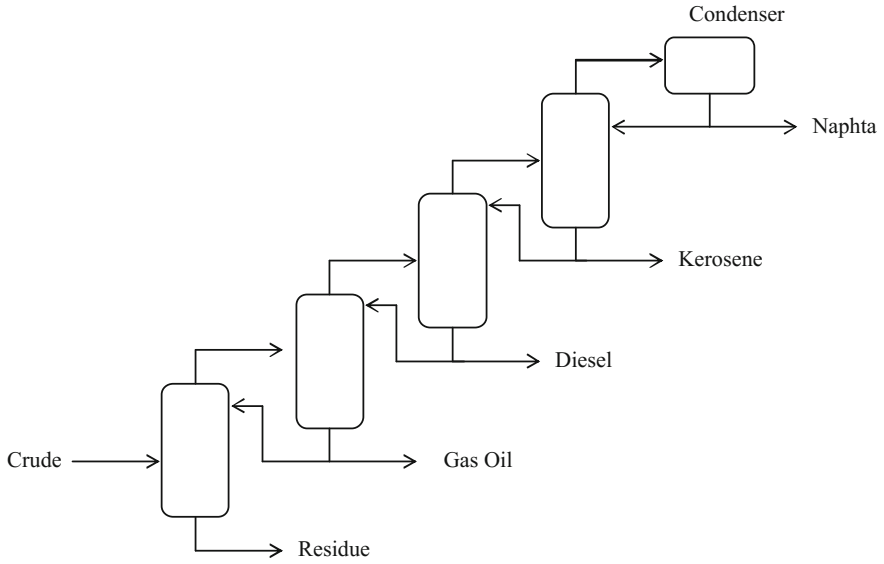


**Fig. 2.6** Conventional distillation as an indirect sequence

Figure 2.6 shows conventional crude oil distillation as an indirect sequence.

The considered fractions are: Naphta, Kerosene, Diesel, Gas Oil and Residue.

In the indirect sequence the heaviest component is removed first in a sharp cut.

Then, the lighter components travel to the next column, where the separation process is repeated.

Conventional crude distillation is an indirect sequence as shown in Fig. 2.6.

In the first column the residue is removed, while gas oil, diesel, kerosene and naphtha moves to the next column in the series. The procedure continues until the components have been completely separated.

In a direct sequence the lightest component is removed first in a sharp cut. Then, the heavier component travel to the next column and the process is repeated.

A direct sequence for crude oil distillation is shown in Fig. 2.7.

Innovative distillation sequences aiming to make use of advantages of direct and indirect sequences have been developed.

A significant relation between direct split and indirect split separation schemes was proposed by Devos et al. (1987). The process consists in successively separating increasingly heavy petroleum cuts at the head of a plurality of columns. Schemes flexibility, and different potential designs have been outlined by several studies (Manley 1993).

Figure 2.8 illustrates the principle of progressive distillation (Devos et al. 1987). The considered fractions are: Naphta-A, Kerosene-B, Diesel-C, Gas Oil-D and Residue-E.

The concept allows flexibility, and several sequence designs have been suggested.

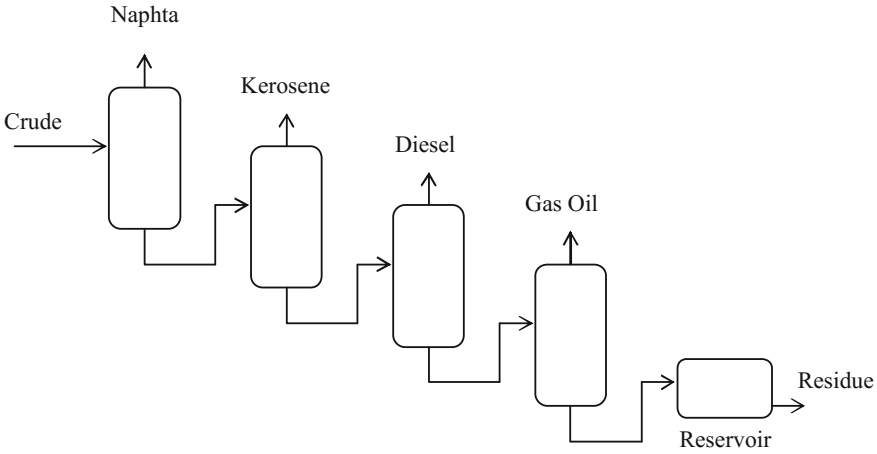


**Fig. 2.7** Conventional distillation as a direct sequence

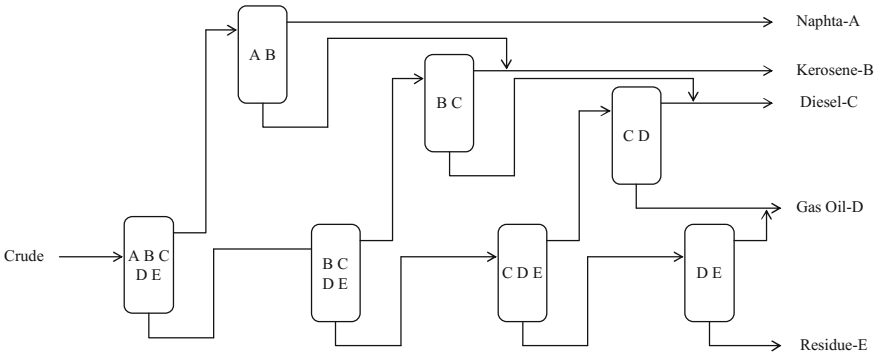


**Fig. 2.8** Illustration of progressive distillation

After the initial separation, the arrangement bifurcates into two series of columns. The light phase from the top series is withdrawn as a product stream, while the heavy phase travel to the next column in the series. The overheads from the bottom series are combined with the bottoms from the top series, while the bottoms from the bottom series travel to the next column.

Progressive distillation is relatively close to direct sequence, but in the progressive distillation the separations are not sharp. A mix of progressive and regressive distillation schemes may increase the sharpness of operations.

### 2.1.4 Lattices for Process Synthesis

Nzeutchap (2006) studied the dual graded graphs associated to the Hopf algebra of planar binary trees and their dual. This is the so-called Loday-Ronco Hopf algebra (Loday and Ronco 1998).

Hopf algebra is both an algebra and the dual of an algebra, the coalgebra, which are compatible (Sweedler 1969; Hivert 2005; Hivert et al. 2005). There is a product rule which describes combining the objects and a coproduct rule which describes separating the objects.

Separation schemes may be organized as partially ordered sets of binary trees with n leaves, ordered by tree rotation operations. These are the so-called Tamari lattices.

A Tamari lattice, is a partially ordered set in which the elements consist of different ways of grouping a sequence of objects into pairs using parentheses.

For instance, for a sequence of four compounds 1234, the five possible groupings are: $((12)3)4$, $(12)(34)$, $(1(23))4$, $1((23)4)$ and $1(2(34))$. Each grouping describes a different order in which the compounds may be combined by a binary operation (see Fig. 2.2). In the Tamari lattice, one grouping is considered before another if the second grouping may be obtained from the first by only rightward applications of the associative law::

$$(a\ b)c = a(b\ c).$$

Applying this law with $a = 1$, $b = 23$, and $c = 4$ gives the expansion $(1(23))4 = 1((23)4)$. So in the ordering of the Tamari lattice $(1(23))4 \leq 1((23)4)$ or, in other words, the separation sequence $(1(23))4$ is earlier than the separation sequence $1((23)4)$.

In this partial order, any two groupings $g_1$ and $g_2$ have a greatest common predecessor, the meet $g_1 \wedge g_2$, and a least common successor, the join $g_1 \vee g_2$.

The Hasse diagram of the Tamari lattice is isomorphic to the vertex-edge incidence graph of an associahedron (Loday 2004). The number of elements in a Tamari lattice for a sequence of $n + 1$ objects is the n-th Catalan number. The combinatorics of the Tamari lattices was studied using Hopf algebras (Loday and Ronco 1998; Foissy 2009).

Figure 2.9 shows the Tamari lattices with 3 nodes.

This lattice corresponds to 4-compounds separation trees.

Transition from a separation scheme to another is accomplished by rotation that is switching between direct and indirect sequencing.

Figure 2.10 shows the Tamari lattices with 4 nodes.

The Tamari lattice from Fig. 2.10 is associated to a 5-compounds separation.

The lattice shows all the possible separation schemes and their interrelationship.

It is a lattice of lattices.

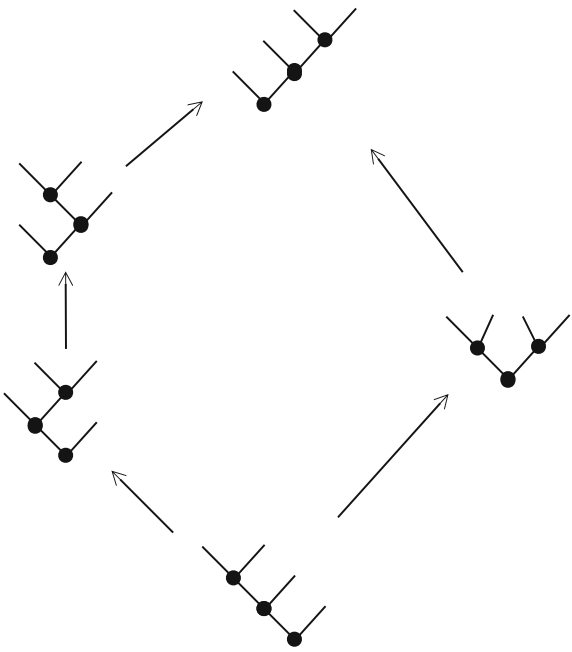

**Fig. 2.9** Tamari lattice of size 3

### 2.1.5 *Integration of Lattices*

Figure 2.11 shows the polytope for lattices configurations.

The notations are:

- K0-substances
- K1-separation trees
- K2-superstructure (lattice)
- K3-super superstructure (lattice of lattices)

K1 illustrates the separation trees. K2 shows a lattice of trees (corresponding to Fig. 2.9).

K3 shows a lattice of lattice of trees (corresponding to Fig. 2.10).

In Fig. 2.11, K1, K2 and K3 are presented without portraying the detailed separation schemes.

Implementing polytope project starts from the sequence K0 → K1 → K2 → K3 and balance this by the reverse sequence: K3′ → K2′ → K1′ → K0′. The reverse way K3′ → K2′ → K1′ → K0′ corresponds to recirculation or integration. This reverses the arrows direction in K1, K2 and K3.

The two sequences should be coupled taking into account that the thermal effect of a separation may be compensated by the thermal effect of integration.

A level in the polytope shown in Fig. 2.11 is the complete structure obtained by a new step for all the trajectories in the U-tree or D-tree. K2 allows all 4-compounds

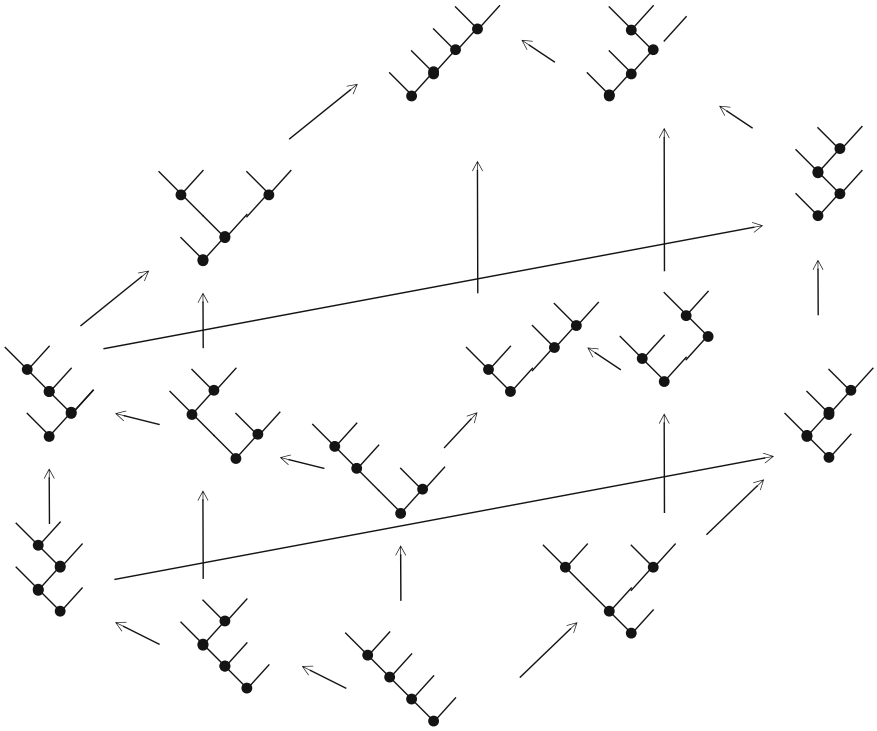

**Fig. 2.10** Tamari lattice of size 4

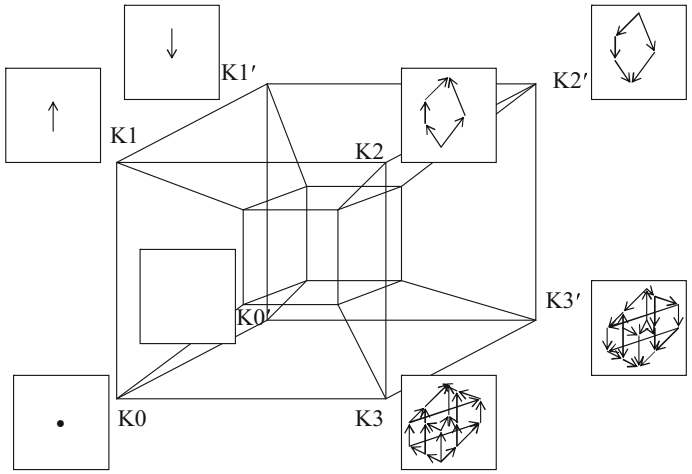


**Fig. 2.11** Polytope for lattices configurations

separations and K3 allows all 5-compound separations. Arrows indicate the relations between separation devices.

## 2.2 Cyclic Separations

### *2.2.1 Cyclic Operations*

In chemical engineering, operating modes as reversed flow for reaction-regeneration energy efficient coupling of endothermic and exothermic reactions, countercurrent flow and induced pulsing flow in trickle beds, unsteady operations, cyclic processes, extreme conditions, low-frequency vibrations to improve gas–liquid contacting in bubble-columns, high temperature and high pressure technologies, and supercritical media, and use of composite structured packing achieving low pressure drop through vertical stacking of catalyst, are now considered for practical application (Ruthven 1984).

Cycling operation methods are of great importance in oil chemistry, in pharmaceutical and food industry, bio-refinery, isotopes separation, hydrogen purification, desalinization, and so forth (Yang 1987). Cyclic separation technologies such as pressure swing adsorption (PSA), temperature swing adsorption (TSA), vacuum swing adsorption, cyclic zone adsorption, simulated moving beds (SMB) chromatography, pressure swing reactor and reverse flow reactor, parameter pumping and so forth, are unsteady non-linear processes difficult to put into practice and to control (Chin and Wang 2004).

In pressure swing adsorption (PSA) processes, gas mixtures are separated by selective adsorption over a bed of sorbent materials. The cyclic nature of these processes arises from the high pressure adsorption phase and the subsequent low-pressure regeneration phase. The PSA cycle was accepted for commercial use in air drying (Dowling et al. 2012).

Thermal swing adsorption (TSA) processes are similar to pressure swing adsorption processes and also separate gas mixture, but here the cyclic nature of these processes arises from the low temperature adsorption phase and the subsequent high temperature regeneration phase. There exist processes that are a combination of PSA and TSA.

A reverse flow reactor is a packed bed reactor in which the flow direction is periodically reversed in order to trap a hot zone within the reactor. In this way even systems with a small adiabatic temperature rise can be operated without preheating the feed stream.

In a pressure swing reactor, reaction and adsorption occur in the same bed.

The adsorption is typically used to purify one of the reaction products. The cyclic nature of a pressure swing reactor arises from the same high pressure adsorption and low pressure regeneration phases as in the pressure swing adsorption.

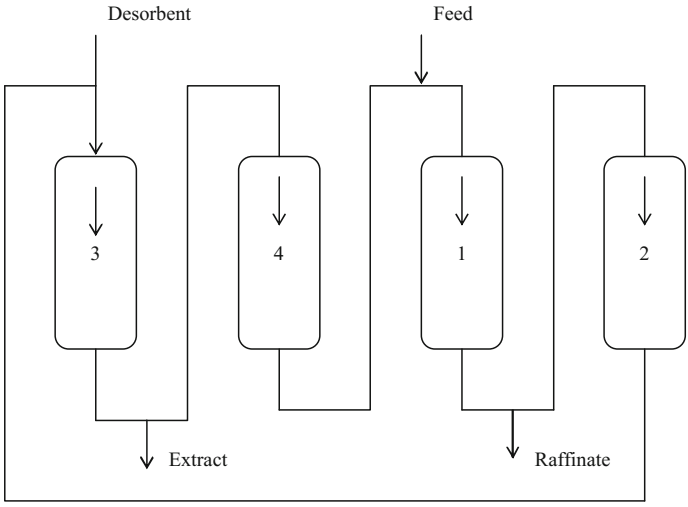


**Fig. 2.12** Linear presentation for simulated moving bed

In a simulated moving bed (SMB) process, the positions of the feed and product streams are periodically moving along the sorbent bed. In this way a flow of the solid sorbent, which flows counter-currently to the gas, is imitated. The aim of a moving bed process is to make more efficient use of the sorbent material.

Numerous cycling separation schemes based mainly on intuition have been reported in literature. An example of SMB schemes is shown in Fig. 2.12.

This is a linear presentation of the SMB cyclic schemes.

Figure 2.13 shows a cyclic presentation of SMB.

As the separation complexity and the number of devices increases it becomes very difficult to formulate a feasible schedule much less an optimal one.

The proposed approach allowing operating cyclic separations in multi-compound high complexity conditions is that of self-evolvable separation systems. These are systems that can change autonomously the schemes and the dynamic behavior and are capable to control and to take advantage of the unexpected events of their environment in increasingly complex ways. Potentially self-evolvable devices are separation systems with emergent, not entirely pre-programmed, behavior.

### *2.2.2 Non-Crossing Partitions*

Cyclic operations may be studied using non-crossing partitions.

Non-crossing partitions only make sense for a set with a linear order. Moreover instead of the linear order {1, …, n} we could also put the points 1, …, n on a circle

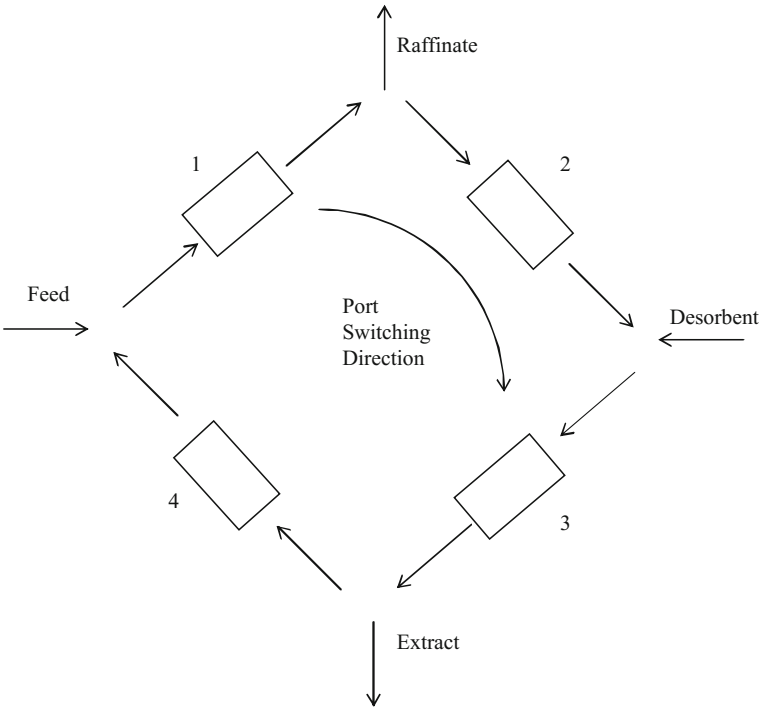


**Fig. 2.13** Cyclic presentation for simulated moving bed

and consider them with circular order. This corresponds to the linear and cyclic presentations of SMB.

Non-crossing is correlated to the fact that there is a natural succession of the operations.

Figure 2.14 shows a crossing partition (a) and non-crossing partition (b).

In this case (a) corresponds to the notation (13)(24) and (b) corresponds to the notation (124)(3).

Consider for instance the notations are: 1-feed, 2-extract, 3-desorbent, and 4-raffinate. There are 4 operations indexed by 1, 2, 3 and 4 and we will consider that it is possible to by-pass some of them but not to cross them. We can group or by-pass some steps, as desorption for instance, but crossing do not corresponds to acceptable solutions since it change the natural order of steps.

Figure 2.14 illustrates this aspect of separation technology. Figure 2.15 contains non-crossing partitions. The notations are obvious. For instance (1234) denotes a series of 4 coupled devices or stages, 1(234) means that 1 is decoupled but 2, 3 and 4 are still coupled, while 1234 means that all the stages are decoupled.

Figure 2.15 shows all possible coupling and decoupling of steps in cyclic operations.

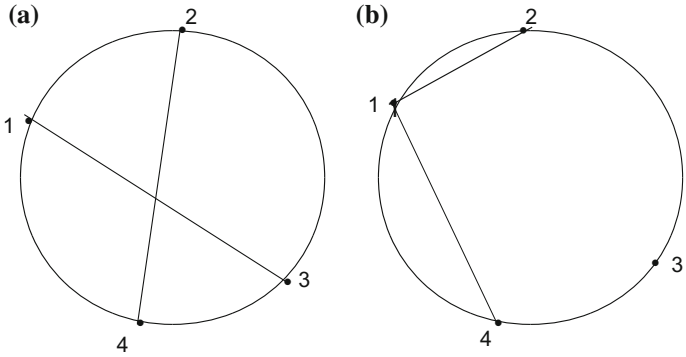


**Fig. 2.14** Crossing and non-crossing partitions

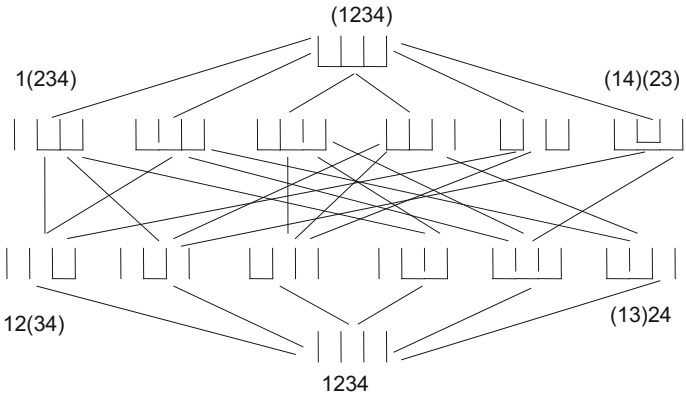


**Fig. 2.15** Non-crossing partitions

Up and down, denoted by U and D, trajectories describe this coupling or decoupling of steps.

Observe that:

$$\mathrm{U}\,((123)4) \;=\; (1234):\ \mathrm{D}\,((123)4) \;=\; 1(23)4 + (12)34 + (13)24 \tag{2.1}$$

$$\mathrm{DU}((123)4) \;=\; 1(234) + (134)2 + (124)3 + (123)4 + (12)(34) \;+ (14)(23) \tag{2.2}$$

$$\begin{aligned}\mathrm{UD}((123)4) = {} & 1(234) + (123)4 + (14)(23) + (124)3 \\ & + (123)4 + (12)(34) + (134)2 + (123)4\end{aligned} \tag{2.3}$$

$$(\mathrm{DU} - \mathrm{UD})((123)4) \;=\; -2\mathrm{x}\;((123)4) \tag{2.4}$$

This calculus illustrates the commutation condition for the lattice of non-crossing partitions (Appendix A).

Studies of the Hopf algebra of non-crossing partitions are due to Novelli and Thibon (2003) and Ebrahimi-Fard and Patras (2015).

### 2.2.3 *Dual Graded Graphs for Evolving Schemes*

Schemes evolving between linear and cyclic sequences may be considered as potential candidates for self-evolvable technologies.

The cycle we refer here is an up and down evolution on the U-tree and D-tree.

Such schemes may be based on the dual Catalan trees as described by Qing (2008), Iordache (2013).

Consider the Catalan tree and its dual shown in Figs. 2.16 and 2.17.

Figure 2.16 shows the Catalan tree U-graph

Figure 2.17 shows the Catalan tree D-graph

Vectors of four digits show the stages in which the four devices of a separation installation are. Consider for instance the notations are: 1-feed, 2-extract, 3-desorbent, and 4-raffinate. In pressure swing adsorption the raffinate refers to the gas which is not adsorbed during the high pressure stage. The compound which is desorbed from the adsorbent at low pressure is the extract product.

Thus the vector 1124 denotes the installation with the first two devices in the feed stage the third in extract stage while the fourth device in raffinate stage.

The Catalan tree U-graph (Fig. 2.16) corresponds to the progress of hierarchical separation schemes while the Catalan tree D-graph (Fig. 2.17) corresponds to regressive schemes with recirculation. Together they describe a cyclical process.

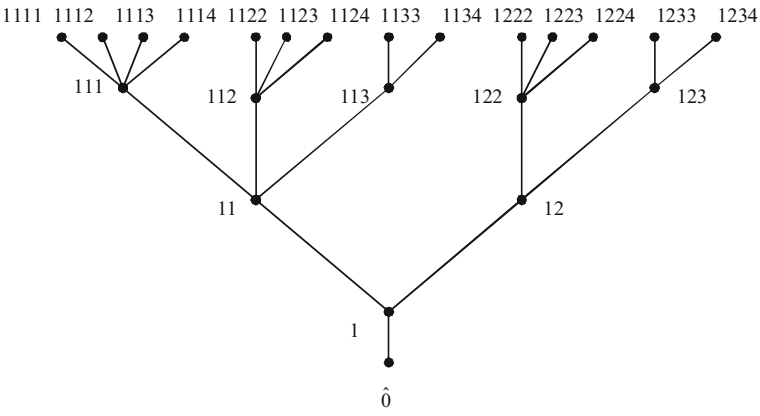


**Fig. 2.16** Catalan tree U-graph

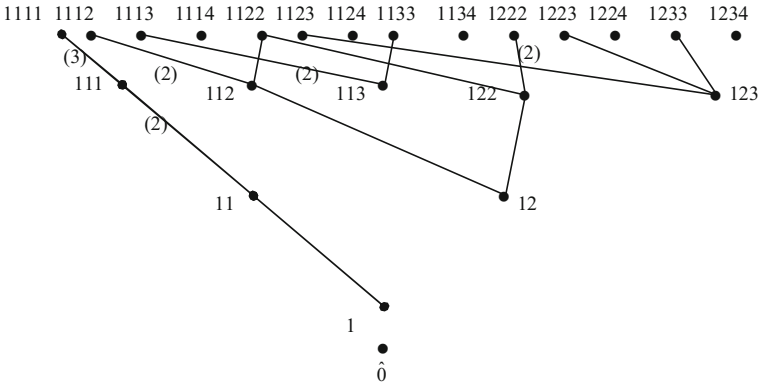


**Fig. 2.17** Catalan tree D-graph

The weights indicated on the connections between two vectors show the number of ways we can obtain one from another in up and down direction.

Figure 2.16 shows the number of ways to pass from a vector to another, only if this is different from one. For instance there are (3) ways to pass from 111 to 1111 depending on the selected position of the new inserted column.

Let the vertex set be the number string of the form $x = a_1a_2a_3\ldots a_n$ with $1 = a_1 \leq a_2 \leq a_3 \leq \ldots \leq n$.

In the U-graph, y covers x, $x \uparrow y$, if and only if, y can be obtained from x by adding a right number to the right end of x.

The U-graph constructs the separation schemes. It is supposed that different steps are related in the natural order of steps in a separation process. In this example the natural order is 1, 2, 3 and 4.

A higher level is a new step and this either replicates the previous step since that step was not completed in just one column or may be one of the subsequent steps in the natural order. After 1 we may have in the U-graph, 11 or 12. After 12 we may have in the U-graph 122 or 123.

In the D-graph, x covers y, $x \downarrow y$, if and only if, y can be obtained from x by deleting $a_i$ from $a_1a_2a_3\ldots a_n$ only if $a_{i-1} = a_i$.

The D-graph reconstructs the schemes. This is done by grouping stages that are identical.

From 122 we may obtain in D-graph 12 and from 1233 we may obtain in D-graph 123. It is a method allowing grouping the previously replicated steps when replication is not more necessary.

The resulting trees are dual.

The significant role of the step "12" is highlighted by the dual graph.

We can consider "12" as coupling the step 1 and 2 as a kind of basic cyclic schemes, from 1 to 2 and from 2 to 1. The four steps separation reduces to a two steps separation (Iordache 2013).

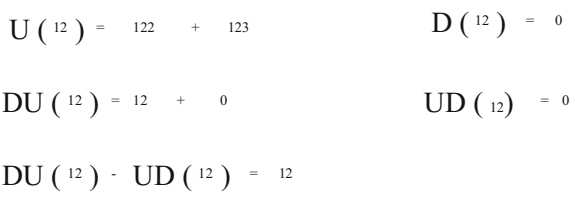


**Fig. 2.18** Commutation condition for Catalan trees

The cyclic character is a consequence of the switching between U-tree and D-tree.

Figure 2.18 illustrates the commutation condition for Catalan graphs.

By 0 in Fig. 2.18 we indicate that the connection is missing.

Observe that the Heisenberg commutation relation: DU-UD = I is verified and the two trees are 1-dual (Appendix A).

The Fibonacci graphs may be another mathematical model useful to describe the correlation of cyclic and linear separation schemas.

Schemas with just two steps are imagined and associated to Fibonacci graphs studied by Fomin (1994).

The vertices of the Fibonacci graph are words on the alphabet {1, 2} and a word w is covered by w′ if w′ is obtained from w by adding a 1 at the end or by changing any 1 into a 2. In the graph that is dual to the Fibonacci graph, w is covered by w′ if w is obtained from w′ by deleting a 1, and the multiplicity of the edge between w and w′ is the number of ways to delete a 1 from w′ to get w.

Suppose that the state "1" corresponds to compression-saturation step and "2" to decompression-purge step. The states of the separation schemas are {1, 2} words. Words are viewed as sequence of columns in the separation schemas.

At any level any a new compression-saturation column is activated and a new digit "1" joins the existing state or one of the existing column are changed in decompression-purge denoted by "2".

Figure 2.19 shows the Fibonacci dual graphs.

Figure 2.20 illustrates the commutation condition for Fibonacci graphs.

The cyclic character is a consequence of the switching between U-tree and D-tree.

The role of the purely decompression-purge steps in one or to columns as "2" or "22" is highlighted by the Fibonacci dual graph.

### *2.2.4 Polytope for Cyclic Operations*

Potentially self-evolvable schemes appear as superposition of dual schemes.

We will consider the coupling of both directions U and D.

U constructs the schemes by divergent including new steps and stages, while D reconstructs this by convergent grouping steps and stages.

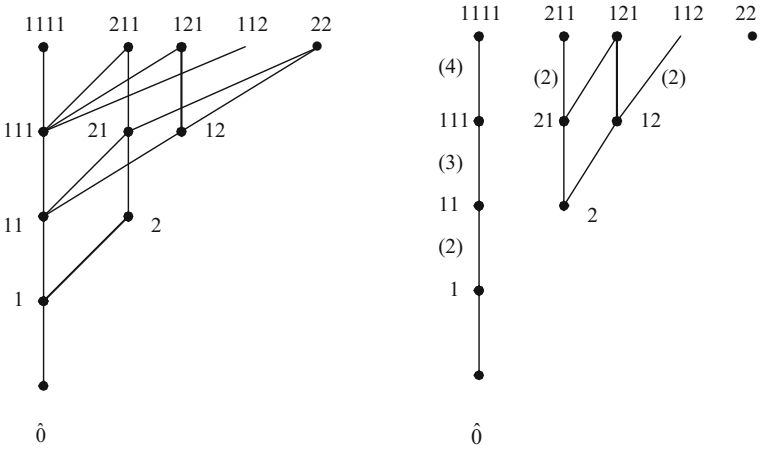


**Fig. 2.19** Fibonacci dual graphs

**Fig. 2.20** Commutation condition for Fibonacci graphs

$$U(_{12}) = {}_{121} + {}_{22} \qquad D(_{12}) = {}_{2}$$

$$DU(_{12}) = {}_{21} + {}_{12} \qquad UD(_{21}) = {}_{21}$$

$$DU(_{12}) \cdot UD(_{12}) = {}_{21}$$

The two ways should be coupled taking into account that the effect of a separation is compensated at least in part by the effect of integration.

Interesting hybrid PSA-distillation processes illustrates the potential of coupling the cycling PSA with the linear separation trees (Ritter et al. 2012).

Figure 2.21 shows the polytope associated to the Catalan trees.

This clarifies the polytope project implementation.

The black dots "•" in Fig. 2.21 correspond to distinct separation sequences.

The polytope serve as guide for the construction and reconstruction of the self-coordinated and self-evolvable separation schemes.

Implementing polytope project starts from the direct sequence S → K1 → K2 → K3 and balances this by the reverse sequence: K3′ → K2′ → K1′ → S′.

Figure 2.21 illustrates the need of reversing the divergence trend of increasing levels, that is, the front face of the polytope, connected to the Self, by mapping it to the back face of the polytope and the corresponding convergent trend of decreasing order of levels.

Smart systems perspectives for separation technologies start to be evaluated and implemented by chemical engineers.

Local distributed process control is considered as a key factor for self-evolvability. This control implies that the energy and chemical supply to be

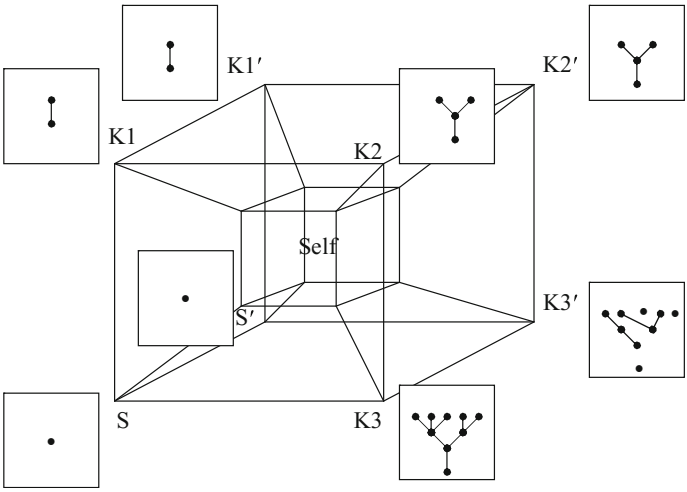


**Fig. 2.21** Polytope for Catalan trees

localized to the site were it is required. It should be based on embedded arrays of local sensors and actuators.

Cyclic operation allows coupling direct and reverse sequences in the polytope projects implementation. When combined with this non-stationary cyclic operation such micro structured programmable devices offer new possibilities for innovative separation schemes.

With this approach one can envision a programmable separation unit coupled to a motherboard and providing operation conditions that adjust automatically to the desired separation. The program may be based on the dual graded trees or more generally on Hopf algebras describing the separation and integration processes.

Increased efficiency, productivity and selectivity could be obtained through smart operation and multi-scale control. Smart separation schemes would involve assemblies of structured, modular separation devices and precise computer control based on information transfer between distributed arrays of local sensors and actuators.

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# Chapter 3
# Molecules and Networks

## 3.1 Periodic Features

### *3.1.1 Smart Drug Delivery Systems*

Recent advances in genomics and in the study of complex diseases have shown the necessity for an alternative way of thinking in medicine and pharmacology, a view in which pathology and physiology results from interactions between many processes at different scales.

The new scientific field of systems biology is correlated to this perspective. It focuses on the study of genes, proteins, biochemical reaction networks and cell populations considered as dynamical systems. Polytope projects provide a conceptual framework and effective tools for studying emergent and immergent features from molecules to organisms and contrary.

The method by which a drug is delivered to organism has a significant effect on its efficacy. The traditional approach is to develop drug delivery systems, DDS, which will release the drug at constant rate, to ensure a required concentration level. The drug application method, that may be oral, inhalation, transdermal and so on, determines the drug distribution in organism.

This traditional approach is not always suitable or effective. Drugs may induce large metabolic degradation, may lead to adverse effects, may saturate the organisms or may decrease in time the bioavailability. The traditional drug application approach neglects the variability of drug effects and of the organism requirements. Additionally, some of the traditional approaches are associated with the very slow progress in the efficacy of the treatment of complex or severe diseases.

The reason of low efficiency of conventional DDS resides in the complexity of drug-organism interaction process and the complexity of some diseases.

It was observed that most organisms are not passive in their requirements or response to drugs. Organisms manifests as dynamic systems which require different amounts of drug at different times, at different sites for different patients.



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Studies in Systems, Decision and Control 92,
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The biological processes and functions are organized in time, as a specific biological time and space structure, as revealed by physiology and anatomy studies. The time structure is characterized by multiple biological rhythms, while the spatial distribution is characterized by multiple scale heterogeneity. Organisms always involve a wide range of scales both in time (femtoseconds for chemical reactions, seconds for metabolism processes, day to months for cells and years in living organisms) and space (nanometers for molecular structures, micrometers for organelles and cells, centimetres for tissues and organs and meters for organisms).

The drug delivery systems should take into account both the temporal and spatial heterogeneity of the organisms. Despite the fact that some diseases and drug delivery-organism interactions are recognized as highly complex, diseases treatments continue to be implemented by drug delivery regimes and procedures were complexity properties are neglected.

The consideration of different scales, from the macroscopic scale to the atomic and sub-atomic scales is becoming more and more important for drug delivery system design. To illustrate the multiple scales issue we may refer to the design of transdermal delivery systems (Shaeiwitz and Turton 2004).

In terms of multi-scale design, a transdermal delivery system illustrates design from the macroscopic scale through the molecular scale. At the macroscopic scale, the transdermal delivery system must be assembled and be customer friendly. At the mesoscopic scale, between macroscopic and microscopic, the pharmacokinetics of the drug should be modeled. At the colloidal scale, adhesion must be understood in order to facilitate selection of a suitable adhesive. At the microscopic scale, the mechanism of transport of the drug through the skin must be understood. The nano scale study concerns the drug mixing with enhancers and excipients. The former may alter the permeability of the external layer of skin most often acting as the limiting resistance, to facilitate drug delivery. The latter are pharmaceutically inactive ingredients such as skin moisturizers usually found in transdermal patches. A molecular-scale design illustration would be to design the drug based on an understanding of the desired pharmacology.

Innovative DDS able to establish the drug application mapping and timing, in order to be adaptive to the unavoidable variability in living organisms, and to perform an active healing, start to be developed and implemented in the last decade.

New domains as chronopharmaceutics and chronotherapy have emerged (Smolensky and Peppas 2007). Significant research was devoted to the design and evaluation of DDS that release a therapeutic agent at a rhythm that matches the biological requirements of a given disease therapy.

Constant drug delivery may become ineffectual and needs to be replaced by a pulse of therapeutic concentration in a periodic manner. This imposed the development of modulated, pulsatile DDS (Sershen and West 2002). In such systems there is rapid and transient release of a certain amount of drug molecules within a short time-period immediately after a predetermined off-release period. Various techniques are available for cyclic delivery like pH, temperature, light, magnetic field, presence or absence of a specific molecule, micro-flora and so on.

To minimize the toxicity associated with the drug delivery, the research focused to the development of modulated drug delivery systems capable of releasing therapeutic agents in response to physiological requirements. These are known as self-regulated or responsive systems.

A major class of modulated drug delivery systems is that in which the pulsatile release of drugs is triggered by external signals. These are known as externally regulated or pulsatile delivery systems. Developments in the field of pulsatile systems based on external triggers such as electrical, ultrasound, magnetic and mechanical have been reported (Sershen and West 2002). Research was done in the field of polymer based temperature-sensitive, pH-responsive, inflammation-responsive and glucose-and other saccharine-sensitive systems; enzyme-based urea-responsive, glucose-responsive and morphine-triggered systems and systems based on antibody interactions.

Hydrogels are three-dimensional, hydrophilic polymer networks capable of imbibing large amounts of water or biological fluids. The networks are composed of homopolymers or copolymers, and are insoluble due to the presence of crosslink such as entanglements or crystallites. Hydrogels are capable to swell in aqueous media. They are used to regulate drug release in reservoir-based, controlled release systems or as carriers in swellable and swelling-controlled release devices. Hydrogels as stimuli-sensitive gel systems modulated release in response to pH, temperature, ionic strength, electric field or specific analyte concentration differences (Peppas and Leobandung 2004).

In such DDS, release can be designed to occur within specific areas of the body.

The skin patches are useful for drug delivery by iontophoresis. Iontophoresis is a technique used to enhance the absorption of drugs across biological tissues such as skin. Patches are either impregnated with drugs or some versions can be used as dispensers of the drugs (Murdan 2003).

To confront the complexity of drug delivery and to go through the frontier of complexity smart drug delivery systems should be implemented and evaluated.

This approach adopts the point of view according to which the drug delivery system cannot be completely pre-programmed but would be actively constructed by interaction with the organism.

Smart systems perspectives for drug delivery start to be evaluated and implemented.

### *3.1.2 Drug Delivery and Dual Graded Graphs*

Chronotherapy describes the use of rhythmic cycles in the application of therapies. Examples are the drug treatments that are administered according to a schedule that corresponds to individual rhythms in order to maximize effectiveness and minimize side effects of the therapy (Sajan et al. 2009).

Chemotherapy takes into account circadian rhythms since the proliferation of normal cells and of damaged cells is gated by the circadian clock and the damaged

cells are less well synchronized. It was established that the detoxification of cytostatic drugs depends on time of administration.

The body's immune system can destroy some cells within a window occurring every 12–14 days (Ashdown 2004; Coventry et al. 2009). By giving low-dose treatment at the right time, researchers succeeded in halting the spread of advanced disease.

The body has an immune cycle during which it swings "on" and "off". When the immune system turns "off", it releases inhibitory cells. Treating organisms at the right time may increase their life.

The timed drug delivery supposes an iterated screening of drugs and drug delivery by interaction with the organism, resources and environment.

Chronotherapy may be based on the binary vectors associated to drugs. These binary vectors are also elements of dual graded graphs. The proposal is to use the vectors trajectories on the U-graphs and D-graphs according to the "up" and "down" periods for the biological rhythms (Ticher et al. 1995; Sharma 2003).

A vector of composition $i = \langle i1, i2, \ldots ik, \ldots \rangle$ may be associated to each drug i, whose components correspond to different characteristic groups of the molecule, in a hierarchical order according to the expected importance of their pharmacological potency. If the m-th portion of the molecule is pharmacologically more significant than the k-th portion, then we have $m < k$. The hierarchical order may be imposed by the physiological mechanism of the drug. The mth step is before the kth step.

The components ik are "1" or "0" according to whether a similar, or identical, portion of rank k is present or absent in molecule i, compared with the reference molecule (Iordache 2012, 2013).

On the other side, binary vectors may be generated using dual graded graphs (Fomin 1994, Appendix A).

The switch from U-tree to D- tree corresponds to the switch from a vector to other vectors and, in our interpretation, from a drug or drugs mixture to another mixture and this "up" and "down" switching may be associated to chronotherapy rhythms.

There are several pairs of dual graded graphs that may be considered for drug delivery systems. The right pair to choose for a specific disease depends on the physiological mechanism of the drug to be tested.

Figure 3.1 shows lifted binary tree and Binword tree. Figure 3.1a shows the U-tree while Fig. 3.1b shows the D-tree. U denotes the "up" operator generating the U-graph while D denotes the "down" operator generating the D-graph.

Lifted binary tree and Binword are dual (Fomin 1994).

The difference between a tree structure and a poset or lattice structure is outlined by the DGG approach. In the U-graph tree each state can be realized in a unique way while in the poset structure of the D-graphs several ways of realization are possible. This multiplicity ensures the flexibility of the dual schemes.

To each pair of dual graded graphs, there is a pair of dual Hopf algebras that may be associated.

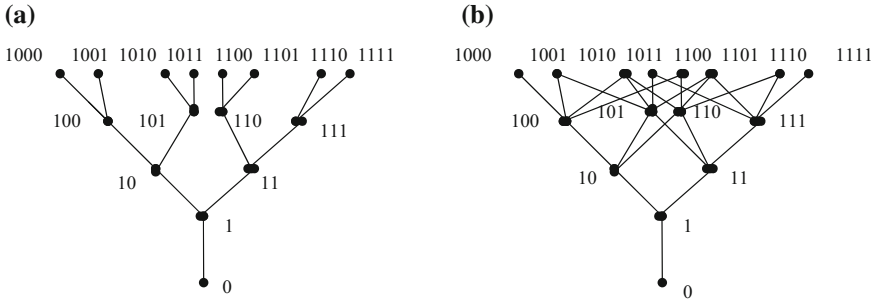



**Fig. 3.1** Lifted binary tree and Binword

**Fig. 3.2** Commutation condition for lifted binary trees and Binword

$$U(11) = 111 + 110 \qquad D(11) = 1$$

$$DU(11) = 11 + 11 + 10 \qquad UD(11) = 11 + 10$$

$$DU(11) - UD(11) = 11$$

Many combinatorial objects have a natural breaking or decomposing structure which gives a coalgebra structure to the graded vector space on such objects (Joni and Rota 1979). Often there is a compatible way of putting pieces together or composing, extending this to a Hopf algebra structure. Sometimes, either the assembling or the breaking process is symmetric, leading to commutative or co-commutative Hopf algebras respectively (Appendix B).

The lifted binary tree and Binword are the graphs associated to the dual Hopf algebras NSym, non-commutative symmetric functions and QSym, quasi-symmetric functions (Hivert et al. 2005; Nzeutchap 2006).

In the lifted binary tree y covers x if it is obtained by adjoining a single "0" or "1" to the end of x. On the other hand x is covered by y in Binword if it is obtained from y by removing a single letter, but not the first. For example 101001 covers 11001, 10001, 10101 and 10100.

Figure 3.2 shows the commutation condition for lifted binary tree and Binword.

The construction of the trees should find its roots in the physiological mechanism of the drug to be tested. Adjoining to the end corresponds to a new step in drug action that is to a new radical in the drug molecule. Removing of a digit but not the first corresponds to the fact that some steps of the physiological mechanisms may be by-passed or blocked.

Figure 3.3 shows another pair of dual graded graphs, the so-called developed binary trees (Iordache 2013).

Figure 3.3a shows the U-tree while Fig. 3.3b shows the D-tree. U and D trees are in duality relation.

They have been studied as infinite 2-nary trees by Fomin (1994).

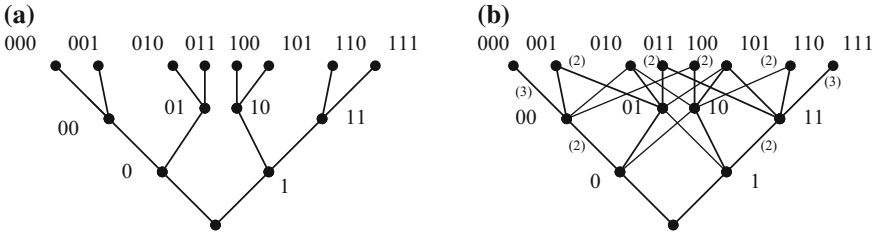



**Fig. 3.3** Developed binary trees

**Fig. 3.4** Commutation condition for developed binary trees

$$U(1) = 11 + 10 \qquad D(1) = \hat{0}$$

$$DU(1) = 2x1 + 1 + 0 \qquad UD(1) = 1 + 0$$

$$DU(1) - UD(1) = 2x1$$

The vertex set is represented by strings of "1" or "0" of finite length. The length of the string is the rank of the element.

For the U-graph shown in Fig. 3.3a, x is covered by y if and only if y can be obtained from x by inserting a number to the right end of x. The D operator corresponds to deleting a letter that is a digit in the associated vector.

In the D-graph a word x of rank k is linked with a word y of rank k − 1 by a vertex having as weight the number of ways to obtain y from x by deleting a letter from x.

The weights are indicated on the tree shown Fig. 3.3b if different than one.

For instance, Fig. 3.3b shows the weight (2) for the vertices connecting 100–10 and 011–01.

Figure 3.4 illustrates the commutation condition for developed binary trees.

### *3.1.3 Chronoterapy Case Studies*

Case studies referring to anesthetics, human immunodeficiency virus inhibitors and to 2-phenylindoles will be presented in more detail.

The first step in quantifying the concept of similarity for molecules of local anesthetics is to list the most important portions of such molecules. Furthermore, the vector of properties $i = \langle i1, i2, \ldots ik, \ldots \rangle$ should be associated to each local anesthetic i, whose components correspond to different characteristic groups of the molecule of anesthetic, in a hierarchical order according to the expected importance of their pharmacological potency. The components ik are "1" or "0" according to whether a similar (or identical) portion of rank k is present or absent in anesthetic i compared with the reference anesthetic. The analysis includes such chemical

compounds that fit the following general scheme: (lipophilic portion)–(intermediate chain)–(hydrophilic portion), since these are the most numerous and have the widest range of uses among the species used in practice of local anesthesia. The lipophilic portion normally consists of at least one phenyl radical, the hydrophilic portion is most often a secondary or tertiary amine, and the intermediate chain commonly has an ester or amide linkage. It is assumed that the structural elements of a local anesthetic molecule can be ranked, according to their contribution to anesthetic potency, in the order of decreasing importance: lipophilic portion > hydrophilic portion > intermediate chain > number of nitrogen atoms > number of oxygen atoms. The lipophilic portion is primarily responsible for the lipid solubility that allows diffusion across the nerve cell membrane, determining the intrinsic potency of local anesthetics. Both the lipophilic and hydrophilic portions determine protein-binding characteristics, which are felt to be the primary determinant of anesthesia duration.

Procaine is a tertiary amine, containing a primary amino group linked to an aromatic ring (Fig. 3.5). In procaine, the lipophilic portion is a phenyl radical, the hydrophilic portion is an amine, the intermediate chain is an ester, there are two azoth N atoms and two oxygen O atoms; obviously, its associated vector is: 11111. Procaine was selected as a reference anesthetic because it was among the first synthetic compound successfully used for regional anesthesia and, in this and most other local anesthetics, the lipophilic portion consists of at least one phenyl radical, the hydrophilic portion is a secondary or tertiary amine, and/or the intermediate chain has an ester linkage.

Torrens and Castillano (2006, 2009a, b, 2010, 2013) presented the results of their drug classification studies in the form of classification trees and periodic tables. In fact the periodic tables show in a different way some of the levels of the classification tree. Periodic tables including the chemical elements periodic table may be represented as trees.

Dual trees outline the increasing and decreasing complexity of compounds.

In the study of local anesthetic a periodic table as shown in Table 3.1 was proposed following Torrens and Castillano study. To simplify the presentation, Table 3.1 contains only few of the studied compounds.

As columns in the table the first three digits for property vectors are selected 010, 100, 101, 110 and 111. Rows are to the next two digits in any vector to complete the five digit characterization: 00, 01, 10 and 11. For instance in the fourth column 101 and second row 01, we will find the anesthetics characterized by 10101 that is benzocaine.

Such tables may be useful for chronotherapy purposes.

Suppose that we start to apply a treatment with dyclonine. It is a 110 compound.

**Fig. 3.5** Procaine

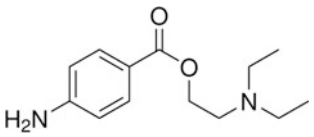


**Table 3.1** Periodic table for local anesthetics

| | 010 | 100 | 101 | 110 | 111 |
|---|---|---|---|---|---|
| 00 | | | | Mexiletine | Cocaine |
| 01 | Dibucaine | | Benzocaine | Dyclonine | Hexylcaine |
| 10 | | | | Lidocaine | |
| 11 | | Phenytoin | | | Procaine |

According to the rule to build U-tree shown in Fig. 3.3a, a digit is added and we look for 1100 (mexiletine) and for 1101 (lidocaine).

In the D direction (Fig. 3.3b) a digit is deleted and we look for 10 (benzocaine) and to 11 (dyclonine). The proposal is to use a mixture dyclonine, lidocaine, mexiletine for the U period and dyclonine, benzocaine for the D period. The selection of a drug in a mixture of drugs characterized by the same vector may be based on therapeutic or economic criteria.

The U and D may correspond for instance, to morning "high activity" and evening "low activity" periods.

For the study of Human Immunodeficiency Virus inhibitors a periodic table as shown in Table 3.2 was proposed (Torrens and Castellano 2009a, b, 2010).

As a reference it was selected the didanosine. The formula is $N_4O_3S_0P_0X_0$ where X = F, Cl. The associated vector is: 111111. The chosen significance order for inhibitor action is N > O > S > P > X. The components in the vectors associated to other inhibitors are "1" or "0" according to whether they are identical, or different if compared with the reference molecule.

Table 3.2 shows only few of the studied compounds.

As columns in the table the first three digits for property vectors are selected 000, 001, 010 and 011. Rows are to the next two digits in any vector to complete the five digit characterization: 01, 10 and 11.

The proposed chronotherapy is based on dual trees shown in Fig. 3.3.

Suppose that we start to apply a treatment with efavirenz. It is a 001 compound

In the U direction (Fig. 3.3a) a digit is added and we look for 0010 (tenofovir) and to 0011 (delaviridine).

In the D direction (Fig. 3.3b) a digit is deleted and we look for 00 (efavirenz) and 01 (lamivudine).

The proposal is to use a mixture evafirenz, tenofovir and delaviridine for the U period and evafirenz, lamivudine for the D period.

The U and D may correspond to "high activity" and "low activity" periods.

**Table 3.2** Periodic table for human immunodeficiency virus inhibitors

| | 000 | 001 | 010 | 011 |
|---|---|---|---|---|
| 01 | | Tenofovir | | |
| 10 | Tipranavir | Efavirenz | | |
| 11 | Amprenavir | Delaviridine | Lamivudine | Emivirine |

A similar methodology may be applied for 2-phenylindoles library design.

Some 2-phenylindoles and their derivative prove to have anti-cancer activity (Basak et al. 2010).

Figure 3.6 shows the molecular structure of the 2-phenylindoles derivatives. Different radicals are denoted by R1, R2, R3 and X (see Table 1, Basak et al. 2010).

For 2-phenylindole derivatives we considered associated vectors as: y = R1, R2, R3, X.

This means that the chosen significance order for drug action is R1>R2>R3>X.

We associate the digit "1" to R1 = H, R2 = H, R3 = $OCH_3$ and X = $C(CN)_2$ and the digit "0" to the radicals that are different from these.

We selected the compound #2 (Table 1, Basak et al. 2010) as reference #2 = 1 1 1 1 1.

Obviously the choice of the set of characteristics and of their hierarchy should be based on drug physiological mechanism and drug efficiency tests.

Table 3.3 shows the radicals pertaining to different 2-phenylindoles derivatives.

Table 3.4 outlines the reference set for 2-phenylindoles derivatives-matrix

Table 3.4 contains the information as Table 3.2 in digitalized form.

The half maximal inhibitory concentration ($IC_{50}$) is a measure of the effectiveness of a compound in inhibiting biological or biochemical function. This quantitative measure indicates how much of a particular drug is needed to inhibit a given biological process by half. Here we focused on derivatives with high $IC_{50}$.

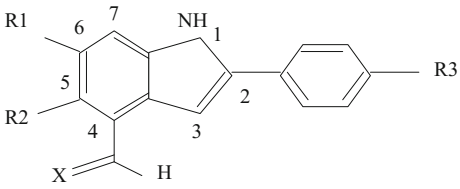



**Fig. 3.6** Molecular structure of 2-phenylindole derivatives

**Table 3.3** Reference set for 2-phenylindoles derivatives

| No | R1 | R2 | R3 | X | $IC_{50}$ (nM) |
|---|---|---|---|---|---|
| #1 | H | H | H | $C(CN)_2$ | 430 |
| #2 | H | H | $OCH_3$ | $C(CN)_2$ | 720 |
| #43 | H | H | H | O | 420 |
| #30 | H | t-Bu | $OCH_3$ | O | 280 |
| #19 | H | n-Hexyl | $CF_3$ | $C(CN)_2$ | 150 |

**Table 3.4** Reference set for 2-phenylindoles derivatives-matrix

| No | R1 | R2 | R3 | X |
|---|---|---|---|---|
| #1 | 1 | 1 | 0 | 1 |
| #2 | 1 | 1 | 1 | 1 |
| #43 | 1 | 1 | 0 | 0 |
| #30 | 1 | 0 | 1 | 0 |
| #19 | 1 | 0 | 0 | 1 |

To illustrate the selection criterion at this level we take into account that the organisms show specific biorhythms. For different regimes for organism the delivery of different 2-phenylindoles mixtures may be beneficial, and ensure increased drug efficiency.

Table 3.4 is useful for chronotherapy purposes.

Suppose that we start to apply a treatment with #43. It is a 110 compound.

In the U direction (Fig. 3.3a) we look to new digits added to 110 that is to 1101 (#1) and to 1100 (#43).

In the D direction (Fig. 3.3b) we look to less digits in the vector 110 that is to 11 (#43) and 10 (#19).

The proposal is to use a mixture #1 with #43 dyclonine for the U period of maximum activity and #19 with #43 for the D period of minimum activity. A permutation between U and D period may be tested too.

As discussed, there are several pairs of dual graded graphs that may be considered for drug delivery systems. The right pair to choose for a specific drug depends on the physiological mechanism of the drug to be tested.

Figure 3.7 shows a polytope for lifted binary and Binword trees.

The black dots "•" in Fig. 3.7 correspond to different vectors in the tree that is to different drugs or mixtures.

Implementing the polytope project starts from the direct sequence S → K1 → K2 → K3 and complements this by the reverse sequence: K3′ → K2′ → K1′ → S′.

The direct sequence corresponds to the U direction while the reverse sequence corresponds to the D direction. The switch from U-tree to D-tree is the switch from a vector to other vectors that is, from a drug or drugs mixture to another mixture and this switching may be associated to chronotherapy rhythms.

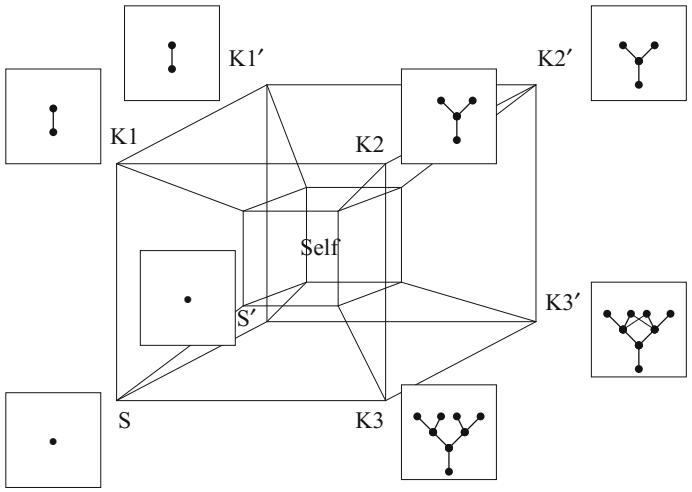



**Fig. 3.7** Polytope for lifted binary trees and Binword trees

### 3.1.4 Periodic Table of Elements

The usual periodic tables may be replaced by classification trees.

Such attempts have been proposed by Bohr as an alternative to usual chemical periodic tables (Jensen 1986).

Figure 3.8 shows a tree-like version of the periodic table. It was also named step-pyramid or Bayley-Thomsen-Bohr periodic table (Jensen 1986).

The last two rows not included in Fig. 3.8 show 32 elements from cesium, Cs to radon, Rn and 32 elements from francium Fr to ununoctium118.

The periodic table of the elements suggests that hydrogen (H) and the helium (He) could be the origin of everything else, a kind of basic blocks.

The construction principle is an evolutionary process applied to atomic species

The chemical periodic table is more close to the U-trees.

It describes the completion of energy levels by electrons step by step according to the exclusion principle.

U and D-trees for atoms are studied in nuclear physics. U corresponds to fusion while D to fission.

Figure 3.9 illustrates nucleosynthesis using tree-like description.

Figure 3.9 appears as a superposition of partially known U-tree of fusion and D-tree of fission.

The nuclear reactions are as follows (Signore and Puy 1999):

1. $n \rightarrow {}^{1}H + e + \nu$
2. ${}^{1}H + n \rightarrow {}^{2}H + \gamma$
3. ${}^{2}H + {}^{1}H \rightarrow {}^{3}He + n$

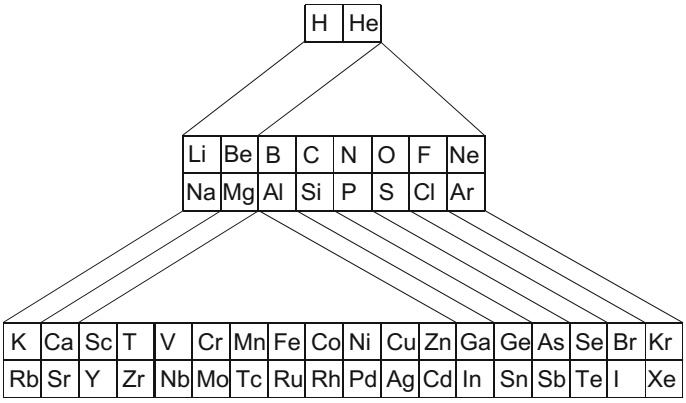



**Fig. 3.8** Tree-like version of the periodic table

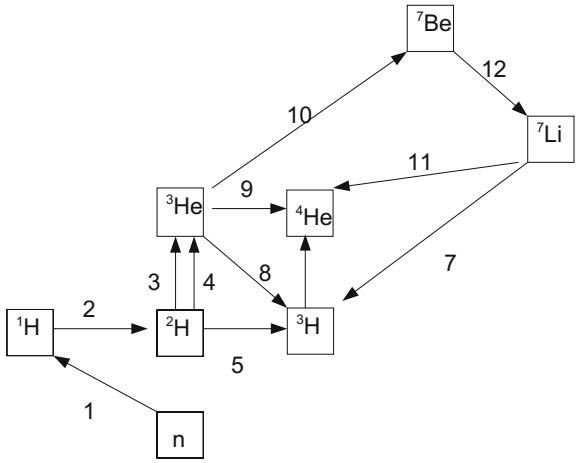



**Fig. 3.9** Trees of nucleosynthesis

4. $^{2}\mathrm{H} + {}^{2}\mathrm{H} \rightarrow {}^{3}\mathrm{He} + \mathrm{n}$
5. $^{2}\mathrm{H} + {}^{2}\mathrm{H} \rightarrow {}^{3}\mathrm{H} + {}^{1}\mathrm{H}$
6. $^{2}\mathrm{H} + {}^{3}\mathrm{H} \rightarrow {}^{4}\mathrm{He} + \mathrm{n}$
7. $^{3}\mathrm{H} + {}^{4}\mathrm{H} \rightarrow {}^{7}\mathrm{Li} + \gamma$
8. $^{3}\mathrm{He} + \mathrm{n} \rightarrow {}^{3}\mathrm{H} + {}^{1}\mathrm{H}$
9. $^{3}\mathrm{He} + {}^{2}\mathrm{H} \rightarrow {}^{4}\mathrm{He} + {}^{1}\mathrm{H}$
10. $^{3}\mathrm{He} + {}^{4}\mathrm{He} \rightarrow {}^{7}\mathrm{Be} + \gamma$
11. $^{7}\mathrm{Li} + {}^{1}\mathrm{H} \rightarrow {}^{4}\mathrm{He} + {}^{4}\mathrm{He}$
12. $^{7}\mathrm{Be} + \mathrm{n} \rightarrow {}^{7}\mathrm{Li} + {}^{1}\mathrm{H}$

## 3.2 Reaction Networks

### *3.2.1 Chemical Reaction Networks*

Reaction networks are viewed as derived from ordinary molecular structures related in reactant-product pairs so as to manifest a chemical super-structure. Such superstructures are candidates for applications in combinatorial chemistry. Notable characterization of a reaction superstructure occurs when such reaction graphs are directed, as for example when there is progressive substitution or addition on a fixed molecular skeleton. Such a set of partially ordered entities is a poset which further manifests a number of special properties, as then might be utilized in different applications (Klein 1986; Klein and Bytautas 2000; Klein et al. 2008).

Focus on the overall super-structural poset goes beyond ordinary molecular structure and brings an extra dimension to conventional stereo-chemical theory. The possibility that different molecular properties vary smoothly along chains of

interconnections in such a superstructure is a natural assumption for a novel approach to molecular property and bioactivity correlations. Different manners to interpolate/extrapolate on a poset network yield quantitative super-structure/activity relationships with some numerical fits, for instance, for properties of polychlorinated biphenyls seemingly being satisfactory. There seems to be perspectives for combinatorial approach (Ivanciuc et al. 2005; Bruggemann and Restrepo 2013).

### *3.2.2 Azines*

Predictive schemas based on similarity comparisons to the corresponding activities of related structures were used for azines characterization (Panda 2013).

The azines have been derived from successive substitution of the ring –CH– of benzene by N atoms.

The special superstructure considered is a substitution-reaction network, which for the N of the benzene-like skeleton appears as in Fig. 3.10. Starting from an unsubstituted compound, N substituents are progressively introduced one after another, with earlier substituents fixed at their different possible positions. When substituents are N atoms, the diagram starts with benzene and ends with hexa-N-benzene, while all the different patterns of substitution occur in between.

Figure 3.11 summarizes the substitution reactions.

N atoms have been indicated by dots and double bonds have been omitted.

The weights indicated on the connections between two compounds show the number of ways we can obtain by one from another in (up, down) direction of the network.

Figure 3.12 illustrates the commutation relation for substitution reactions.

Commutation relations have been introduced in the study of differential posets (Stanley 1988, 1990.

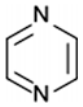
In the polytopic frame, atoms associated to the level K0, chemical molecules are associated to K1, while chemical reaction networks to K2.

K3 corresponds to interaction of reaction networks or in other words to super superstructures.

We can identify:

- S(K0)-Atoms
- K1-Molecules
- K2-Reaction Networks
- K3-Networks of Reaction Networks

**Fig. 3.10** Pyrazine



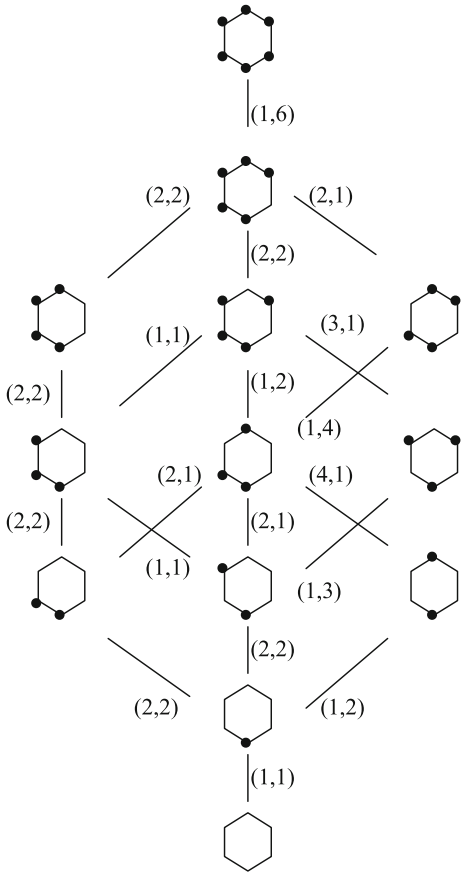



**Fig. 3.11** Azines substitution reactions

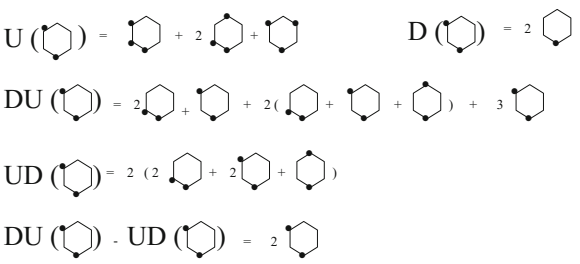



**Fig. 3.12** Commutation relation for azines substitution reactions

The direct sequence describes successive substitution of the ring –CH– of benzene by N atoms while the reverse sequence describes the reverse process. This doesn't imply reversibility of all the involved chemical reactions.

The Self should coordinate the interaction of the substitution networks with the reverse substitution networks in duality relation.

### 3.2.3 *Hemoglobin Oxygenation*

Figure 3.13 shows the addition-reaction poset for oxygenation of hemoglobin (Ackers and Doyle 1992; Edelstein 1996).

Hemoglobin has two symmetric conformational state T and R. T is denoted by a square R by a circle in Fig. 3.13. An x shows the inclusion of oxygen.

The weights indicated on the connections between two states show the number of ways we can obtain by one from another in (up, down) direction of the network.

A simpler reaction network is that involved with the oxygenation of hemoglobin —where oxygen $O_2$ molecules may be adsorbed to any one, or more, of the four component myoglobin units (Dickerson and Geis 1969; Klein et al. 2008).

Figure 3.14 shows another addition-reaction poset for oxygenation of hemoglobin.

Here the great bulk of the structure of the myoglobin unit is suppressed to retain the skeletal framework of the appropriate symmetries.

The weights indicated on the connections between two structures show the number of ways we can obtain one from another in (up, down) direction.

With the summary diagram of Fig. 3.14, each position displayed there may be interpreted as entailing a mix of conformations.

Figure 3.15 illustrates the commutation condition for hemoglobin oxidation.

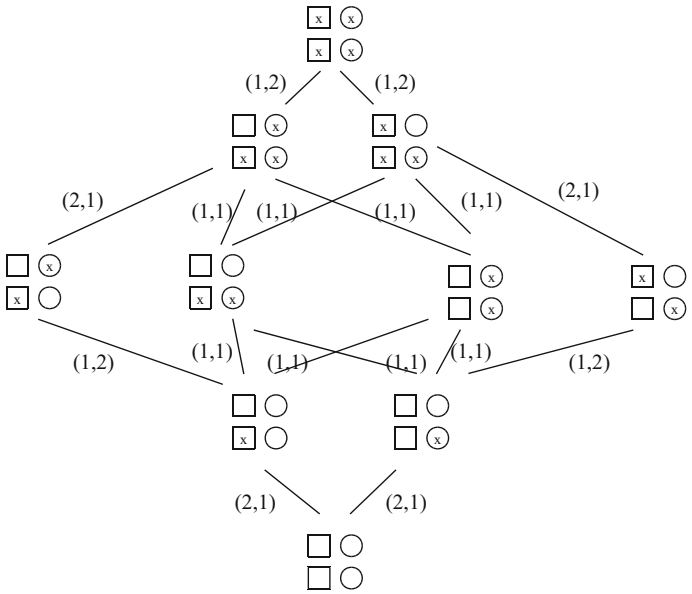



**Fig. 3.13** Oxygenation of hemoglobin

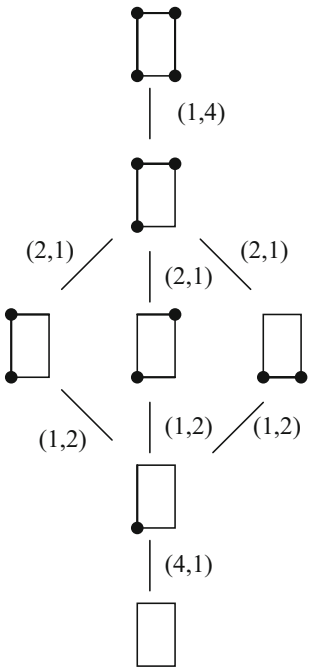



**Fig. 3.14** Addition-reaction poset for oxygenation of hemoglobin

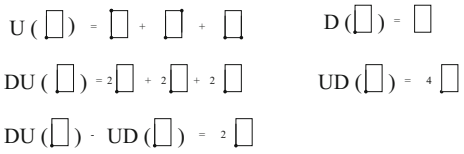


**Fig. 3.15** Commutation condition for hemoglobin oxidation

## *3.2.4 Adsorption of Polar Species*

The adsorption of polar species at the surface of a cell or micelle is illustrated in Fig. 3.16 (Klein and Bytautas 2000).

The species may be adsorbed with either their (+) or (−) end directed to the micelle, indicated here as an arrow. In Fig. 3.16 the four arrows indicate the orientations of each of the adsorbents on the surface.

Up and down steps on the lattice shown in Fig. 3.16, denoted by U and D, trajectories describe the steps in the orientation of adsorbents.

The commutation condition is of interest since it can be correlated to the adsorption environment. Observe that:

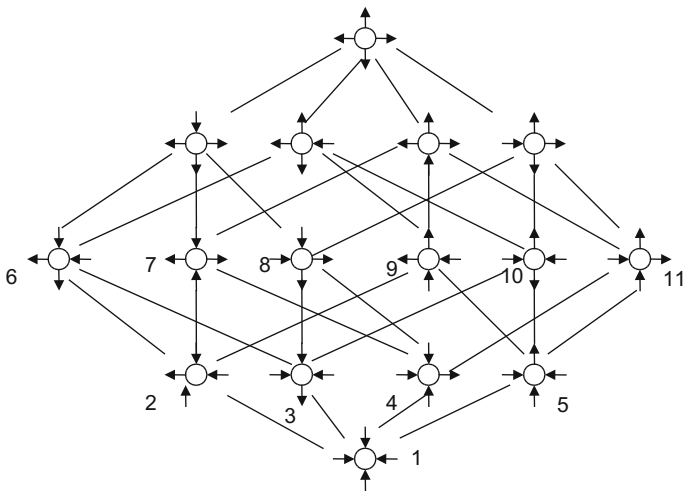



**Fig. 3.16** Orientation of adsorbents on the micelle surface

$$\mathrm{U}(3) = 6 + 8 + 10 : \mathrm{D}(3) = 1 \tag{3.1}$$

$$\mathrm{DU}(3) = \mathrm{D}(6 + 8 + 10) = 2 + 3 + 3 + 4 + 3 + 5 \tag{3.2}$$

$$\mathrm{UD}(3) = \mathrm{U}(1) = 2 + 3 + 4 + 5 \tag{3.3}$$

$$(\mathrm{DU} - \mathrm{UD})(3) = 2 \times 3 \tag{3.4}$$

This calculus illustrates the commutation condition for the lattice of adsorbents orientation (Appendix A).

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# Chapter 4
# Conditioned Walks

## 4.1 Restricted Permutations

### *4.1.1 Placements and Packing*

Floor plan design is an important step in physical design of very large scale integration VLSI circuits. It is the problem of placing a set of circuit modules on a chip to minimize total area and interconnection cost. In the early stage of physical design, most of the modules are not yet designed and thus are flexible in shape and are free to move (Young et al. 1999; Shen and Chu 2003).

The packing design is based on restricted permutations.

Figure 4.1 justifies the term of restricted permutations. Figure 4.1a illustrates why starting from 2 and avoiding the central shadowed cell we need to forbid the (41) line. The associated notation is: 2(41)3. Figure 4.1b illustrates why starting from 3 and avoiding the central cell we need to forbid the (14) line. The associated notation is: 3(14)2.

The standardization word std (u) is the unique permutation having the same inversions as the word, u. A permutation $\sigma$ is a Baxter permutation if for any subword $u = u_1u_2u_3u_4$ of $\sigma$ such that the letters $u_2$ and $u_3$ are adjacent in $\sigma$, std (u) is not 2413 or 3142. In other words $\sigma$ is a Baxter permutation if it avoids the generalized permutation patterns 2(41)3 and 3(14)2 (Babson and Steingrımsson 2000).

Baxter permutations are useful in the study of combinatorial objects as rectangular partitions, twin binary trees, and planar bipolar orientations (Ackerman et al. 2004; Duluck and Guibert 1996, 1998; Bonichon et al. 2010).

Hopf algebras have been introduced in combinatorics to encode the disassembling (coproduct) and assembling (product) of combinatorial objects.

The relation between dual graded graphs, Hopf algebras and restricted permutations is of interest for packing and placement studies (Fomin 1994; Giraudo 2011, 2012).



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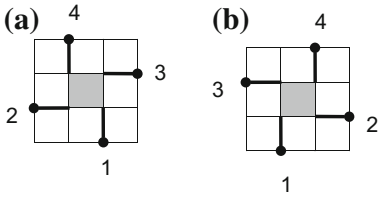



**Fig. 4.1** Restricted permutations

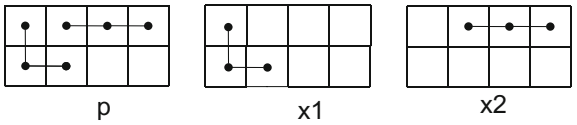



**Fig. 4.2** Placements

As a first example we consider the placements problems that appear in the study of puzzles and circuits (Joni and Rota 1979).

Figure 4.2 illustrates the placements of circuits.

Several flat pieces or circuits are to be assembled into a required form for example a rectangle of shape $2 \times 3$ as shown in Fig. 4.2. The board is a $2 \times 3$ rectangle. There are 2 pieces each formed by tree dots in Fig. 4.2.

A placement of some of the pieces on the board is a subset of the board obtained by placing some of the pieces on the board without overlapping. Two placements covering the same squares by distinct set of pieces or by pieces placed in different positions are considered to be different. The pieces in a placement need not be adjacent. To every placement p, specified by the occupied squares and the position of the pieces we associate a variable x(p) and we denote by V the free module over the integers spanned by the variables x(p) and the variable 1, which denotes the trivial placement of no pieces.

We need to define the comultiplication on the module V. The definition of comultiplication is in fact a natural rendering of the combinatorial operation of cutting up an object into a set of pieces.

If p and q are placements we say that q is a sub-placement of p if the pieces used in q are a sub-multiset of the pieces in p, and they are placed in the same positions.

There is a partial ordering of placements.

For any placement p, let us list all the pairs (q, r) such that:

- q and r are sub-placements of p
- q and r do not overlap
- the union of q and r is the placement p

The coproduct is defined as:

$$\Delta x(p) = \sum x(q) \otimes x(r) \tag{4.1}$$

Here the sum ranges for all such pairs. For example if p, x1 and x2 are the placements shown in Fig. 4.2 then:

$$\Delta x(p) = 1 \otimes x(p) + x1 \otimes x2 + x2 \otimes x1 + x(p) \otimes 1 \tag{4.2}$$

The comultiplication is co-associative. The counit $\varepsilon$ is defined by:

$$\varepsilon(1) = 1; \quad \varepsilon x(p) = 0 \text{ for all } \quad x(p) \neq 1 \tag{4.3}$$

Another example concerns the problem of feeling a surface by pair of non-interacting circuits (Giraudo 2011, 2012; Iordache 2013).

Figure 4.3 illustrates the relation between twin trees and surface packing in the up U direction. The circuits with filled circles and that with unfilled circles should not interact.

The top of Fig. 4.3 refers to surface containing $6 \times 3$ cells. The 3 dots and 3 circles correspond to components to be interconnected as twins.

Obviously we need to consider at lower levels surfaces with $4 \times 2$ cells and $2 \times 1$ cells.

For U-graph, each twin develops in a half of the $2 \times 1$, $4 \times 2$, $6 \times 3$ available surfaces by addition of new dots or circles.

Figure 4.4 illustrates the relation between twin trees and surface packing in the down D direction.

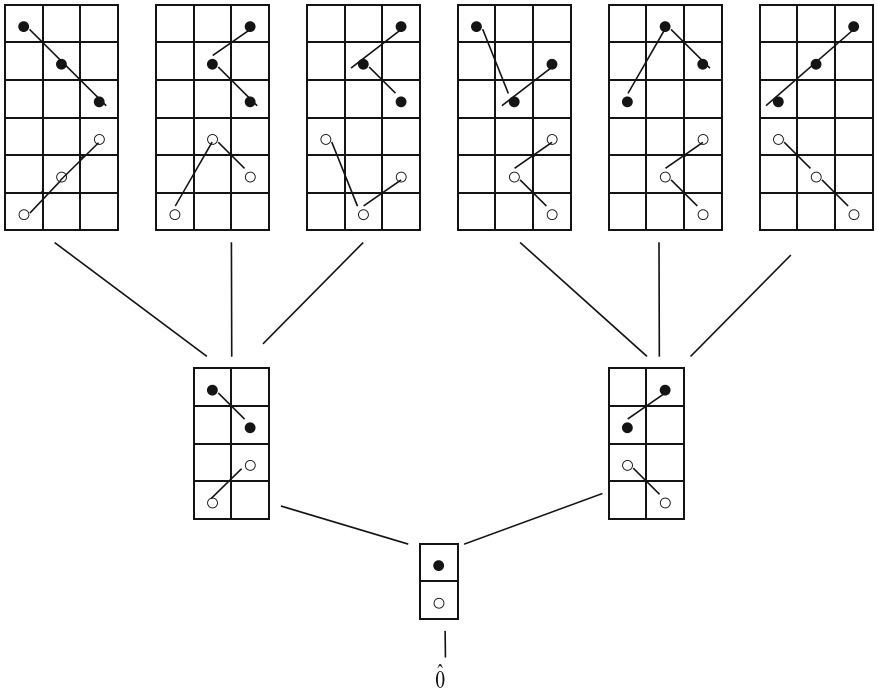



**Fig. 4.3** Twin trees and packing U-graph

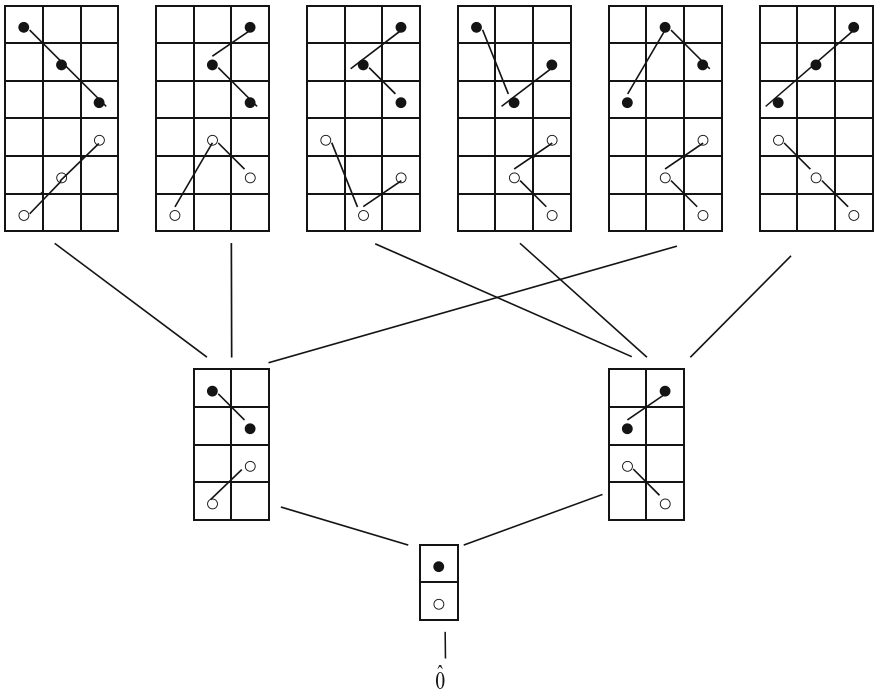



**Fig. 4.4** Twin trees and packing D-graph

For D-graph each twin decreases in a half of the $6 \times 3$, $4 \times 2$, $2 \times 1$ available surfaces by deletion of dots or circles.

Figure 4.5 shows in a simplified form the U-graph for packing.

Figure 4.6 shows in a simplified form the D-graph for packing.

One interesting direction in component integration is to make the system as compact as possible, to couple the divergent packing stages described by U-graphs to convergent unpacking stages described by D.

Figure 4.7 shows the polytope for packing.

The black dots "•" in Fig. 4.7 correspond to pairs of twin trees allowing different packing.

Implementing the polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

The direct sequence corresponds to the U direction while the reverse sequence corresponds to the D direction.

The interaction between the dual directions should be coordinated by the Self.

Pairs of twin binary trees, rectangular partitions, planar bipolar orientations and many other combinatorial objects may be studied in this general framework.

Nzeutchap (2006) conjectured that to each pair of dual graded graphs, there is a pair of dual Hopf algebras that may be associated.

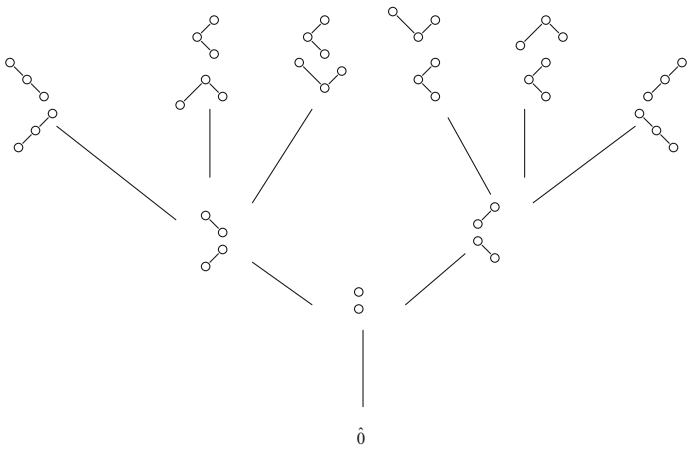



**Fig. 4.5** U-graph for packing

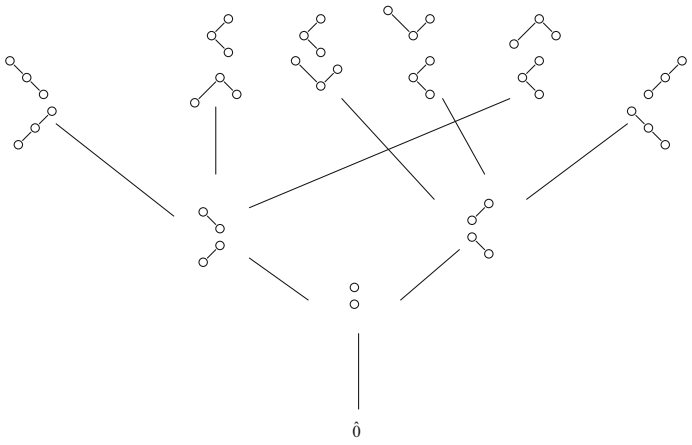



**Fig. 4.6** D-graph for packing

The Hopf algebras and the dual graded graphs for twin binary trees were studied by Giraudo (2011, 2012).

### *4.1.2 Templating and Twin Trees*

An intensively studied area of reversible chemical reactions under thermodynamic control is the dynamic combinatorial chemistry, due to its many possible applications, including drug discovery and advanced functional materials (Lehn 1999, 2002).

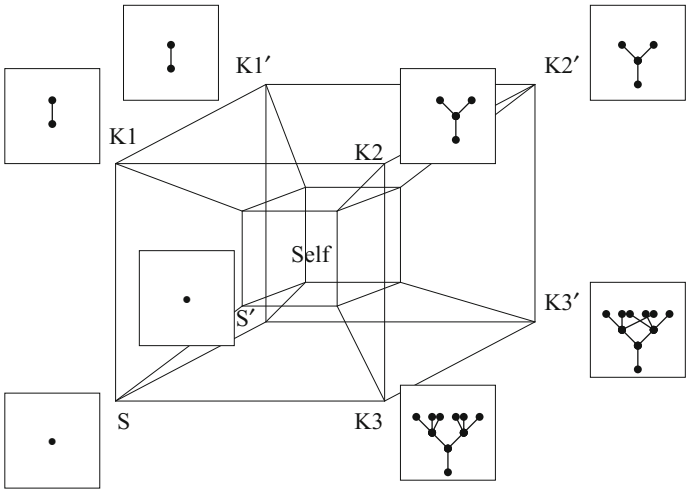



**Fig. 4.7** Polytope for packing

A dynamic combinatorial library (DCL) of products is formed when a mixture of compounds react with one another under thermodynamic control. The products in the library can be constructed from covalent or non-covalent interactions. The composition of the DCL depends on the thermodynamic stability of each of the products. Therefore it is possible to alter the distribution of products if the system is subjected to external influences that alter the relative free energies.

The "lock and key" approach is useful to explain the manipulation of a DCL.

When a library is established, a guest or host template molecule can be added that binds selectively through non-covalent interactions to one particular product. The removal of this product results in a shift in the equilibrium. According to the principle of Le Chatelier, the system restores itself to equilibrium by replacing the removed product which is again removed by the presence of the template. The process continues and the system is exhausted of monomers.

Figure 4.8 shows a schematic representation of thermodynamic templating.

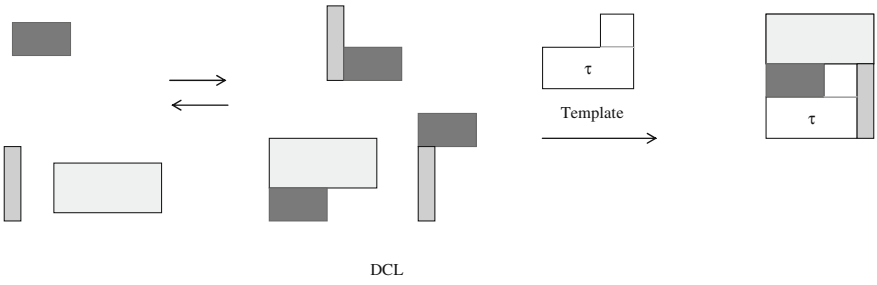



**Fig. 4.8** Thermodynamic templating

Molecules of different shapes form the DCL. The template is denoted by τ. The DCL is amplified towards one particular product when a template acts as a host or a guest to selectively remove that product from the mixture.

A number of functional groups, including esters, borate esters, disulfides, hydrazones, imines, oximes and alkenes are employed in dynamic covalent chemistry (Lehn 1999, 2002).

Figure 4.9 shows the twin trees resulting by templating of τ.

This illustrates the templating in media with restricted mobility as gels or solid solutions for example. In an oriented field, the templating of τ may be done by attachments in down or left direction as the first tree shows in Fig. 4.9 or in up or right direction as the 2nd tree shows in Fig. 4.9. Twin trees corresponding will result (Dulucq and Guibert 1998; Yao et al. 2003). The field generating the two orientations may be electric, magnetic, gravitational, thermal and so on (Hulliger et al. 2000, Pham et al. 2015).

Figure 4.9 refers to the order ABCDFE with D playing the role of the template τ.

The template τ may be included or not by the twin trees.

Suppose that the construction starts from C. Attachments may be left to B or down to E.

From B the attachment goes left to A while from E goes left to τ and then down to F.

Suppose that the construction starts from F. Attachments may be up to A or right to E.

From A the attachment goes right to τ then up to B and right to C.

To obtain the augmented binary tree to each node we add a left child node with label "0" if the node has no left child and a right child node with label "1" if it has no right child. The first bit encountered is always "0" and the last bit encountered is always "1". Therefore we ignore these two bits in labeling a binary tree.

The trees shown in Fig. 4.9 are labeled as 11001 and 00110.

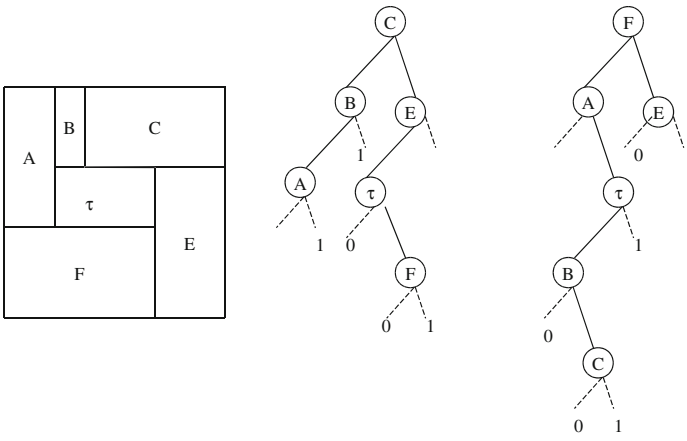



**Fig. 4.9** Twin trees by templating

Observe that the twin trees are identical only as basic modules as A, B, C and so on and only in the final form. Considered as molecules the twins may differ as molecular mass since the bridges between the basic modules may be different.

They differ as history of developments. This kind of twin trees is of interest for advanced functional materials and smart materials (Hulliger et al. 2000; Pham et al. 2015).

Also this may be important for drugs since in most cases the building molecular blocks or radicals are more significant for drug activity than the bridges between blocks.

The building blocks geometric distribution may be another variable for drug activity as significant as chirality.

Supramolecular chemistry offer more opportunities for twin trees via templating.

Templating and bipolar orientations allows obtain compounds with the same basic modules composition but with different history of interrelations between components.

## 4.2 Self-Avoiding Walks

### *4.2.1 Folding and Meanders*

Folded structures may be of different origins like physical, chemical or mathematical (Cheung et al. 2011).

Folding has an important place in polymer chemistry. It is a simple elementary transformation allowing for changes in the conformation of long linear molecules.

It may be viewed as a particular realization of self-avoiding walks. Typically one considers a chain made of n identical constituents, which is folded onto itself with the spatial constraint that constituents should not interpenetrate. The image is that of a folded strip of n stamps. The combinatorial problem of enumerating all the compact foldings of a closed polymer chain happens to be equivalent to that of enumerating meanders that is configurations of a closed road crossing a river through n bridges (Di Francesco et al. 1997a, b).

The meander problem is one of these fundamental combinatorial problems with a simple formulation, which resist the repeated attempts to completely solve them. This is due to the long-range memory involvement in any folding problem. Folding involves non-Markovian processes.

The compact folding problem of a polymer chain was studied by Di Francesco et al. (1997a). A long closed polymer chain of say 2n identical monomers was considered. The question was to count the different ways of folding the whole chain onto itself, forbidding interpenetration of monomers. By compact folding, we mean that all the monomers are packed on top of each other. Accordingly, folding appears as a simple realization of objects with self-avoiding constraints. The image of the folding of a closed strip of 2n stamps is that of all stamps piled up on top of each other.

The equivalence between this folding problem and the meander problem is obvious. Drawing a line (river) across the 2n constituents (bridges) of the folded polymer, and pulling them apart, produces a meander of order n. The folding of a closed polymer chain and the meander problem are therefore identical. By analogy, we were led to define the meander counterpart of the folding problem of an open polymer chain, the so-called semi-meanders. The latter are defined in the same way as meanders, except that the river is now semi-infinite, that is, it has a source, around which the semi-meander is allowed to wind freely.

Di Francesco et al. (1997b) studied the meander and semi-meander problems in the framework of the Temperley-Lieb algebra. This study is based on a one-to-one correspondence between multi-component semi-meanders and reduced elements of the Temperley-Lieb algebra.

Legendre (2014) reviewed the stamp folding problem, the number of ways to fold a strip of n stamps, and the related problem of enumerating meander configurations.

The study of equivalence classes of foldings and meanders under symmetries allows to characterizing and enumerating folding and meander shapes.

It is assumed that the stamps are labeled 1, ... , n, consecutively along the unfolded strip. The strip is folded into a stack, one stamp wide and n stamps tall, where the horizontal segments represent the stamps, whereas the vertical segments represent the perforations. Stamps are numbered the same on both sides, so that it does not matter which side is up in the final packet.

Let Tn denote the set of folding of n stamps, where we regard two foldings to be the same whenever they are reflections of one another over a vertical line, the stamps being stacked up as in Fig. 4.10.

Figure 4.10 shows the 16 foldings of 4 labeled stamps constituting the set T4 (Legendre 2014). Observe that any folding can be represented by a permutation by listing the labels of the stamps from top to bottom. We identify a folding with its associated element in the set of permutations Sn, so that a permutation pertaining to a folding is called a folding. For example, the permutation (1324) is not a folding because a crossing occurs.

The set Tn of foldings of n labeled stamps can be portioned into r(n) disjoint orbits of size n under the action of the circular permutation C = (23 … n1). The set Rn, the n-folding with leaf 1 on top is the set of representatives of the orbits of C in Tn.

The foldings in the first column of Fig. 4.10 constitutes the set R4.

The set Rn can be constructed inductively using a tree of n levels deep as shown in Fig. 4.11. Figure 4.11 shows elements of the tree describing the set Rn.

The root of tree, at the level 1, is the folding constituted of a single leaf. Level n of the tree describes Rn and comprises r(n) nodes. To each folding at the level n, a leaf labeled n + 1 is appended to leaf n. The new leaf is inserted in any possible position with the constraint that leaf 1 must stay on top, leading to all descendant nodes.

Figure 4.11 illustrates the tree of foldings.

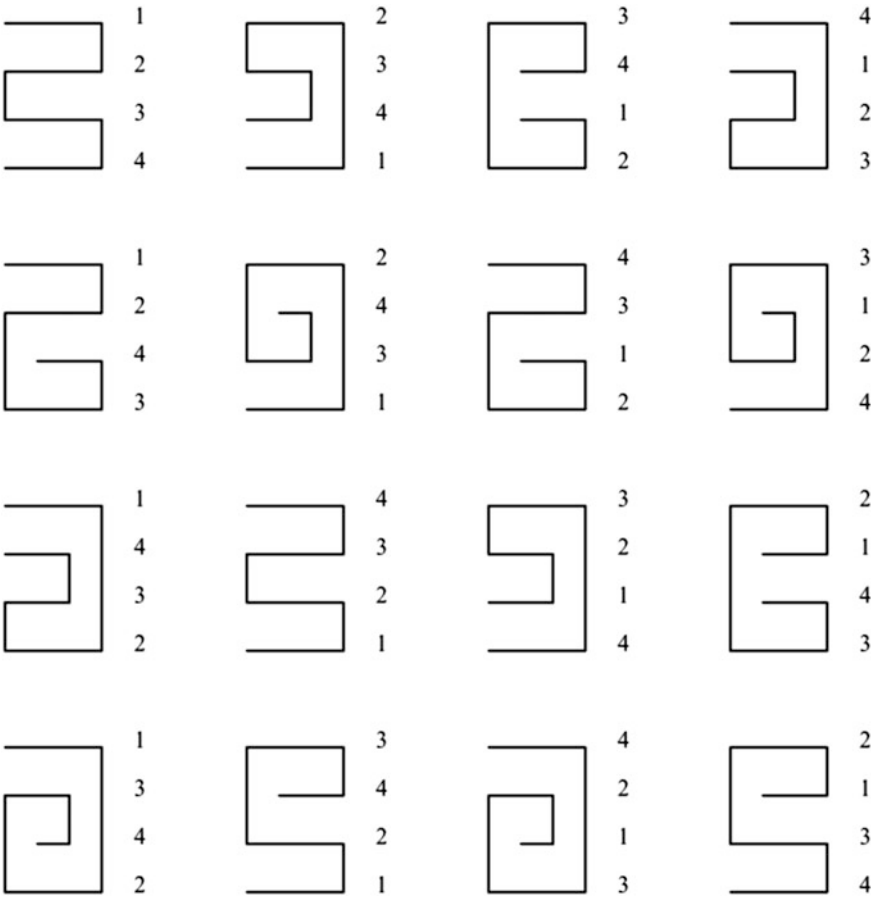



**Fig. 4.10** The foldings of 4 labeled stamps

It shows the sets Rn. At a given level of the tree, each folding in the left sub-tree can be paired uniquely with a folding in the right sub-tree by keeping leaf 1 in place and rotating the leaves around leaf 2.

### *4.2.2 Self-Avoiding Polygons*

The problem of self-avoiding walks is one of simplicity of definition hiding difficulty of solution.

The problem was introduced by theoretical chemists as a model of a polymer in a dilute solution. It became a combinatorial model for of phase transition of interest for mathematical physicists (Guttman 2012; Beaton et al. 2012).

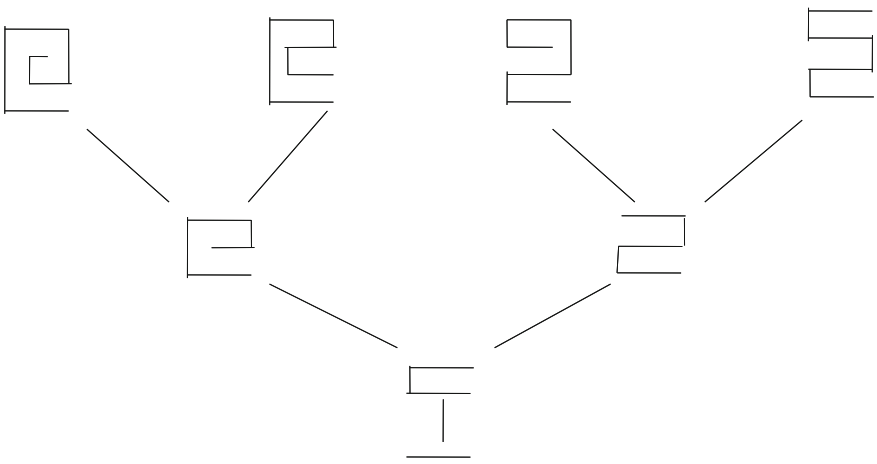


**Fig. 4.11** Tree of foldings

Figure 4.12 shows a self-avoiding walk on the square lattice.

If the end-point of a self-avoiding walk is adjacent to the origin, an additional step joining the end-point to the origin will produce self-avoiding circuits or self-avoiding polymers.

If we ignore the knowledge of the origin and distinguish circuits only by shape, we refer to self-avoiding polygons (Zhao 2014).

Figure 4.13 shows some of the 8-sided polygons on the square lattice.

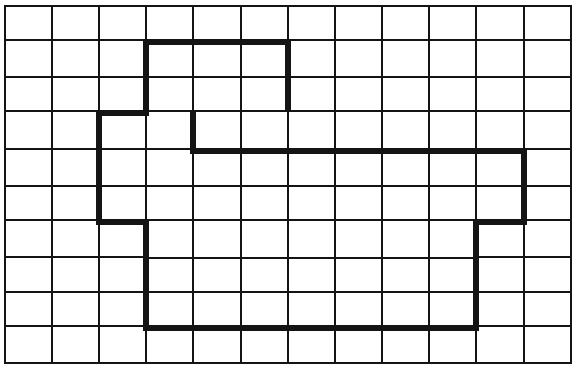
Self-avoiding polygons may be constructed by edge insertion as shown in Fig. 4.14.

Figure 4.14 illustrates the insertion of parallel edges. There are eight ways of inserting parallel edges into the basic shape square. In fact there are two different outcomes as we ignore the duplicates ones.

The generating graph of self-avoiding polygons is shown in Fig. 4.15.

The Hopf algebra of self-avoiding polygons was studied by Zhao (2014).

**Fig. 4.12** Self-avoiding walk



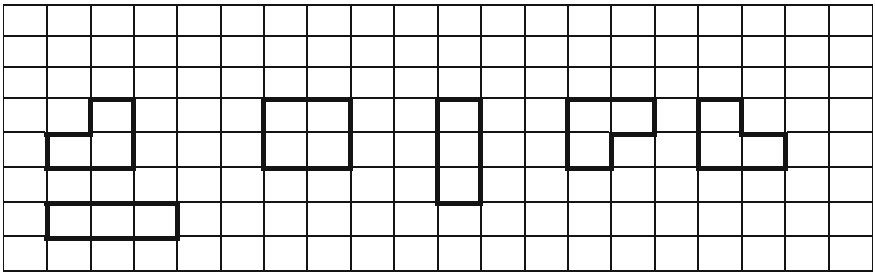


**Fig. 4.13** Self-avoiding polygons

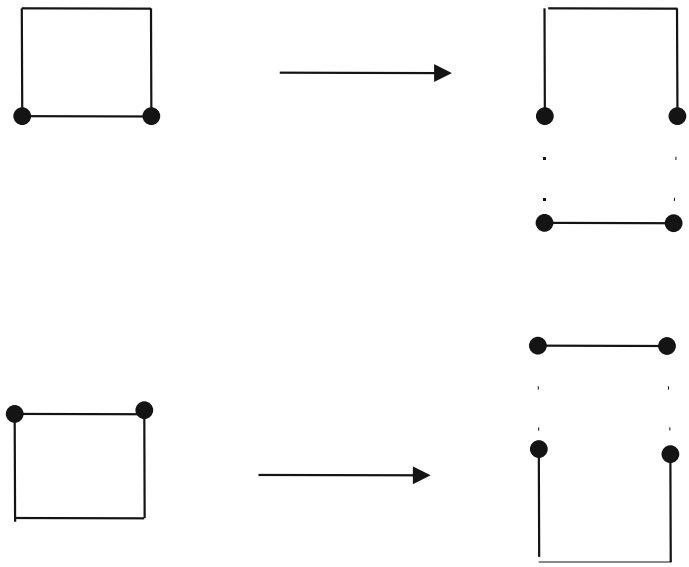


**Fig. 4.14** Inserting parallel edges

We can consider the product $\nabla$ as a disjoint union (Sweedler 1969, Appendix B).

Zhao (2014) defined two coproducts, corresponding to admissible vertical cuts and admissible horizontal cuts.

Figure 4.16 shows an example of coproduct $\Delta_w$ for admissible vertical cuts.

Figure 4.17 shows an example of coproduct $\Delta_w$ for admissible horizontal cuts.

For both types of cuts Hopf algebras of self-avoiding polygons are resulting.

These two Hopf algebras capture some properties of the generating process and are significant if we have to build a modular construction vertically or horizontally.

If we limit the graph generation to the basic bricks $2 \times 1$ or $1 \times 2$ the generated tree is a 2-differential Young lattice is shown in Fig. 4.18 (Shimozono and White 2001; Bishop and Killpatrick 2007).

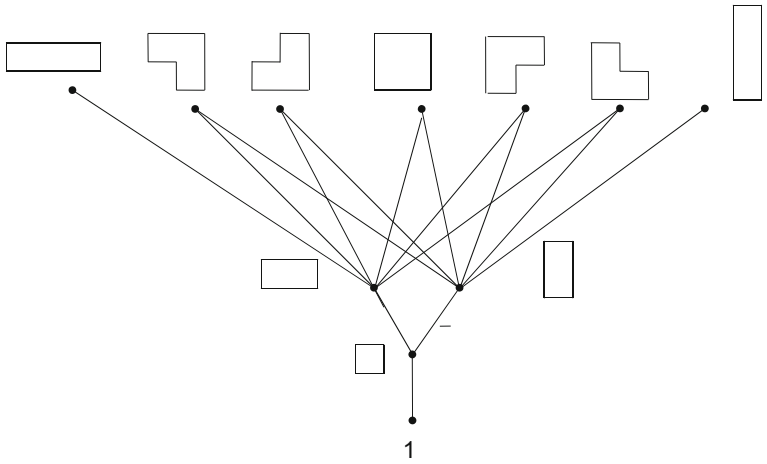



**Fig. 4.15** Tree of self-avoiding polygons

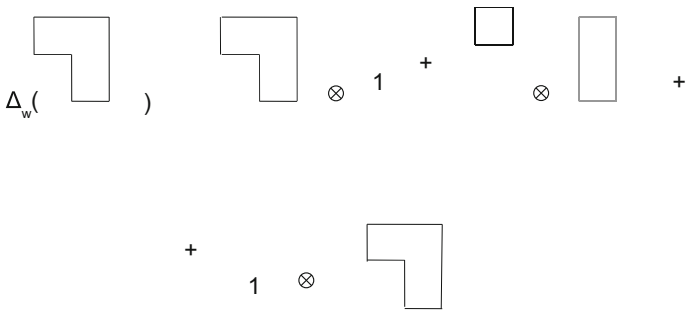



**Fig. 4.16** Coproduct for vertical cuts

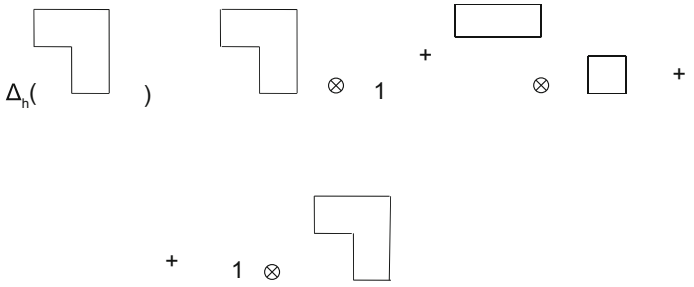



**Fig. 4.17** Coproduct for horizontal cuts

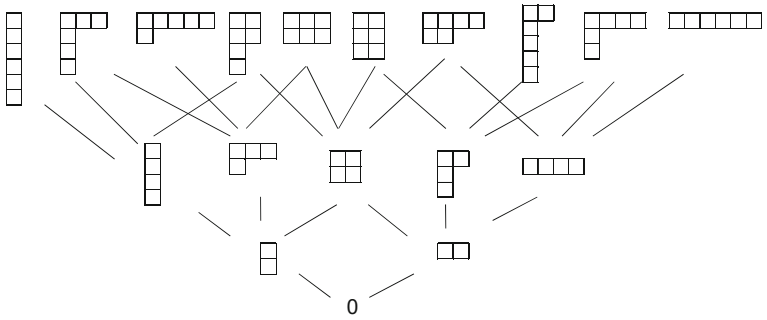



**Fig. 4.18** A 2-differential Young lattice

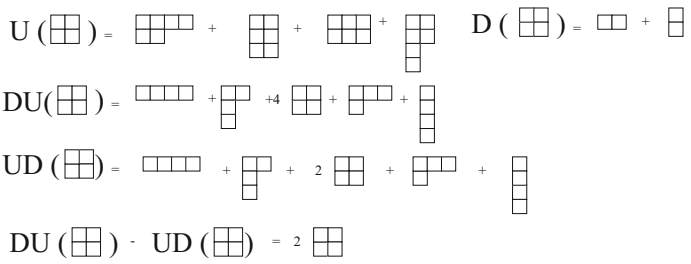



**Fig. 4.19** Commutation condition for 2-differential Young lattice

Figure 4.19 illustrates the commutation condition for the 2-differential Young lattice.

In this case r = 2 (Appendix A).

With molecules represented as graphs it is natural to view chemical reactions as rewriting rules applied to molecular graphs (Benkö et al. 2003).

A chemical reaction is a breaking, forming and changing of bonds. The conservation rules and valence rules can be imposed on rewriting rules to take into account that the chemical reactions are stoichiometric.

Figure 4.20 illustrates graph rewriting rule (top) and graph rewriting steps a, b, c (bottom).

The host graph is shown in Fig. 4.20a. A left graph is resulting and this evolves towards the right graph according to the graph rewriting rule. This is shown on the top of Fig. 4.20.

Then the right graph is reattached to the active radical as shown in Fig. 4.20b, c.

Benkö et al. (2003) studied the generic properties of chemical networks and proposed an artificial chemistry model based on graph rewriting. The simulation of unimolecular reactions is a direct application of rewrite rule to a molecule.

Behr et al. (2016) described graph rewriting in the frame of combinatorial Hopf algebras.

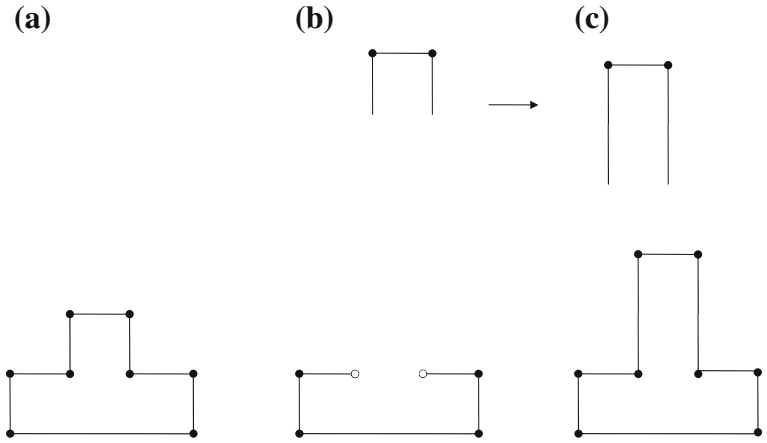



**Fig. 4.20** Graph rewriting

Motivated by the desire to understand the combinatorics of graph rewriting systems a formulation of graph rewriting itself that is based on the concept of diagrammatic combinatorial Hopf algebras was proposed.

The classical example of the Heisenberg-Weyl algebra of creation and annihilation of indistinguishable particles can alternatively be interpreted as the algebra of discrete graph rewriting. To pass from the special case of discrete graph rewriting to the case of general graph rewriting required every aspect of the framework of diagrammatic combinatorial Hopf algebras as a guideline for the construction.

The study of conditioned walk in random conditions is a more recent domain of interest.

This concerns stochastic processes the context of combinatorial Hopf algebras (Diaconis et al. 2014; Pang 20014).

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# Chapter 5
# Assembling and Configuring

## 5.1 Self-assembling

### *5.1.1 Self-assembly of Tiles*

Self-organization refers to pattern-formation processes via interactions among similar components or events internal to a given system without external influences. In this way, organization emerges at the global level as a result of local information exchanged among the constituents of the system. The achieved patterns or self-organized structures are the collection of entities arranged due to cascades of iterative interactions across space and time where complexity unfolds progressively (Drees et al. 2012).

The main differences among physical, chemical, biological or cognitive self-organizing systems lie in the complexity of their components and their governing laws.

For instance, entities of biological systems like the cell are far more complex than physical elements such as crystals. At the physical or chemical level, only physical laws govern the system whilst in biological systems genetically controlled components that is information processing, are also influencing the behavioral interactions among the living entities.

The way in which components interact is critical to understand how self-organization works in numerous systems. Two important mechanisms of interaction are positive feedback and negative feedback. The former takes an initial change in a system and reinforces it in the same direction as the initial deviation. In contrast, negative feedback reinforces changes in the opposite direction thus breaking and shaping the process, and hence inhibiting any positive feedback process that may be at work. Positive and negative feedback corresponds to



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Studies in Systems, Decision and Control 92,
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construction and deconstruction allowing self-organization. The connection with Hopf algebra is understandable. Roughly speaking a Hopf algebra is both an algebra and the dual of an algebra, the coalgebra, which are compatible (Joni and Rota 1979; Hivert 2005). There is a product rule which describes construction, composing or assembling the objects and a coproduct rule which describes deconstruction, decomposing or disassembling (Blasiak 2010).

Self-organization in many systems also arises from multiple interactions among individuals transferring information via signals.

Weak chemical bonds are useful to design and grow self-assembled nanostructures. Under thermodynamic equilibrium molecules assemble using several types of non-covalent intermolecular interactions, for example hydrogen or ionic bounds, and evolve into relatively stable structures.

DNA assembly employs complementarity and hydrogen bonding for molecular self-organization by weak bonding.

Several major experimental developments make use of DNA for constructing nanostructures, for information processing and as a material for nanotechnology. Adleman (1994) proposed an approach to information processing with bioprocesses that allowed solving combinatorial problems by making use of specific set of DNA molecules.

DNA-based computing consists of four basic operations: encoding, hybridization, ligation and extraction. Problem solutions are obtained through an exhaustive parallel search by means of the pattern recognition intrinsic to DNA hybridization that is to self-construction of complementary DNA strands. Involved chemical reactions such as the activity of restriction enzymes, ligases polymerases or simple hybridization can operate in parallel and this explains the possibility to solve complex problems by DNA-based computing.

Cellular automata architectures describing DNA self-constructed circuit patterns for various forms of DNA tiles have been studied by Winfree (2000).

DNA self-assembly using rigid square tiles have been studied prevalently.

However it was observed that the tilling need to be flexible and the tiles should be recycled through alternating assembly and disassembly stages. The self-construction and reconstruction operation may be programmable using both glued and un-glued tiles (Carbone and Seeman 2002).

Interesting models have been devoted to the study of self-assembly of flexible tiles (Jonoska et al. 2011).

The models using flexible junction molecules are based on DNA branched junction molecules with flexible arms extended to free sticky ends.

Sticky end types a, b, c, a̲, b̲, c̲ and so on are different types of un-adjoined arms sticking off of molecules. Two sticky ends which are able to adjoin such as those of type a, and underlined a, are known as complementary sticky ends.

A tile type represents a branched junction molecule with a certain arrangement of sticky end branches.

An edge formed by joining two complementary sticky ends is called a bond-edge type.

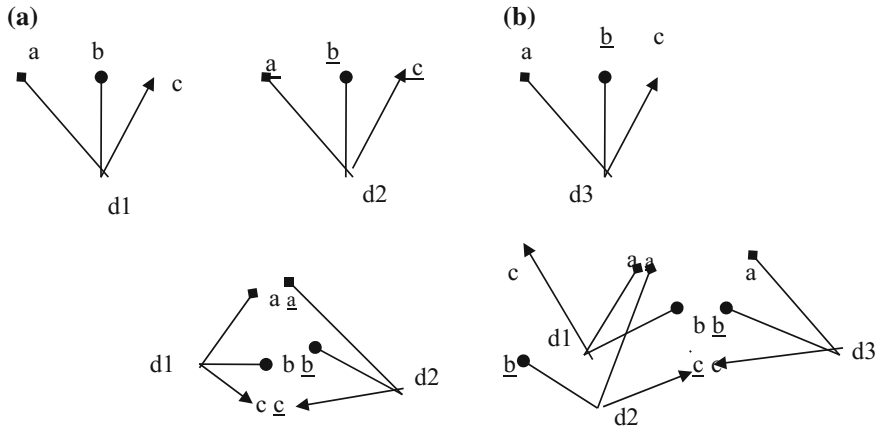


**Fig. 5.1** Tiles and complexes

A pot type P is a set of tiles such that for any sticky end type a on a tile in P, the complementary sticky end of type $\underline{a}$ also exists on some tile in P.

A complex is an arrangement of tiles from a pot type P with as many adjoined complementary sticky ends as possible with the given tiles.

A complete complex has no un-adjoined sticky ends hanging off of itself.

For this model a problem to solve is encoded in tiles and a solution of the problem is obtained if and only if a complete complex, that is a complex without sticky ends, can assemble.

The principle of tiling is illustrated in Fig. 5.1 (Jonoska and McColm 2000).

Three compounds may exists in two complementary forms, a, b, c and $\underline{a}$, $\underline{b}$, $\underline{c}$.

Three tiles are considered here. They are denoted, d1, d2, d3.

A complete complex (a) and an incomplete complex (b) are represented in Fig. 5.1 (bottom).

Between trees, several interactions may arrive at the next level of assembling.

The process of flexible assembly is illustrated in Fig. 5.2. For any radical as a, b or c compound having the complements $\underline{a}$, $\underline{b}$, or $\underline{c}$, are involved. Tiles are denoted, d1, d2, d3 and d4.

Coupling of complementary pairs is incomplete and some radicals remains free.

However, the incomplete complexes may interact at higher levels of tiling.

This corresponds to the computing task.

Figure 5.2 describes the tiling in the upward direction. The resulting U-tree takes an initial construction in the system and reinforces it in the same direction as the initial construction. The D-tree would reinforce changes in the opposite direction thus breaking and reshaping the tree. U-tree and D-tree corresponds to construction and deconstruction allowing self-organization. Dual trees describing the tiles assembly and disassembly should be implemented as polytope projects for bio-inspired computing.

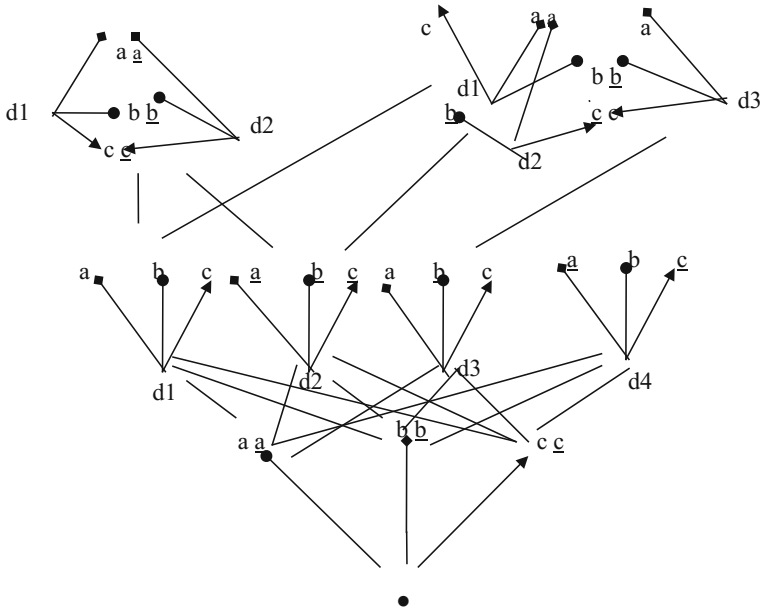


**Fig. 5.2** Tiling process

### *5.1.2 Computation in Cells*

One particular area of study in the field of cellular computing concerns the computational capabilities of gene assembly in unicellular organisms called ciliates (Landweber and Kari 1999; Kari and Mahalingam 2010).

Ciliates, unicellular protozoa named for their wisp-like cover of cilia, possess two types of nuclei: an active macronucleus containing the functional genes, and a functionally inert micronucleus that contributes only to genetic information exchange. In the process of conjugation, after two ciliates exchange genetic information and form new micronuclei, they have to assemble in real-time new macronuclei necessary for their survival. This is accomplished by a process that involves reordering some fragments of DNA from the micronuclear DNA (permutations and some inversions) and deleting other fragments. The process of obtaining the macronuclear DNA from the micronuclear DNA, by removing the non-coding sequences and permuting the coding fragments to obtain the correct order, is called gene rearrangement (Prescott 1994; Kari and Mahalingam 2010). The function of the various non-coding eliminated sequences is unknown and they represent a large portion of the micronuclear sequences.

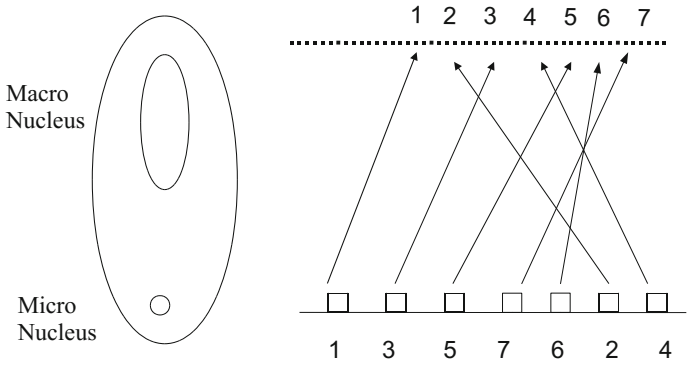


**Fig. 5.3** Gene rearrangement

An example is the micronuclear *Actin I* gene in *Oxytricha nova* is composed of 9 coding segments present in the permuted order 3-4-6-5-7-9-2-1-8, and separated by 8 non-coding sequences. Instructions for the gene rearrangement that is gene unscrambling, are apparently carried in the micronuclear DNA itself. Pointer sequences present at the junction between coding and non-coding sequences, as well as certain RNA templates, permit reassembly of the functional macronuclear gene (Prescott 1994; Kari and Mahalingam 2010).

In the macronucleus, gene-sized chromosomes assemble from their scrambled building blocks. Telomere repeats mark and protects the surviving ends.

In the micronucleus, coding regions of DNA are dispersed over the long chromosome.

Figure 5.3 illustrates the principle of gene rearrangement in ciliates.

Reassemble during macronuclear development allow forming the functional gene copy on top.

Computation in living cells can be described with the assembly/disassembly or insertion/deletion, doubling/contracting processes studied in combinatorial analysis with dual graded graphs and Hopf algebras.

### *5.1.3 Permutation Trees*

Observe that genes rearrangements may be described by permutations.

Ignoring internal eliminated sequences, segments in micronuclear DNA can be viewed as permutations of the final macronuclear sequence.

The nuclear dualism of ciliates, that is the existence of micro and macro nucleus, suggests that dual permutation trees may be useful for gene rearrangements modeling (Fomin 1994; Appendix A).

Figure 5.4 shows the dual graded graphs of permutation trees.

Figure 5.5 illustrates the commutation condition for permutation trees (Appendix A).

The permutation graphs have been considered also as trees of elementary design of experiments (Iordache 2012, 2013). Gene rearrangements may be viewed as design of experiments embedded in biological systems.

Figure 5.6 illustrates the polytope for permutation trees.

The black dot "•" in Fig. 5.6 corresponds to a permutation that is to an arrangement.

Rearrangements modify the permutation vectors as content.

Implementing the polytope project starts from the direct sequence S → K1 → K2 → K3 and complements these by the reverse sequence: K3′ → K2′ → K1′ → S′.

It is a switching between arrangement and rearrangement processes.

More general study of permutations would involve the Hopf algebra introduced by Malvenuto and Reutenauer (1995).

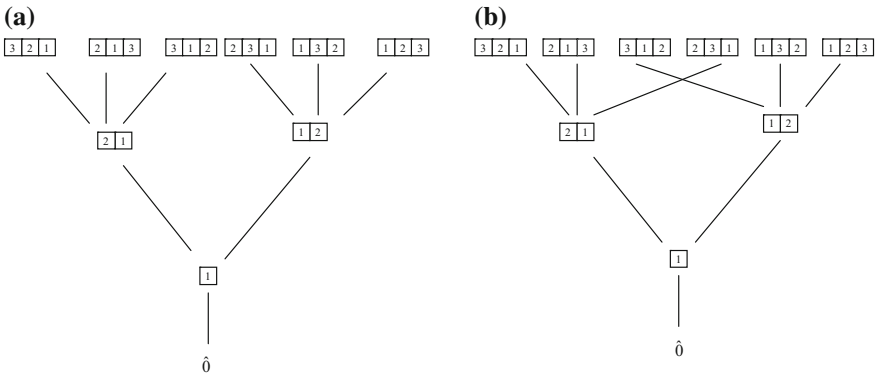


**Fig. 5.4** Dual permutation trees

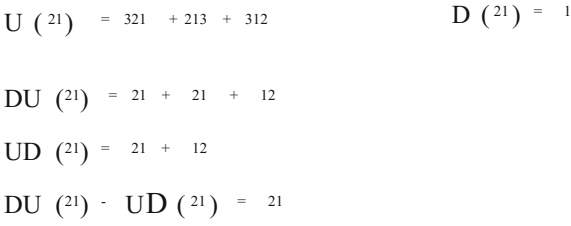

**Fig. 5.5** Commutation condition for permutation trees

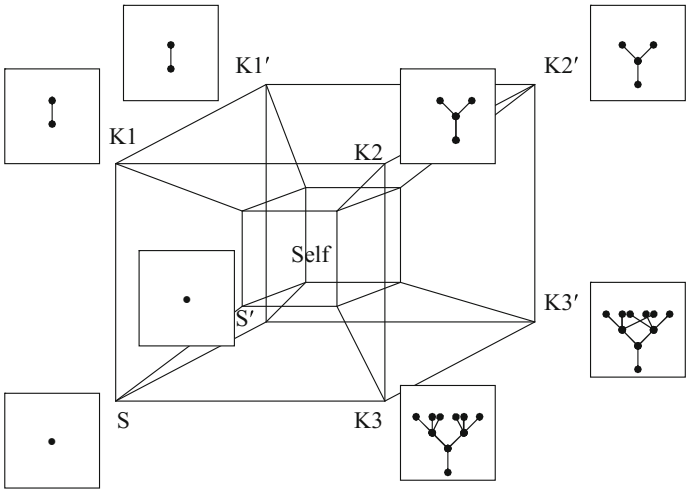


**Fig. 5.6** Polytope for permutation trees of gene rearrangement

## 5.2 Self-reconfiguring

### *5.2.1 Metamorphic Robots*

Metamorphic robotic systems are collections of mechatronic modules that can dynamically self-reconfigure (Chirikjian 1994). A change in the macroscopic morphology results from the locomotion of each module over its neighbors.

Application for structures reconfiguration in times of emergency, reveal the importance of previously knowing all the possible configurations that a predetermined finite number of modules can assume (Chirikjian 1994; Drees et al. 2012).

There are some interesting questions in the literature of modular and metamorphic robots which are sometimes implicit in the context (Chen and Burdick 1995, 1998)

- How to enumerate all possible configurations that a metamorphic robotic system can assume
- How to find the optimal configuration for a predetermined task
- How to plan the movement of a metamorphic robot system, that is, how to determine a sequence of module movements required to go from a given initial position to a desired goal configuration (Pamecha et al. 1996; Chiang and Chirikjian 2001).

Chen and Burdick (1995) consider the problem of finding an optimal module assembly configuration for a specific task. Their solution was formulated as a discrete optimization procedure.

Pamecha et al. (1996) proposed lower and upper bounds to the number of moves needed to change such systems from any initial to any final specified configuration. Pamecha et al. (1996) introduced the concept of distance between metamorphic robot configurations and demonstrate that this distance satisfies the formal properties of a metric.

These metrics are applied to the automatic self-reconfiguration of metamorphic systems for computing the optimal sequence of movements required to reconfiguration.

The problem of enumerating the set of kinematically distinct modular robot assembly configurations from a given set of modules was also addressed.

Martins and Simoni (2009) focuses on numeration of planar metamorphic robots configurations.

The general problem is how to enumerate the basic set of all the non-isomorphic configurations of a metamorphic robotic system or, in other words, how many different kinematic chains may be spanned by a given finite set of modules. By different kinematic chains, it is meant all the non-isomorphic configurations of a metamorphic robotic system. Other configurations may be obtained later by basic operations of group, reflection symmetry and mirror symmetry.

The motion planning problem for a self-reconfigurable metamorphic robotic system is to determine a sequence of robot motions required to go from a given initial configuration to a desired goal configuration.

It would be desirable to design an optimal algorithm that minimizes the number of steps required to reach the final configuration. However, there is no simple solution for computing the optimal sequence of moves required to reconfigure.

The reason is that the search space, that is, the number of possible sequences of configurations, grows exponentially with the number of modules in the system. It is a combinatorial optimization problem.

Martins and Simoni (2009) studied the problem of determination of all possible non-isomorphic kinematically configurations with a determined number of modules.

Figure 5.7 shows the enumeration of all non-isomorphic metamorphic robot configurations with up to four square modules.

The bold lines show where the new modules may be added for the next level of configuration. These bold lines control the robot configurations. Some configurations are discarded due to isomorphism with previously generated configurations.

Figure 5.8 shows some configurations for a metamorphic robot with 3 square modules which may move relative to a fixed hatched square base (Chiang and Chirikjian 2001).

The initial configuration is shown in Fig. 5.8a shows while Fig. 5.8d shows the final configuration. More intermediary steps should be considered according to the algebra of reconfiguration.

Similar reconfigurations have been described as partition diagrams (Ruch 1972; Sauerbrei et al. 2006).

Figure 5.9 shows a partition diagram. The initial uniform partition of the 4 objects (1111) evolves toward the final grouped partition (4000).

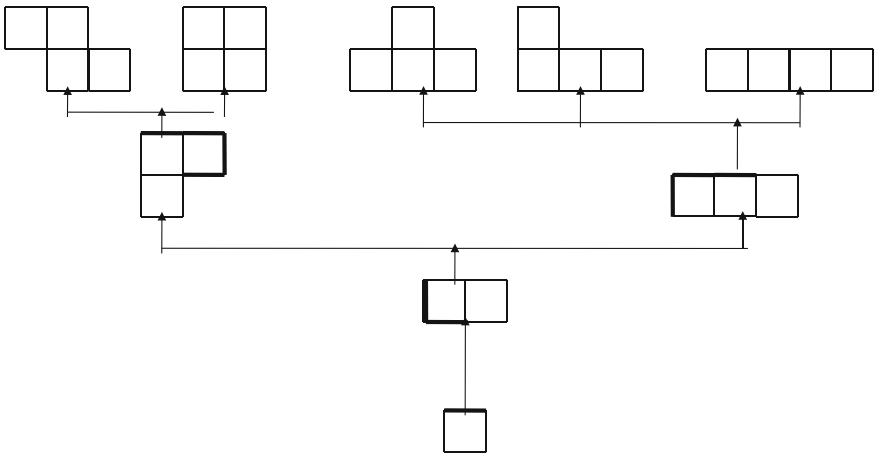

**Fig. 5.7** Enumeration of all non-isomorphic metamorphic robot configurations

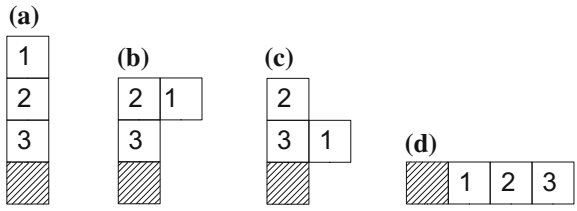


**Fig. 5.8** Reconfiguration sequence

Figures 5.7, 5.8 and 5.9 suggest that dual trees describing the construction and deconstruction may be considered for modeling robots reconfiguration. A more general model is combinatorial Hopf algebra where the product and coproduct respectively encode how to configure and how to split or reconfigure combinatorial objects.

### *5.2.2 Construction and Deconstruction*

Figure 5.10 illustrates the duality construction (Fig. 5.10a) deconstruction (Fig. 5.10b).

It outlines the DGG encountered in the study of Hopf algebras (Bergeron et al. 2012).

The U-tree describes the construction while the D-tree describes the deconstruction.

Figure 5.11 illustrates the commutation conditions for dual constructions.

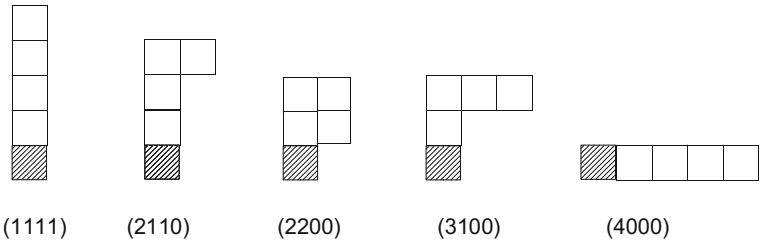


**Fig. 5.9** Partition diagram

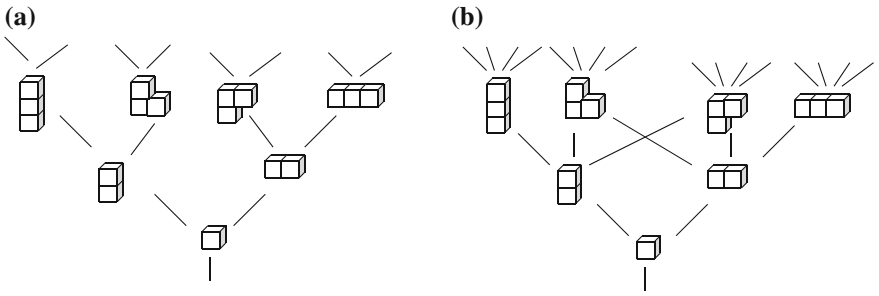


**Fig. 5.10** Dual construction and deconstruction

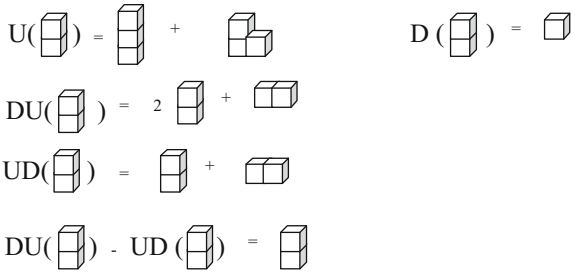


**Fig. 5.11** Commutation conditions for dual construction and deconstruction

A self-evolvable construction should be able to swing between dual constructions.

Reconfigurable tableau or lattices may be built by cube-shape modular constructions (Aloupis et al. 2009; Gilpin and Rus 2010; Tolley and Lipson 2011).

Figure 5.12 shows the polytope for dual construction and deconstruction.

The black dots "•" in Fig. 5.12 corresponds to different automata or assembly of cubic cells.

The Self should coordinate the interaction of the construction and deconstruction ways in duality relation.

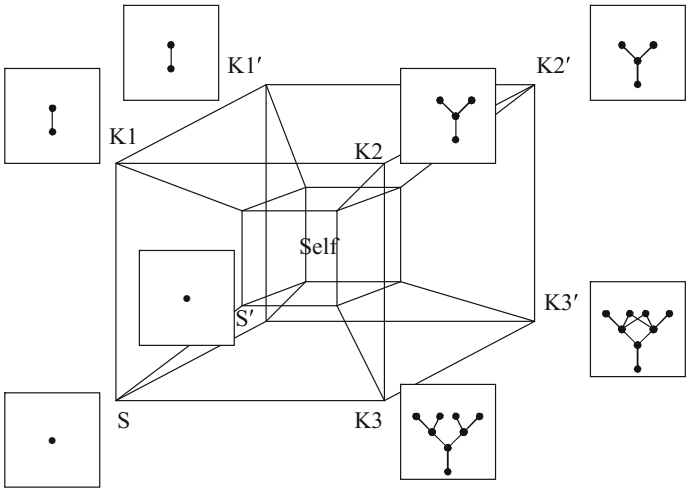


**Fig. 5.12** Polytope for dual construction and deconstruction

### *5.2.3 Shifted Shapes*

The process of forming shapes through assembly and disassembly is illustrated in Fig. 5.13.

A regular block of material results by modules assembly characterized by the operator U. Once this material structure is completed, the modules not needed in the final structure detach from the neighbors. The process is described by the operator D.

Once these extra modules are removed, we are left with the final shape.

The process is governed by the operators U and D introduced in the study of differential posets (Stanley 1988, 1990).

Assembly and disassembly are dual concepts.

An interesting example of dual graded graphs illustrating the construction and the deconstruction study is represented by the shifted shapes.

Figure 5.14 shows the diagonal of shifted shapes. This is the set of cells that are leftmost in their rows. They are darkened in Fig. 5.14.

Figure 5.15 shows the dual graded graphs of shifted shapes.

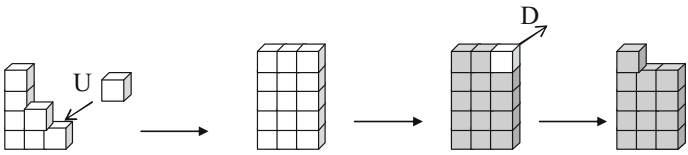


**Fig. 5.13** Assembly and disassembly

**Fig. 5.14** Diagonal of a shifted shape

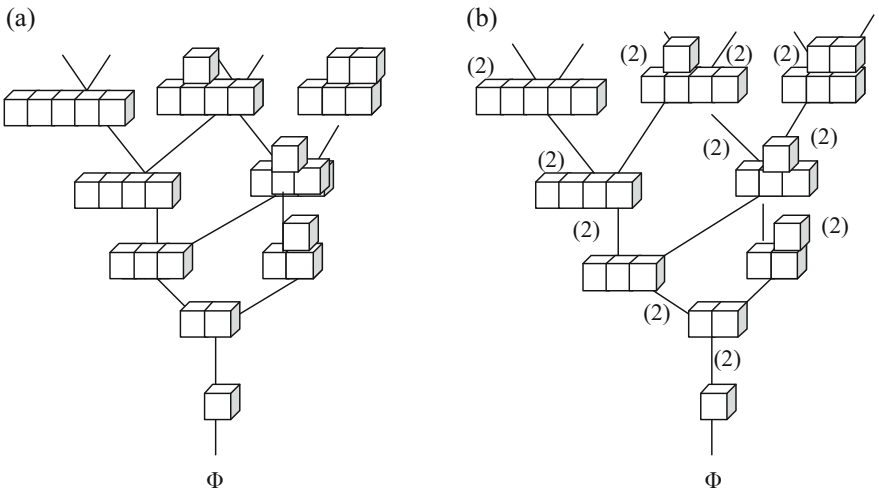


**Fig. 5.15** Dual graphs for shifted shapes

The dual graded graph of shifted shapes SY = ($G_1$, $G_2$) was studied by Fomin (1994).

The set of shifted Young diagrams of n having strictly decreasing row lengths, indexes the vertices having rank n. There are no multiple edges in G1 where elements x and y are adjacent if $|y| = |x| + 1$ and $x \subset y$ as diagrams.

One obtains G2 from G1 by changing an edge of weight one to an edge of weight (2) if x is obtained from y by removing a non-diagonal element.

Figure 5.16 illustrates the commutation conditions for shifted shapes.

Figure 5.17 shows the polytope for shifted shapes.

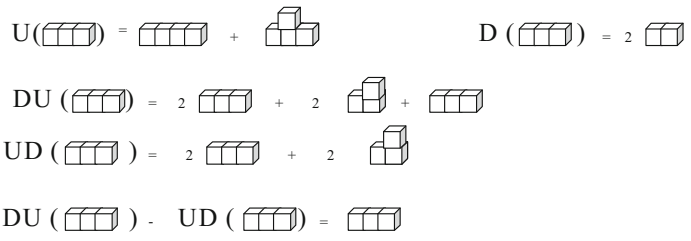


**Fig. 5.16** Commutation conditions for shifted shapes

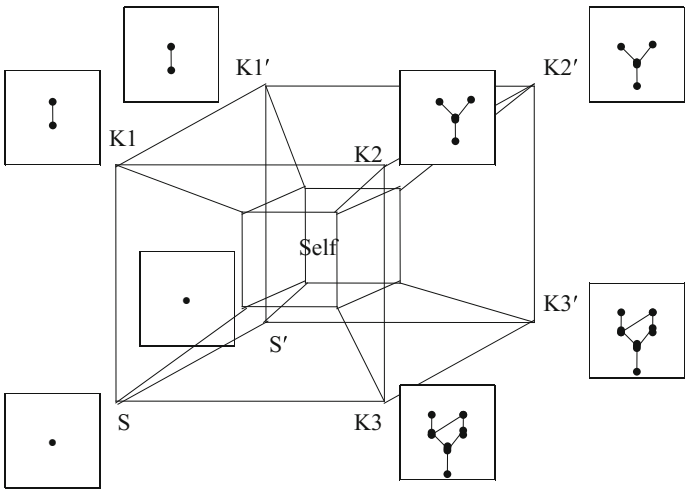


**Fig. 5.17** Polytope for shifted shapes

The black dots "•" in Fig. 5.17 corresponds to different construction steps.

Implementing the polytope project starts from the direct sequence S → K1 → K2 → K3 and complements these by the reverse sequence: K3′ → K2′ → K1′ → S′.

The dialogue of assembly disassembly processes is mediated by the Self.

Such processes have been studied in robotics for modular shape description (Goldstein et al. 2005; Yim et al. 2007; Tolley and Lipson 2011; Schweikardt and Gross 2011).

Figure 5.18 illustrates the assembly by disassembly.

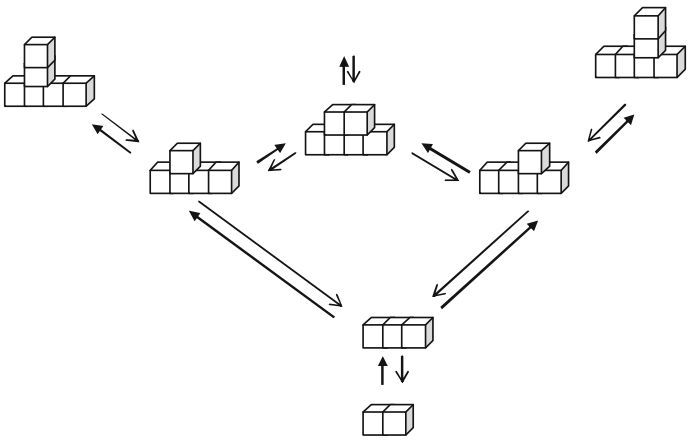

**Fig. 5.18** Assembly by disassembly

The assembly planner samples the graph of all possible paths to assembly by starting with the complete structure and removing one cube at a time until the existing state is revealed Reversing the disassembly sequence reveals a valid assembly sequence (Tolley and Lipson 2011).

Gilpin and Rus (2012) presented an innovative approach to rapidly configure active objects using a large collection of smart particles (sand, pebbles, tiles, cubes) capable of communicating and bonding with their neighbors. Traditional manufacturing create devices using a hierarchical approach that is organized as a sequence that includes mechanical design, fabrication, electronic design, boards production, assembly and finishing. In contrast, it is possible to package the necessary mechanical, perceptual and computational capabilities in small, smart building blocks that integrate actuation, sensing communication and control. Reconfiguration in the system proposed by Gilpin and Rus (2012) consists of selecting the correct aggregation of these modules for a required shape or design.

This work builds on a body of research addressing programmable matter, modular self-reconfiguring systems and smart systems.

### *5.2.4 Skew Strip Shapes*

Assemblies planning relating to identical rectangular robots moving on the plane that form planar structure locally like a brick wall have been studied by Seo et al. (2016).

Assembly planning is considered as a variant of robot motion planning where the goal is to assemble parts into one object.

Rectangles or rhombs can fill the plane without gapes and the pattern is structurally sound as in concrete masonry structures.

Such a structure is shown in Fig. 5.19.

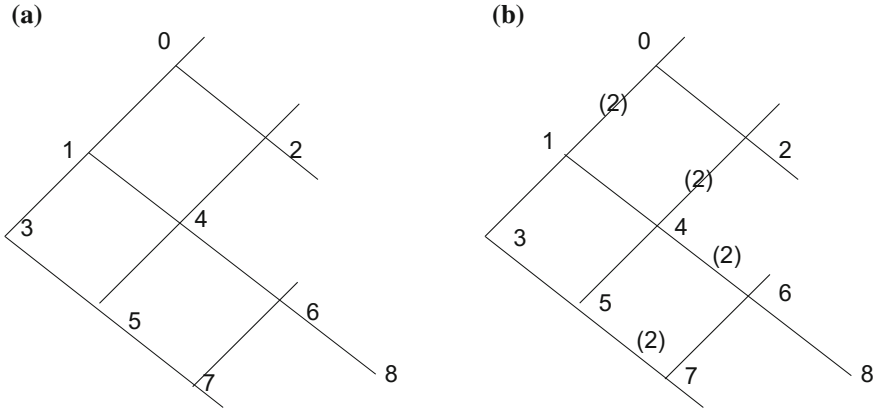


**Fig. 5.19** Lattices of skew strip shapes

The assemble process is described by the U-lattice while the disassembly is described by the D-lattice. The elements that can be for instance sensors, actuator or smarts are denoted by 0, 1, 2, 3, and so on. These are the elements of a distributive lattice (Fomin 1994).

Figure 5.19a shows the U-lattice while Fig. 5.19b shows the D-lattice.

The weight function is 1 if q covers a single element and (2) otherwise.

Figure 5.19 shows the weight, only if this is different from one.

Observe that:

$$\mathrm{U}(4) = 1 + 2; \quad \mathrm{D}(4) = 5 + 2 \times 6 \tag{5.1}$$

$$\mathrm{DU}(4) = 3 + 4 + 2 \times 4; \quad \mathrm{UD}(4) = 3 + 4 + 2 \times 4 \tag{5.2}$$

$$\mathrm{DU}(4) - \mathrm{UD}(4) = 0 \tag{5.3}$$

In this case the two lattices are 0-dual.

The dual lattices frame offers an assembly planning algorithm for constructing planning structures of a brick wall pattern out of rectangular modular robots which can dock to each other.

Given an assembled structure the algorithm can be used for self-disassembly planning by following disassembly presidencies.

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# Chapter 6
# Devices and Technologies

## 6.1 Microreactors

### *6.1.1 Microtechnology and Chemical Plants*

Chemical, biochemical and pharmaceutical industries, were among the first to make an interdisciplinary move into the promising field of Microtechnology (Ehrfeld et al. 2000; Ehrfeld 2007). Chemical engineers are intensively analyzing the possibilities offered by the strategy of miniaturization and integration to realize a radical change in design methods for modern chemical plants (Ehrnfeld and Ehrnfeld 2001).

The research and development work started in the late 1970s, and the term process intensification was used to characterize the novel concept. The intention was to achieve much lower investment, operating, and maintenance costs for chemical plants, without decreasing their production capacity, by means of a dramatic reduction in plant size (Jensen 1999, 2001; Pohar and Plazl 2009). The technological progress even in standard plant items has proven that this concept has a realistic basis. One may consider, on the one hand, a standard stirred-tank reactor with a cooling jacket having a volume of about 10 $m^3$ and, on the other hand, a potentially equivalent reactor for the same production capacity consisting of a static mixer and a compact heat exchanger having a volume of about 0.1 $m^3$. This comparison demonstrates the superiority of continuous operation over batch processing with regard to specific plant volume and its importance in process intensification. Many other examples exist, such as spinning disk reactors, vortex scrubbers, reactor-mixing systems, and, multifunctional reactors, which integrate reactions and unit operations.

The recent development of process intensification directs to the novel field of microreaction technology. Because of the small characteristic dimensions of microreaction devices, mass and heat transfer processes can be strongly enhanced, and, consequently, initial and boundary conditions as well as residence times can be



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precisely adjusted for optimizing yield and selectivity. Microreaction devices are evidently superior, due to their short response time, which simplifies the control of operation. In connection with the extremely small material holdup, nearly inherently safe plant concepts can be realized. Microreaction technology offers access to advanced approaches in plant design, like the concept of numbering-up instead of scale-up and, in particular, the possibility to utilize novel process routes not accessible with macroscopic devices.

Microfabrication methods have to be introduced into chemical engineering in order to profit from the potential advantages of microreaction technology. Although this is a difficult task, several chemical companies have successfully started to utilize microreaction technology for commercial syntheses of fine and special chemicals.

Effort must still be spent to transfer further promising research results into commercial application and to get away from traditional strategies in chemical engineering.

Enhancement of heat transfer and mass transfer processes is a natural effect of miniaturization.

Diffusion, thermal conductivity, and viscosity are physically similar phenomena that involve the transport of a physical quantity through a gas or liquid. The driving forces for the corresponding transport fluxes of mass, energy, and momentum are the gradients in concentration, temperature, and velocity, respectively, where in all three cases the fluxes are in the same direction as the gradients. For given differences in these properties, a decrease in the characteristic dimensions results in an increase in these gradients and, correspondingly, in higher mass and heat transfer rates as well as in higher viscous losses. Accordingly, mixing and heat exchange systems with extremely high transfer rates per unit volume can be realized by miniaturization; on the other hand, however, the effect of viscous losses has to be taken into account.

In addition of the effect of decreasing linear dimensions on the corresponding gradients, the effective surface area for exchange processes has to be considered.

With decreasing characteristic dimensions, the surface-area-to-volume ratio of the system increases. This allows the corresponding enlargement of the specific interface area, that is, of the area per unit mass or unit volume, for transfer processes. In connection with the enhancement of the gradients, the driving forces for heat and mass transfer, extremely efficient mixers and heat exchangers can be realized by miniaturization. The amount of material in a system is reduced with the reciprocal third power of the characteristic dimensions, and, consequently, the response time of the microdevice is extremely reduced so that in most cases large differences concerning temperatures and concentrations are diminished immediately.

In many cases highly exothermal chemical reactions can be performed under isothermal conditions using the channels of micro heat exchangers as reaction volumes. Research on this subject started in the late 1980s, when micro heat exchangers with extremely high transfer rates per unit volume were produced by means of advanced mechanical micromachining methods. Specific heat transfer

rates of more than 20 kW/cm$^3$ have been achieved, and a broad spectrum of materials has been successfully applied.

A wide variety of micromixers are also available that allow mixing times in the millisecond range. They utilize mainly the concept of multi-lamination, where two streams of fluids are split into a large number of small streams and fed alternately into an inter-digital flow system, where they merge into a joint stream.

Other concepts are based on the principle of splitting, side-to-side arrangement, and further splitting to generate an increasing number of streams with different compositions, as known from large-scale static mixers. Vortex-type micromixers have also been applied. A wide range of applications for micromixers exists in the fields of gas–liquid suspensions and liquid–liquid emulsions, with extremely small bubble and droplet sizes, respectively. High uniformity concerning size distribution is achievable. In particular, the specific power consumption for generating suspensions and emulsions is much lower than in the stirring devices or high-pressure jets usually applied in the macroscopic range. Accordingly, micromixers are promising tools to improve the performance of phase transfer and other exchange processes.

Inherent process restrictions in miniaturized devices require innovative design solutions.

Miniaturization inevitably results in a number of process restrictions, and completely new problems arise, too. There are the problems of blockage of microstructures by solid particles and fouling effects. Corrosion might be much more dangerous for microscopic than for macroscopic devices (Ehrfeld 2007).

Modular and flexible production as well as a continuous sensory control of production and real-time optimization, which are also aspects of industry 4.0 in the chemical industry has long been under study.

Modularization and flexibility relate primarily to two areas: in-house batch processes or non-continuous production of small quantities and international value networks.

Chemical industry has been working at the modularization of chemical plants and container modules with microreactors as building blocks of small-scale production systems, especially for fine and specialty chemicals. Design guidelines were established and implemented in demonstration plants with a backbone infrastructure for docking container modules. With a container more than 1000 kg of a product can be produced. The container corresponds to flow rates of about 10–100 kg/h. If a malfunction of a module in a container or within a module, such as a seal leak, the entire module is replaced. The modular systems are more robust than a production of small quantities in the laboratory.

Modular production equipment for the fine and specialty chemicals and pharmaceutical industries is of interest for the introduction of new products into the market. With previous concepts equipment for new products were initially underutilized, with the containers can be satisfied in a start-up phase of market demand. By increasing or decreasing the number of containers for a product we can flexibly responds to demand, without running the risk of underutilized large system of investing.

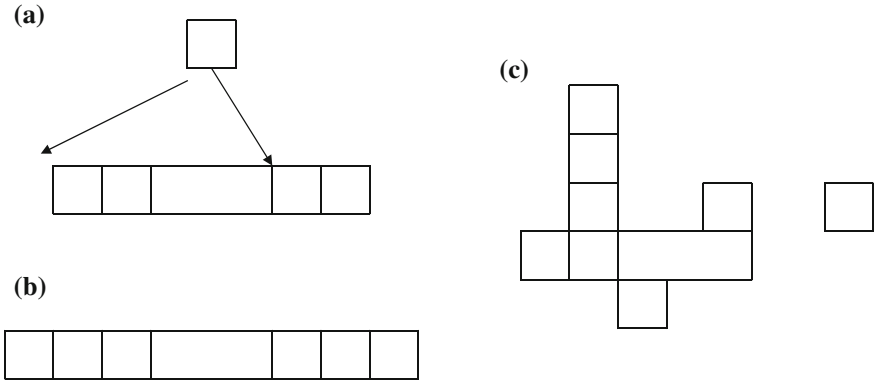


**Fig. 6.1** Modular Micro Reaction System

Figure 6.1 shows a Modular Micro Reaction System and illustrates the module insertion rules.

The (a) part in Fig. 6.1 shows the initial system and the microreactor to be inserted (sealing plate).

Usually the extreme cells are clamping modules.

The (b) part shows the resulting system. The (c) part shows a screen shot of the operator surface.

Obviously Modular Micro Reaction Systems can be described with the insertion/deletion processes studied in combinatorial analysis with dual graded graphs and Hopf algebras.

### *6.1.2 Dual Graded Graphs for Microreactors*

Cells or boxes denoted as 1, 2, 3 and so on, corresponds to peculiar process steps or microreactors.

They are distributed in tableaux as that shown in Fig. 6.1. This corresponds to assemblies of microreactors in series or parallel. The rule of partition of the set of microreactors, the rules of insertion of new microreactors, depends on the technology goal (Iordache 2013).

As an example of partition of objects we will consider the SYT-tree and Schensted graphs in duality (Fomin 1994).

Figure 6.2 shows the DGG formed by SYT-tree and Schensted graphs.

For the SYT-tree the vertices are the standard Young tableaux which are linked if one is obtained from another by defining a box with the maximal entry (Yong 2007). The dual graph for the SYT-tree is the Schensted graph. To construct this we need to make use of Schensted insertion algorithm (Fomin 1994).

Let $\tau$ be a Young tableau. Assume $a_0$ is not an entry of $\tau$. In the first row of $\tau$, find the minimal entry which is greater than $a_0$ say $a_1$ and replace it by $a_0$.

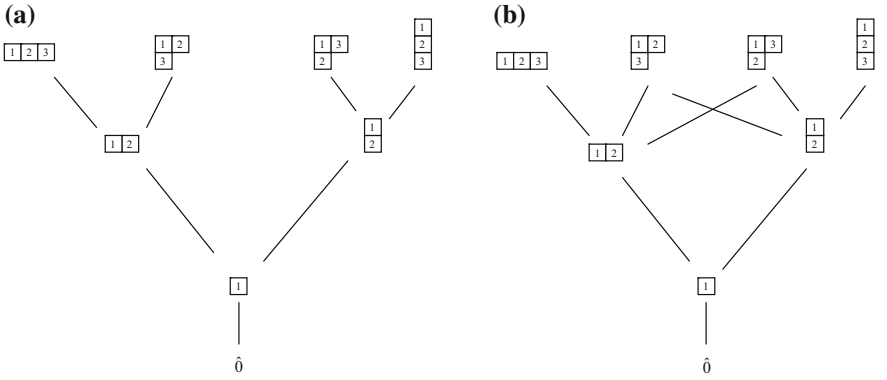


**Fig. 6.2** SYT-tree and Schensted graphs in duality

Then insert $a_1$ into the second row in the same manner, replacing the minimal entry $a_2 > a_1$; $a_2$ goes to the third row, and so on until some $a_i$ is greater on or equal to the elements of the (i + 1) row.

The label $a_i$ is placed into a new box added to this row. The resulting tableau is said to be obtained by Schensted inserting $a_0$ into $\tau$.

The U-graph (Fig. 6.2a) corresponds to distributive hierarchical partitions schemes while the D-graph (Fig. 6.2b) corresponds to dual redistributive schemes of partitions.

The objects, as for instance chemical compounds to be separated or mixed, or stages in a technology to be performed or microreactors, are those that define the elements of the Young tableaux and the insertion algorithm. The insertion algorithm should be based on technological considerations.

The collective behavior among the cells or microreactors demands an analysis of their local edge-to-edge interactions in order to understand the causes by which large structure emerges.

Sequences of entering compounds may be considered as words.

Series corresponds to horizontally positioned devices, in succession, while parallel corresponds to vertically positioned devices for instance a distillation column with two zones, enrichment and stripping or an adsorption column with two adsorbents. The compounds are retained or separated in a zone.

Figure 6.3 shows the commutation condition for SYT-tree and Schensted graphs.

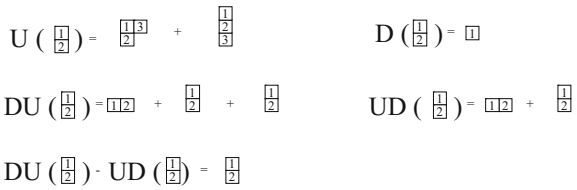


**Fig. 6.3** Commutation condition for SYT-trees and Schensted graphs

Observe that the commutation relation: DU-UD = I is verified and the DGG is 1-dual.

Such commutation relations have been introduced in the study of differential posets (Stanley 1990).

Structure obtained as superposition of the dual graded structures allows more flexibility than that based on a graded graph only.

It contains "up" transitions, U, in the partition schemas and "down" transitions, D, in the repartition schemes.

Observe that transitions between devices may be in some cases reversible that is up, U, and down, D, or irreversible, that is just up U or just down D.

This corresponds to several interactions between parallel and series configurations.

The partition schemas are not pre-determined and may evolve that is schemas allow separation of different elements in different devices making the system as compact as possible by reversible coupling the parallel and series stages.

The operator U describes the partition process starting from cells.

It is the direct way: S → K1 → K2 → K3.

The operator D describes the dual repartition process.

It is the reverse way: K3′ → K2′ → K1′ → S′.

Figure 6.4 shows the polytope of dual partitions.

The black dots "●" in Fig. 6.4 correspond to particular partitions of objects.

The Self allows and coordinates the interaction of the two ways in duality relation.

Microreactors systems are examples of tableaux as shown in Fig. 6.1. They are combinatorial objects and we are interested in the association and disassociation of microreactor systems. The polytope project starts from the direct sequence

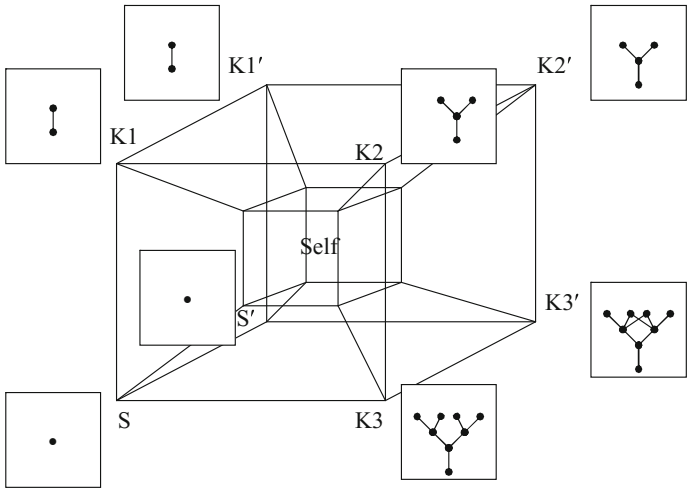


**Fig. 6.4** Polytope for SYT-trees

$S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

It is a switching between association and disassociation processes in technological scheme.

Hopf algebras encode the disassociation or decomposition (coproduct) and association or composition (product) of combinatorial objects (Joni and Rota 1979).

A more general study of SYT trees would involve the Hopf algebra of Young tableaux (Poirier and Reutenauer 1995).

### 6.1.3 Set Partitions

Cells or boxes denoted as 1, 2, 3 and 4, corresponds to particular process steps or to microreactors. The challenge is to assembly this set of cells.

A combinatorial Hopf algebra on set partitions was studied by Rey (2007).

It is based on the Bell order of set partitions as defined by Rey. This partial order admits the Tamari order as suborder. Recall that a Tamari lattice, is a partially ordered set in which the elements consist of different ways of grouping a sequence of objects into pairs using parentheses.

To any permutations of the steps or microreactors a tableau is associated.

Figure 6.5 shows the Bell order on set partitions of size 2 and 3.

Figure 6.6 shows the Bell order on set partitions of size 4.

Notice that the Bell order on set partitions of size 4 is a lattice.

Figure 6.7 shows the dual trees for Bell order on set partitions.

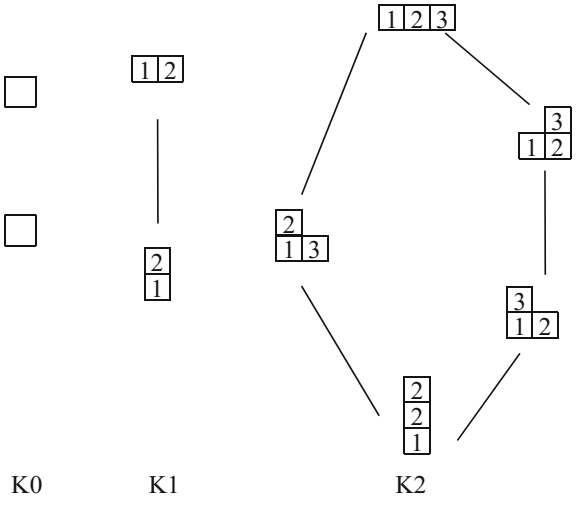


**Fig. 6.5** Bell order on set partitions of size 2 and 3

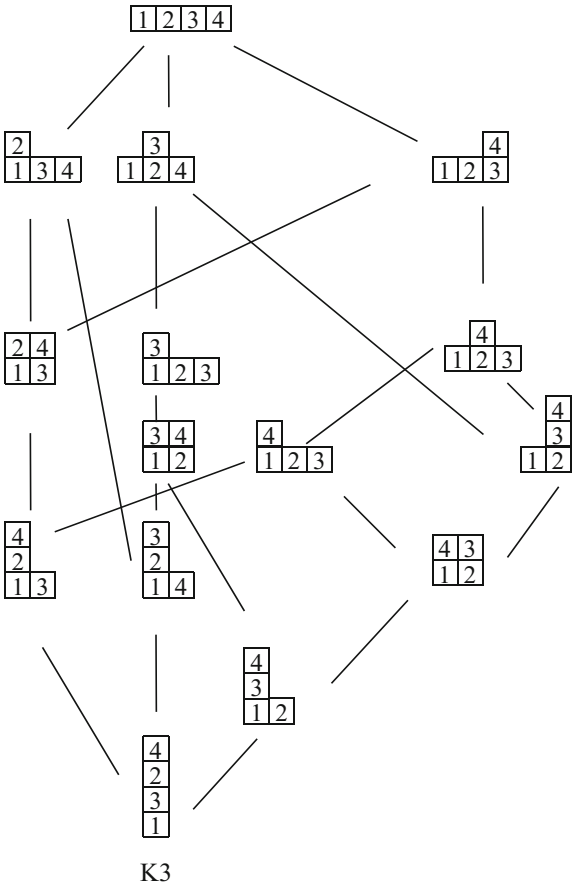


**Fig. 6.6** Bell order on set partitions of size 4

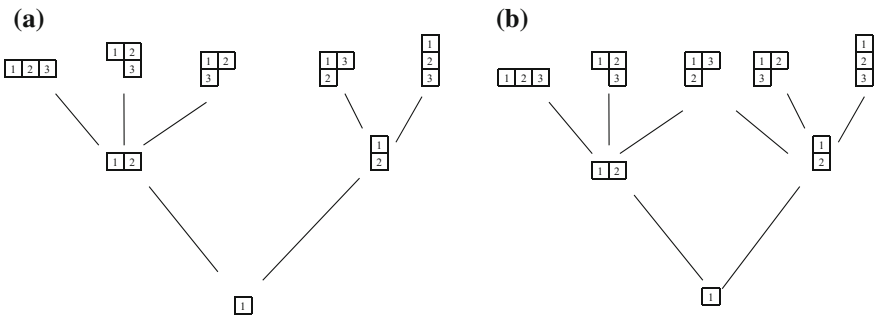


**Fig. 6.7** Dual trees for Bell order on set partitions

The U-graph (Fig. 6.7a) corresponds to distributive hierarchical partitions schemes while the D-graph (Fig. 6.7b) corresponds to dual redistributive schemes of partitions.

The objects as for instance stages or chemical compounds to be separated or mixed are those that define the elements of the tableaux and the insertion algorithm. The insertion algorithm should be based on technological considerations.

Series may corresponds to horizontally positioned devices, in succession, while parallel corresponds to vertically positioned devices for instance a distillation column with several zones, or an adsorption column with several adsorbents. The compounds are retained or separated in a zone or microreactor.

Figure 6.8 shows the polytope for lattices configurations.

The notations are:

- K0-substances, stages, microreactors.
- K1-set partition of size 2.
- K2-set partition of size 3.
- K3-set partition of size 4.

K1 illustrates the separation tableau. K2 shows a lattice of tableaux.

K3 shows a lattice of lattice of tableaux.

The polytope project implementation starts from the sequence $K0 \rightarrow K1 \rightarrow K2 \rightarrow K3$ and should balance this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow K0'$. The reverse way $K3' \rightarrow K2' \rightarrow K1' \rightarrow K0'$ corresponds to integration. This reverses the arrows direction in K1, K2 and K3′.

A level in the polytope shown in Fig. 6.8 is the complete structure obtained by a new step for all the trajectories in the U-tree or D-tree. K2 shows all 3-compounds tableau and K3 shows all 4-compound tableaux. Arrows indicate the relations between tableaux.

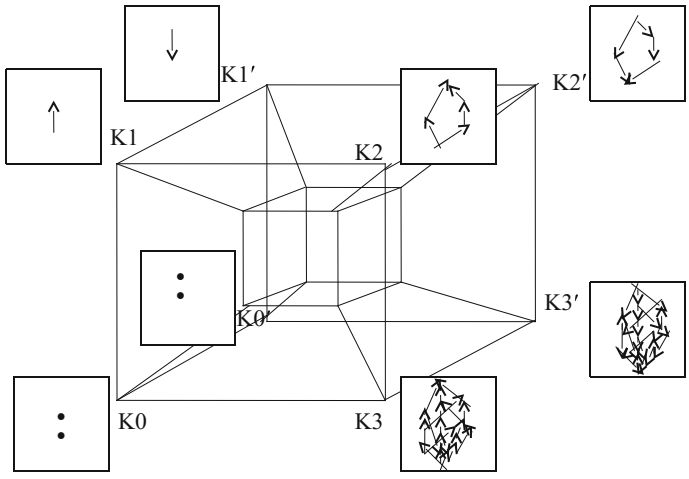


**Fig. 6.8** Polytope for Bell order on set partitions

### 6.1.4 Numbering-up and Chains

Microstructured reactors are known to provide high heat and mass transfer rates for liquid–liquid two-phase systems when used as a single channel. For industrial scale production, scale-up of microstructured reactors is essential to achieve throughput in the required range which is done by numbering-up of a single channel. The important issues are uniform flow distribution and identical slug size in all channels.

Microreaction technology offers access to advanced approaches in plant design, like the concept of numbering-up instead of the conventional scale-up.

Figure 6.9 illustrates scaling-up (Fig. 6.9a) and numbering-up (Fig. 6.9b).

Numbering-up is preferred over the conventional scale-up because the performance can be preserved and operational capacity of the industrial reactor can be achieved.

In the case of single phase flow, flow distribution with minimum energy consumption is the only key issue in the numbering-up for high throughput. However, in two-phase slug-flow, in addition to flow distribution, the slug size should be uniform in all parallel channels as it affects the performance of the microstructured reactors.

There are two ways to number-up microstructured reactors for two-phase reactions (Kashid et al. 2010).

Figure 6.10 shows internal numbering-up and external numbering-up.

The main functional element of the experimental set-up is numbered-up in former case while the whole laboratory set-up is replicated in the latter case.

The scheme of internal numbering-up is shown in Fig. 6.10a. As can be seen, two liquids are mixed in the mixing zone and the biphasic mixture is distributed in several parallel microchannels. The advantage is that it reduces the cost associated with the pumping and mixing equipments as only two pumps and one mixing element is used. However, the distribution of biphasic mixture into parallel channel is a challenging task.

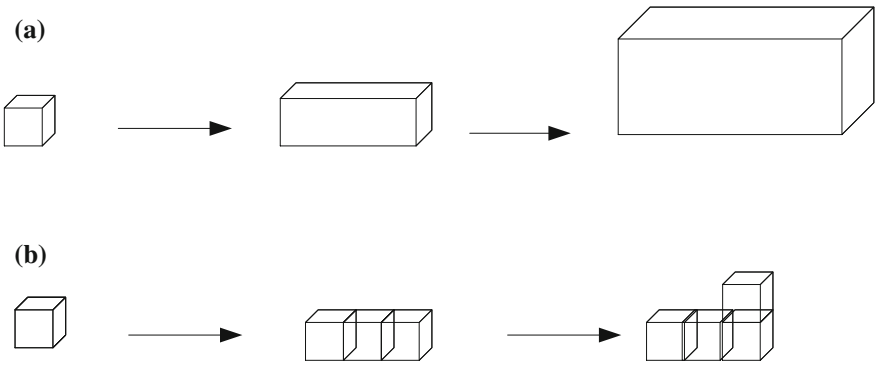


**Fig. 6.9** Scaling-up and numbering-up

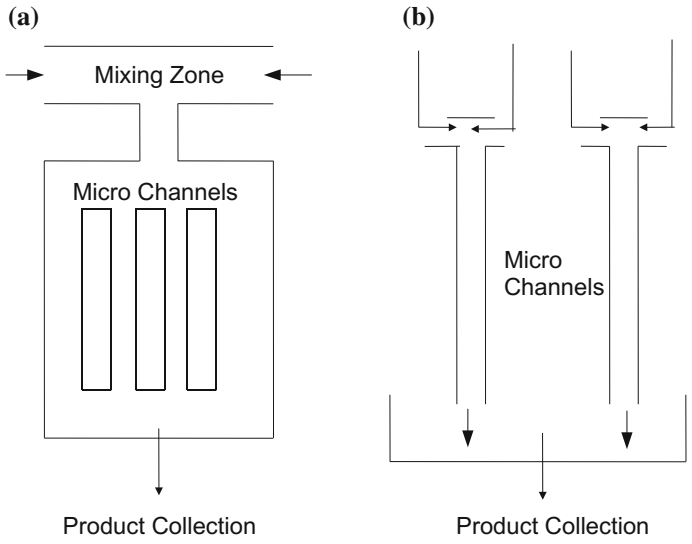


**Fig. 6.10** Numbering-up

To distribute fluid in parallel channels, equal pressure drop in all channels is required.

If the pressure drop is similar in all channels at different slug sizes, the performance of each channel differs from the other due to different interfacial area. A common approach to overcome this problem in microfluidic devices is to use a bigger manifold to uniform the pressure across all channel inlets. Such a manifold can modify the performance from the plug flow and the advantages of single channel can be vanished. Another method is to put obstacles at the channel inlets to increase the pressure in the distributor zone but such an approach also results in misdistribution due to two-phase flow.

The schematic of external numbering-up is depicted in Fig. 6.10b.

It shows that two fluids are introduced to the mixing element of two-phase micro reactors which are arranged in parallel. The arrangement shows that the laboratory set-up is replicated depending on the required throughput. The advantage is that the performance of single micro reactor can be preserved in a high throughput facility. Higher equipment cost and larger set-up size limits the use of this approach.

Numbering-up and numbering-down can be modeled using chains (Fomin 1994).

Figure 6.11 shows dual graded graphs for chains.

The weights indicated on the connections between two chains show the number of ways we can obtain by one from another in “up” and “down” direction.

Figure 6.11 shows the number of ways to pass from a chain to another, only if this is different from one.

Figure 6.12 illustrates commutation condition for chains.

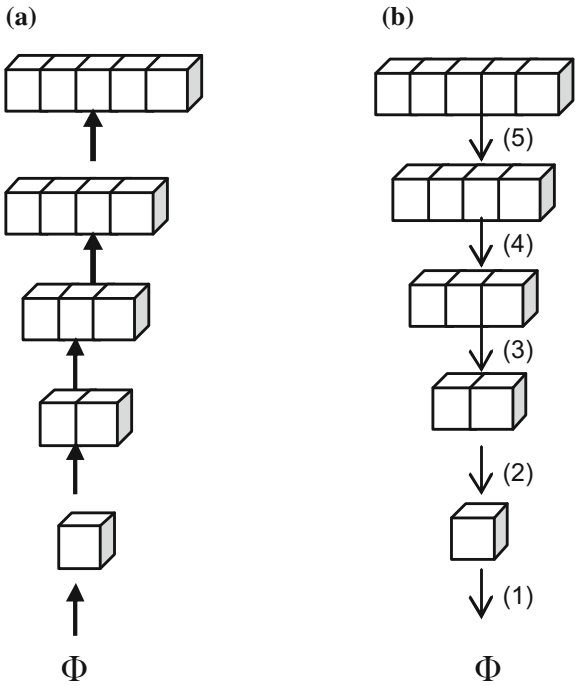


**Fig. 6.11** Dual graded graphs for chains

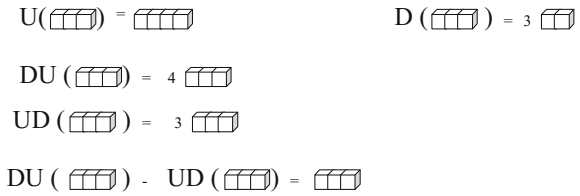


**Fig. 6.12** Commutation conditions for chains

The polytope for chains is shown in Fig. 6.13. A dot corresponds to a microreactor.

Implementing the polytope project starts from the direct sequence S → K1 → K2 → K3 and complements this by the reverse sequence: K3′ → K2′ → K1′ → S′.

It is a switching between numbering-up and numbering-down processes.

Applications of microreactors in process engineering will involve not only miniaturization and intensification but also advanced process control and systems design as well. Micro structured devices facilitate polytope projects implementation. This means innovation opening the way to completely novel synthesis routes, unexplored operating regimes and dynamic operation.

Conventional developments for microreactors are looking for intense operations and compact design. A more active approach involves not only geometrical

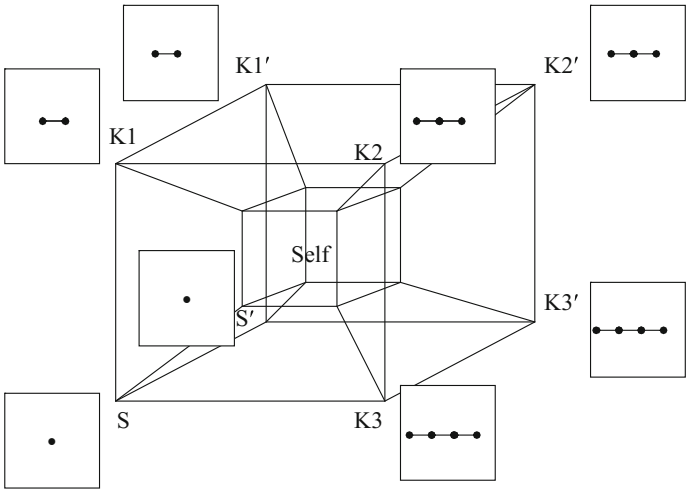


**Fig. 6.13** Polytope projects for chains

microreactors but also sensors and actuators to allow smartness and self-evolvability.

Smart systems perspectives for technologies start to be evaluated and implemented by engineers. Some aspects related to smart systems in chemical engineering have been highlighted by Villermaux (1996).

Local distributed process control was considered as a key factor for self-evolvability. This control implies that the energy and chemical supply to be localized to the site were it is required. It should be based on embedded arrays of local sensors and actuators.

Microreactors or multi-sectioned reactors have potentialities for self-evolvability. When combined with non-stationary cyclic operation such micro structured programmable devices offer new possibilities for innovative chemical synthesis (Matlosz 1995).

Cyclic operation allows coupling direct and reverse sequences in a polytope project implementation.

With this approach one can envision a programmable reactor unit mounted on a motherboard and providing reaction conditions that adjust automatically to the desired synthesis (Matlosz et al. 2001). The program may be based on the algebra generating dual graded trees or Hopf algebras.

Figure 6.14 shows an electrochemical programmable reactor (Vallières and Matlosz 1999).

Figure 6.14a shows the conventional packed bed reactor while Fig. 6.14b shows the micro-sectioned design. Anode sections are separated by insulating sections.

Increased efficiency, productivity and selectivity could be obtained through intelligent operation and multi-scale control. The so-called smart design would

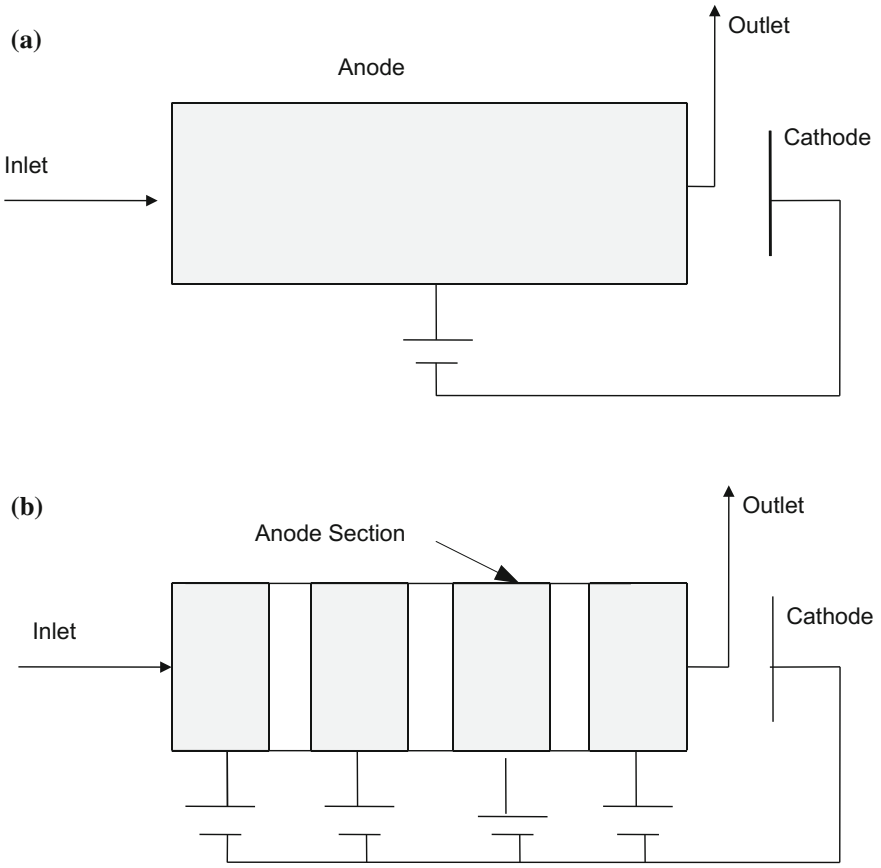


**Fig. 6.14** Programmable reactor

involve assemblies of structured, modular components and precise computer control based on information transfer between distributed arrays of local sensors and actuators.

A large variety of chemical microsensors and microactuators has been developed.

Thanks to developments in silicon microtechnology a large variety of micro fluidic systems have been fabricated enabling the composition of a complex analysis system by integrating different components on a motherboard.

A further step in the realization of microsystems is the addition of microreactor to the system. Such a microreactor may be used to mix chemical reagents, to carry out a thermally induced chemical reaction. A microchemical system results by integration of sensors, controllers, actuators, fluidics and reactors (van den Berg et al. 1996).

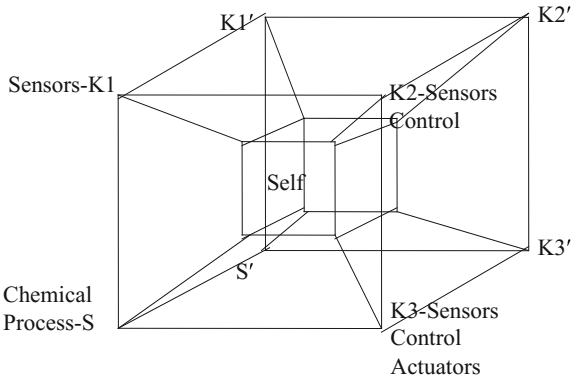


**Fig. 6.15** Polytope for microchemical systems

Mixed circuit boards containing fluid channels, electrical circuitry and silicon based modules have been described by van den Berg et al. (1996). The example of electrochemical microreactor was presented in detail.

Figure 6.15 shows a polytope for microchemical systems.

Figure 6.15 shows different states of integration:

- S-Chemical Process.
- K1-Sensory Systems.
- K2-Sensory and Control Systems.
- K3-Sensory Control and Actuators Systems.

The microchemical system relates the Chemical Process to Sensors/Control/Actuators closing the gap between S and K3.

Implementing polytope project for microchemical systems starts from the direct sequence S → K1 → K2 → K3 and complements this by the reverse sequence: K3′ → K2′ → K1′ → S′.

For the polytope shown in Fig. 6.15 one could identify for instance:

- K3′-De-actuating.
- K2′-Un-control.
- K1′-De-sensing.
- S′-New Chemical System.

Direct sequences interact with reverse sequences and it is the mix and equilibrium of both that counts.

It should be emphasized that similar problems have been encountered in the study of programmable matter (Goldstein et al. 2005) and self-reconfigurable automata (Yim et al. 2007; Cheung et al. 2011; Gilpin and Rus 2012).

Gilpin and Rus (2012) presented a new approach to rapidly manufacturing active devices using a large collection of smart cells as tiles or microreactors capable of communicating and bonding with their neighbors. It is possible to package the necessary mechanical, perceptual and computational capabilities in small, smart

building blocks that integrate actuation, sensing communication and control. Manufacturing in the system proposed by Gilpin and Rus consists of selecting the correct aggregation of these modules for a required shape or design.

## 6.2 Timed Automata

### *6.2.1 Heaps of Pieces and Timed Automata*

The supervisory control theory, is a method for automatically synthesizing supervisors that restrict the behavior of a plant such that as much as possible of the given specifications are fulfilled (Ramadge and Wonham 1987).

The plant is assumed to spontaneously generate events. The events are controllable or uncontrollable. The supervisor observes the string of events generated by the plant and might prevent the plant from generating a subset of the controllable events. However, the supervisor has no means of forcing the plant to generate an event.

In its original formulation the supervisory control theory considered the plant and the specification to be modeled by formal languages, generated by finite automata.

Time consideration using heaps of pieces and timed automata theory have been discussed by Peeters et al. (2007) and by Su et al. (2012).

A heap is a collection of pieces say b1, b2, …, ranged one upon the other, sometimes also sideways to form a heap (see Fig. 6.16).

Pieces can only move vertically so the heap in Fig. 6.16 would be a stable arrangement (Viennot 1989).

Let B be a set of pieces with a symmetric and binary relation R. A heap is a triple (P, $\leq$, L) where (P, $\leq$) is a poset and L is a labeling of the element of P by elements of B such that:

(1) If x, y $\in$ P and L(x) R L(y), then either x $\leq$ y or y $\leq$ x
(2) The relation $\leq$ is the transitive closure of the relation from (1)

For the heap shown in Fig. 6.16 the pieces are B = {b1, …, b5} and relations are:

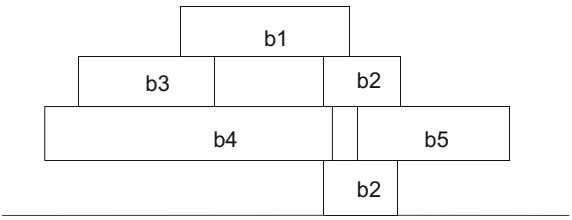


**Fig. 6.16** Heaps of pieces

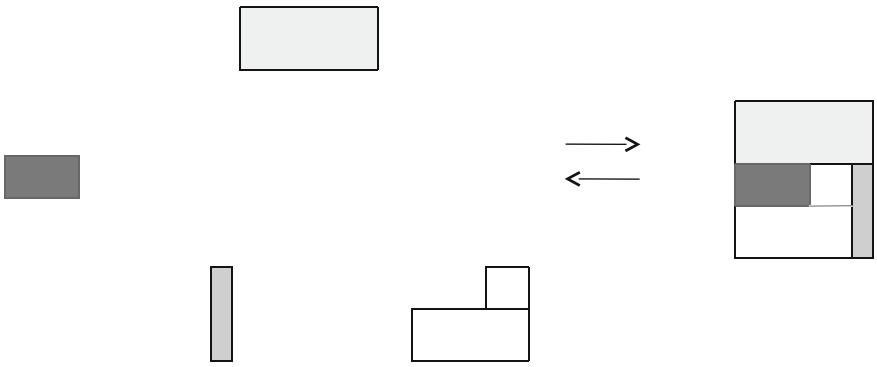

**Fig. 6.17** Heaps representation

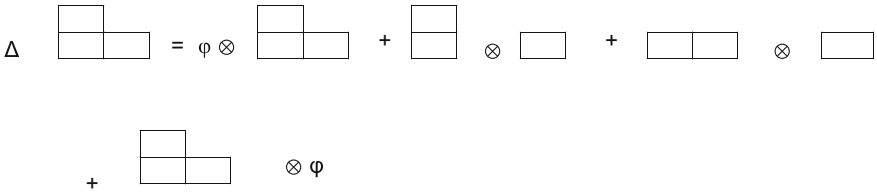


**Fig. 6.18** Coproduct of heaps

b1Rb2, b1Rb3, b1Rb4, b2Rb4, b3Rb4 and b2Rb5.

Figure 6.17 shows more complex heaps, inspired by the tilling scheme.

Bultel and Giraudo (2016) studied the Hopf algebra associated to heaps of pieces (Sweedler 1969, Appendix B).

Figure 6.18 illustrates the coproduct.

The coproduct takes into account the admissible cuts of heaps.

The product describes the acknowledged rules to connect heaps.

### *6.2.2 Paint Factory*

The system that is chosen to illustrate the use of heap of pieces for timed automata is a scaled-down model of a paint factory (Peeters et al. 2007). Time is associated with the plant automata and pieces are defined and applied on the paint factory case.

Figure 6.19 illustrates the heap representation of the sequence s = abc.

We consider three pieces a, b and c.

The elements r1, r2 and so on are called resources.

The heap shown in the right side of Fig. 6.19 is a sequence of pieces piled up in logical order (Peeters et al. 2007).

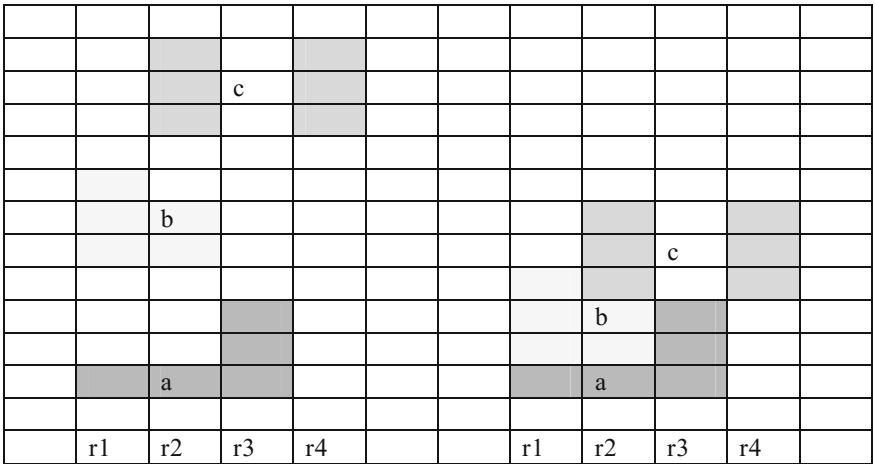


**Fig. 6.19** Heap representation of a sequence

The heaps algebra is used as model of paint factory is shown in Fig. 6.20.

The scaled down model is a mixing device, with some fluids as input and a mixture of these fluids as the output. The different fluids in this model are represented by ink colored liquids. Mixing of these fluids leads to fluids with different

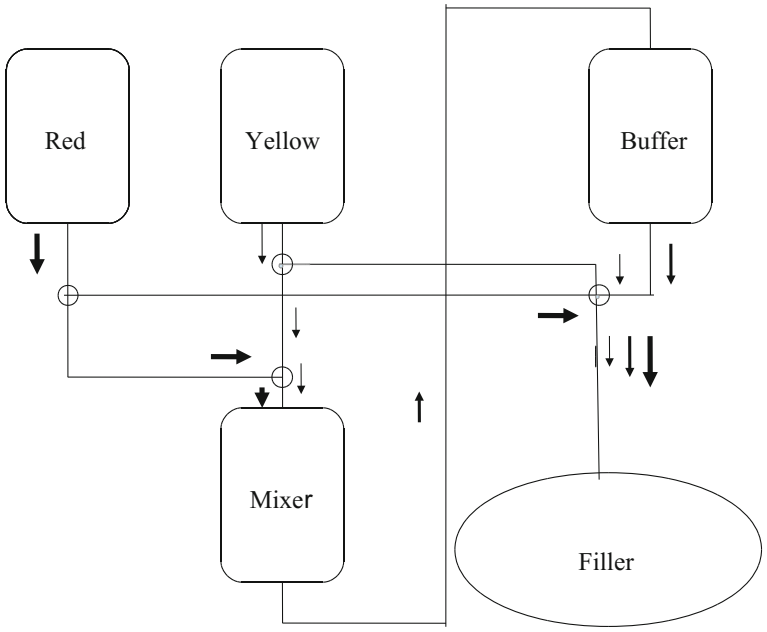


**Fig. 6.20** Paint factory

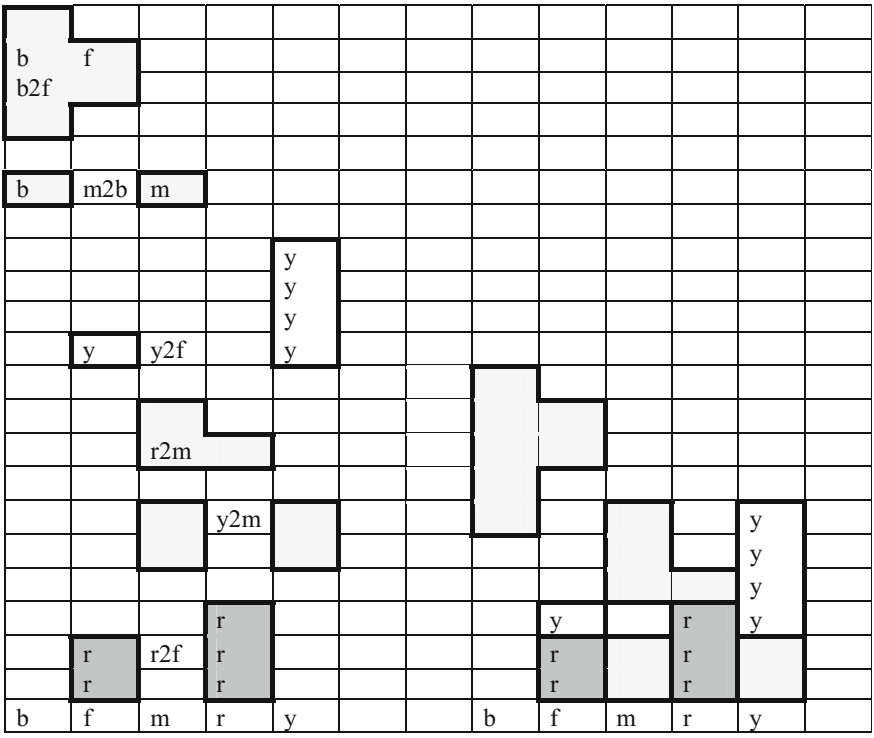


**Fig. 6.21** Heaps of pieces associated to paint factory

colors and the model is therefore better known as the paint factory. The inputs for the paint factory are fluids with the primary colors red, r, and yellow, y. The output can be both primary colors and secondary colors as orange. The primary colors can be injected into cups directly in the filling station or injected in the mix vessel, in order to be mixed. To transport the fluids the either the mix vessel or the filling station, the paint factory is equipped with a set of valves, pumps, vessels, sensors and pipes.

Figure 6.21 shows the heaps of pieces associated to paint factory.

The notations are: b-buffer, f-filler, m-mixer, r-red, y-yellow. They correspond to resources.

In the left part of Fig. 6.21 there are the pieces having a signification b, f, m, r, and y.

Dark cells correspond to red, white cells to yellow and intermediary shadow cells to orange mixtures. Notations as b2f means buffer to filler, y2m means yellow to mixer and so on. The pieces occupying a common vertical position corresponds to events occurring concurrently. Heaps are obtained by letting pieces to fall vertically.

The heap is shown in the right part of Fig. 6.21. It describes the timed automata.

The heap of pieces offers a compact data structure to keep track of the time delays in the timed automata.

The implementation of a polytope project allows taking into account not only the assembly of pieces as shown in Fig. 6.21 but also disassembly and re-assembly of these pieces.

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# Chapter 7
# Concepts and Knowledge

## 7.1 Engineering Design

### *7.1.1 Inferential Design Theory*

Developed by Arciszewski and Michalski (1994), the inferential design theory (IDT) proposes a framework for the integration of multiple conceptual design methods (Michalski 1993).

This theory is interesting due to the combination of concepts and knowledge parts that it proposes. To a certain extent, this combination implements a degree of creativity in the system.

IDT is claimed to be a unified framework due to its multi-strategic aspect. However, this theory does not explain the type of necessary knowledge at the conceptual design stage.

Figure 7.1 illustrates the general frame of IDT. The duality concept-knowledge is outlined.

Inferential design theory considers the memory as a combination of a representation space, design goals, initial knowledge background knowledge, and new knowledge, and sees concept generation as an inference process in which these basic elements are processed via deduction, analogy, or induction.

The results can be new knowledge and/or concepts. The theory also provides design knowledge transmutations which develop the initial processes of deduction, analogy, and induction.

Several types of knowledge transmutation are developed in inferential design theory, such as; replication/destruction, insertion/deletion, agglomeration/decomposition, association/disassociation, and so on.

Table 7.1 shows some pairs of knowledge transmutations. For any pair two opposite transmutations are given.

Alkharouf and Michalski (1996) presented the multi-strategy task-adaptive learning using dynamically interlaced hierarchies. Several basic knowledge



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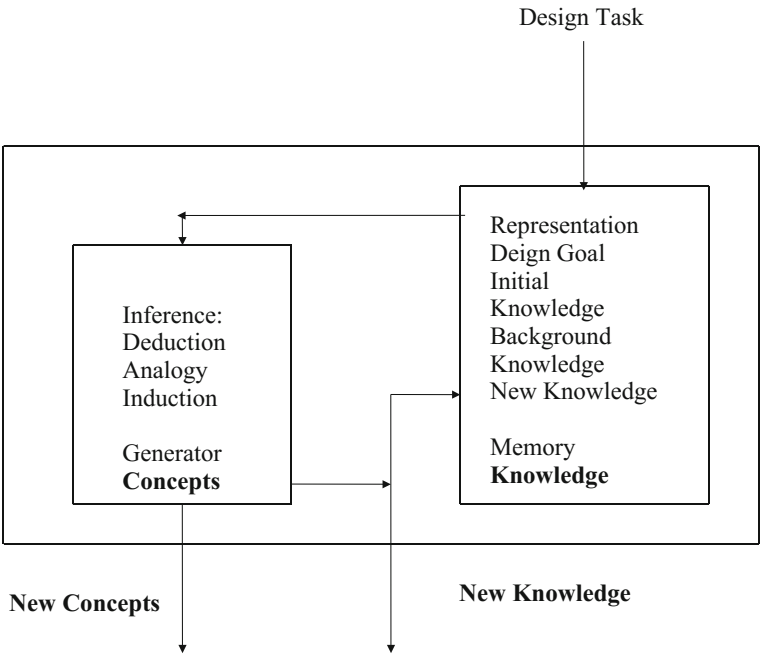


**Fig. 7.1** Inferential theory of learning

**Table 7.1** Transmutations

| | | |
|---|---|---|
| 1 | Association | Disassociation |
| 2 | Selection | Generation |
| 3 | Agglomeration | Decomposition |
| 4 | Characterization | Discrimination |
| 5 | Randomization | Reformulation |
| 6 | Insertion | Deletion |
| 7 | Replication | Destruction |
| 8 | Unsorting | Sorting |
| 9 | Generalization | Specialization |
| 10 | Concretion | Abstraction |
| 11 | Similization | Disimilization |

transmutations can be integrated using a knowledge representation based on dynamic interlaced hierarchies.

The implemented system includes an interactive graphical user interface for visualizing knowledge transmutations performed by the system. To a pair of transmutations, a pair of graph trees is generated. The two trees are similar. The idea behind the dynamically interlaced hierarchies learning is to apply a sequence of transmutations that transfer a given input into one or more outputs that satisfy a learning goal or in other words a particular project.

The dual aspects of knowledge transmutation types is significant. This suggests studying inferential design in the frame of dual graded graphs and Hopf algebras.

Hopf algebra is both algebra and the dual of algebra, the coalgebra, which are compatible. There is a product rule which describes association of the objects and a coproduct rule which describes the disassociation (Sweedler 1969; Joni and Rota 1979; Blasiak 2010).

The aspects recorded in first column in Table 7.1 are more close to the product rule while the last column aspects are more close to the coproduct rule.

The organization of inferential design theory integrates several concepts present in other design theories as concept-knowledge theory, axiomatic design theory and infused design theory.

### *7.1.2 Dual Graded Graphs for Design*

Hatchuel and Weil (2009) introduced concept-knowledge CK, theory to describe the design process (Agogué and Kazakçi 2014). A comparison between CK theories and IDT reveals similarities and differences (Choulier et al. 2011; Bernard et al. 2014).

The structure of knowledge developed in CK theory does not explicitly consider the transmutations that represent a powerful tool in inferential design theory.

In CK design theory a design process begins with a set of propositions that are accepted as true. They are in the knowledge K-space. The starting point of a particular design process is a proposition that is neither true nor false that is written in the concept C-space.

The design process consists in using proposition known in K to refine and expand the proposition in C and to use the proposition in C to create new true proposition in K (Hatchuel et al. 2002, Le Masson et al. 2006).

Concepts have the potential to be transformed into propositions of K but are not themselves elements of K.

In CK theory the design is a dual expansion process. It creates new concepts and new knowledge. This duality suggests using dual graded graphs for design purposes.

Most applications of CK theory utilize a tree for concepts C, but overlook the tree structure for knowledge K. This contrasts in part with the tradition to consider the trees of knowledge as basic knowledge representations (Maturana and Varela 1987; Sowa 2000).

It should be noted that more recent research develops the tree-like structure for both concepts and knowledge (Kazakçi 2013).

Kazakçi proposed design processes similar to that shown in Fig. 7.2.

Here the concept tree is a binary tree (Fig. 7.2a). This corresponds to the digit representation of concepts. The “0” and “1” corresponds to alternatives. More digits may be used if multiple variants or options should be considered.

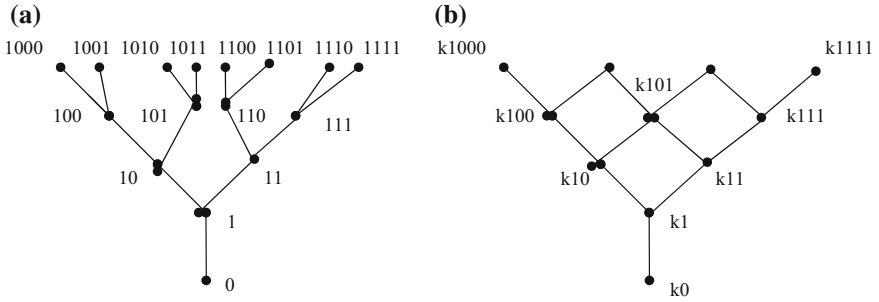


**Fig. 7.2** Concepts tree and knowledge tree

The reticulated tree presentation of knowledge shown in Fig. 7.2b was correlated to intuitionism (Kazakçi 2013).

Obviously there exists a correspondence between the elements of the tree of concepts and the reticulated tree of knowledge considered as a pair of trees.

States of knowledge may be resulting from the concept tree states by grouping.

For instance the knowledge state denoted here by k101 may be the source for concept states 101 and 110.

More general frames with two binary trees inspired by DGG (Fomin 1994) may be useful for design theory. The two trees shown in Fig. 7.3 are proposed for concepts and knowledge representation.

The U-tree from Fig. 7.3a is associated to concepts while the D-tree from Fig. 7.3b corresponds to the associated knowledge that may be redundant.

The D-tree is a reticulated tree. The difference between a tree structure and a reticulated tree or lattice structure is outlined by the DGG approach. In the U-graph tree each state can be realized in a unique way while in the lattice structure of the D-graphs several ways of realization are possible. This multiplicity ensures the flexibility of the dual schemas.

Figure 7.4 shows an example of concept-knowledge analysis based on the Manhattan project (Lenfle 2012).

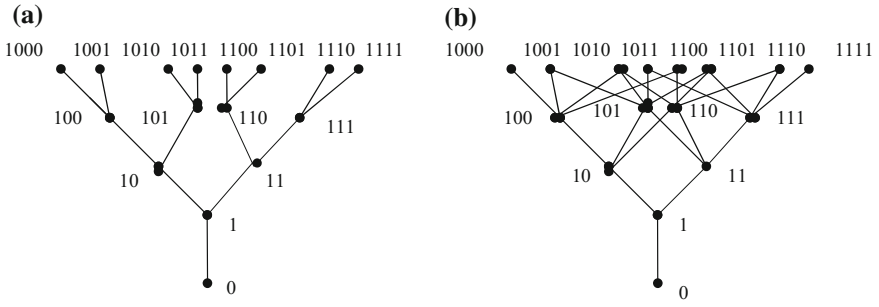


**Fig. 7.3** Dual graded graphs for concepts and knowledge

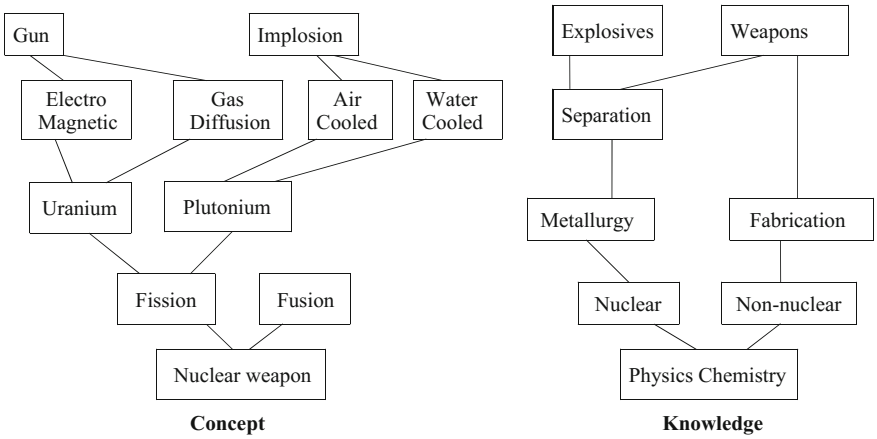


**Fig. 7.4** Concepts and knowledge trees for Manhattan project

The concept tree refers to the particular project: to use nuclear processes to design and build weapons.

The knowledge tree refers to the involved scientific and technological knowledge.

It shows the variants examined in different stages of the project.

Both concepts and knowledge are organized as reticulated trees.

It was a fission route giving the A-bomb and a fusion route giving the H-bomb.

The fission line was pursued initially.

The fissionable materials have been U235 and Pu239.

Separation of U235 from U238 was a difficult task. To perform this task 7 different methods have been identified in 1941 among which 3 have been used. Some separation methods as centrifugal separation have been discarded early but have been used later. Centrifuge separation, with gaseous diffusion, are now the main industrial processes to enrich uranium.

Producing plutonium involve the design and construction of nuclear reactors and the associated chemical engineering separation plants.

A number of variants as gun method or implosion method have been proposed for weapon design.

Observe that the knowledge tree reflects the long time development of technologies and sciences that allowed the fulfilling of the particular project formulated in the concept tree.

It is a duality relation between the two trees. They stand out as parallel and complementary.

The duality concept-knowledge as encountered in IDT and CK theories may be correlated to the Piaget and Garcia (1989) psychogenesis theory of science and technology.

Piaget and Garcia elaborated the hypothesis that there exists a parallelism between the particular problem solving and the historical development of the

involved sciences and technologies. The short history of an individual problem solving, that is the problem ontogeny, or in other words the concept tree, is considered as parallel to the evolutionary long history of a lineage that is, the problem phylogeny, or in other words the knowledge tree. According to Piaget and Garcia, ontogeny parallels phylogeny because the two are subject to similar external constraints. This general mechanism is relevant to both particular problem solving and to scientific activity itself.

Two trees in duality have been used in the axiomatic design theory too (Suh 1998; Goncalves-Coelho 2004; Malaek et al. 2015).

Suh uses a particular ontological structure. According to Suh design happens in two domains the functional requirements domain, FR and to design parameters domain DP.

FR is equivalent to what we want to achieve. FR is satisfied by defining and selecting the design parameters DP, in the physical domain.

Figure 7.5 shows the axiomatic design trees.

The two trees correspond to functional requirements, FR and to design parameters DP.

The work of the designer is to build a mapping between FR and DP trees.

Figure 7.6 shows an example of axiomatic design and zigzagging.

It refers to the goal to preserve a material by refrigeration.

The design parameters refer to compressor and fan. For these the functional requirements should be established. The zigzagging starts from FR0. From this the designer goes to the physical domain to conceptualize a design and determine its corresponding DP0.

Then the designer come back to the functional domain to create FR1 and FR2 at the next level that collectively satisfy the highest level FR. FR1 and FR2 are then the functional requirements satisfying the highest level DP1.

Zigzagging between the two trees corresponds to the interaction associated to the dual graded graphs. This suggests using both up, U and down D transitions in the axiomatic design.

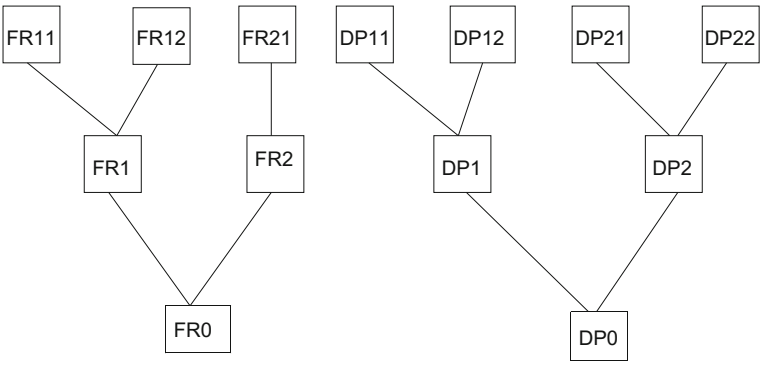


**Fig. 7.5** Axiomatic design trees

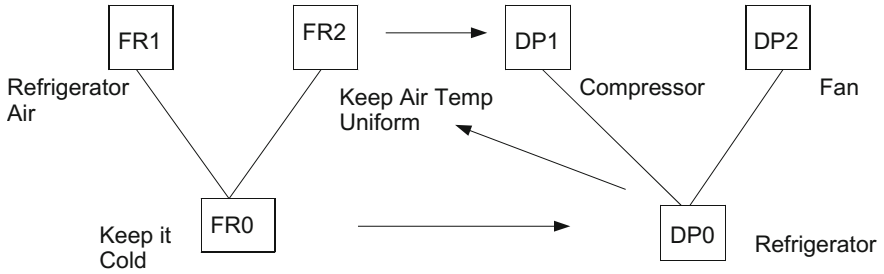


**Fig. 7.6** Axiomatic design zigzagging

Infused design is an approach for establishing effective collaboration between designers from different engineering fields (Shai and Reich 2004). Infused design has demonstrated new forms of creativity by generating designs by studying and transferring across disciplines designs.

Certain engineering domains may be considered as dual to one another. For instance there exists a duality between electrical and mechanical systems. This relation is systematically established through graphs representation. The two graphs are the original graph representation (OGR) describing the domain considered as original and the dual graph representation (DGR) describing the domain where the original information will be transferred.

DGR is more close to U-graphs while OGR is more close to D-graphs in previous representations.

The designs benefit from transfer between the two graphs.

The duality aspects encountered in many design theories is significant.

This suggests studying inferential design in the frame of dual graded graphs and Hopf algebras. There is a product rule which allows association or assembly of the objects and a coproduct rule which allow the disassociation or disassembly.

The evolutions on U-tree, concepts trees, FR-trees, DGR, are more close to the product rule while that for the D-trees, knowledge trees, DP-trees, OGR are more close to the coproduct rule.

The dual graded graphs theory applied for IDT, CK design, axiomatic design and infused design follows the natural trend to unify and standardize the design and control methods.

### *7.1.3 Algebra of Design*

Shapes are part of our everyday experience and play important roles in engineering design activities. Shapes come without apparent structure, therefore rendering any division into parts possible. The attempt to describe a shape inevitably leads to structuring the shape in terms of its certain parts or to shape decomposition.

This should be completed by the dual process of shapes composition or decomposition (Stiny 1991).

A computational framework of composition appropriate for the architectural and engineering design was outlined by Kotsopoulos (2005). Schemata and rules are put into use for the generation of compositions from scratch.

Figure 7.7 illustrates shapes compositions.

In any design, spatial elements are put together to form spatial compositions.

The dual processes of shape decompositions and their grammars have been studied too (Krstic 2005).

Computations with shapes may be conducted in the framework of shape grammars and related shape algebras (Stiny 1991).

Figure 7.8 illustrates the shape decomposition.

The shape in Fig. 7.8 may be described as the projection of a table having legs and a board.

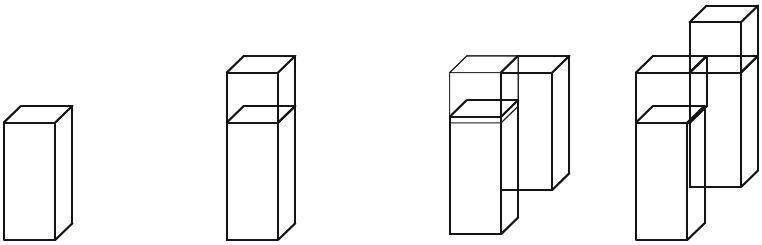

**Fig. 7.7** Shapes compositions

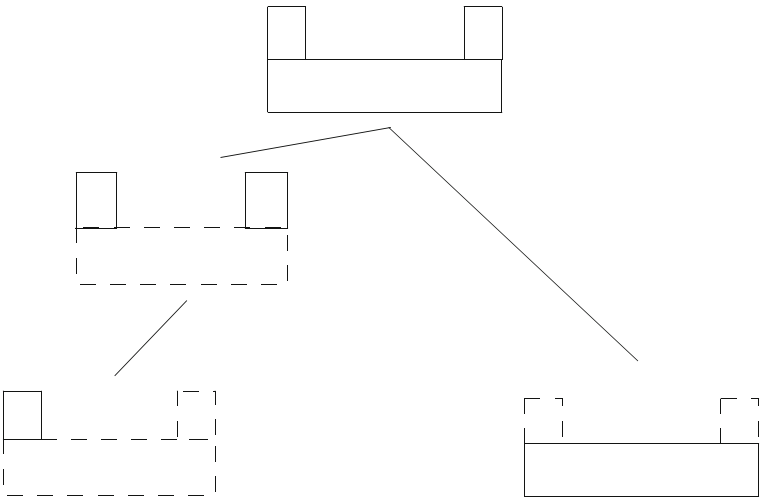

**Fig. 7.8** Decomposition of a shape

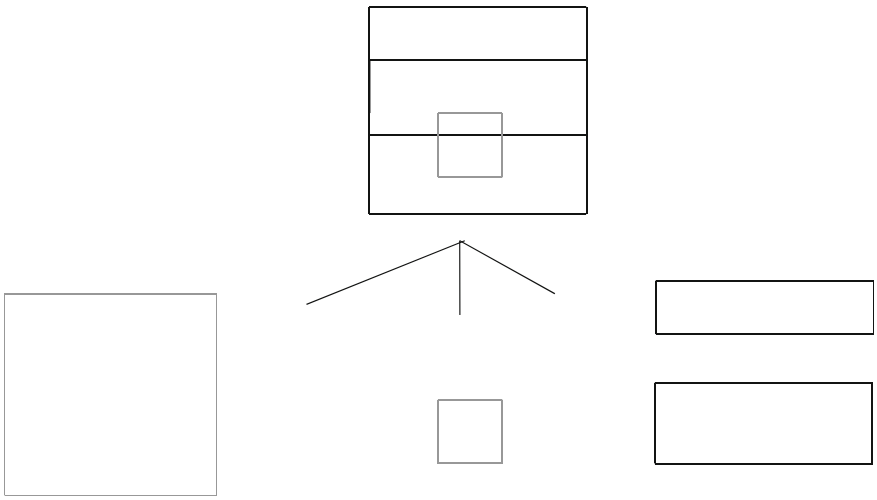

**Fig. 7.9** Decomposition of a construction

The dashed lines denote the decomposed elements of the shape.

Decompositions often appear in place of shapes functioning as their approximations.

Figure 7.9 shows another example of decomposition. The initial complex construction is decomposed in component shapes.

Figure 7.10 illustrates both the composition and decomposition (Babson and Chan 2000).

It suggests that the appropriate models for engineering design should be bialgebras and Hopf algebras. The algebra describes compositions and the coalgebra the decompositions.

To ensure reversibility for constructions and deconstructions Hopf algebras should be assigned to engineering designs.

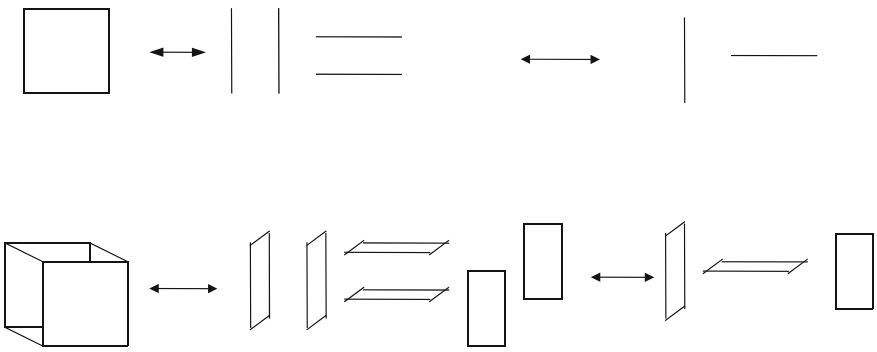

**Fig. 7.10** Composition and decomposition

## 7.2 Concept Analysis

### 7.2.1 Contexts and Concepts

The formal concept analysis, FCA, is a theory of data analysis which identifies conceptual structures among data sets.

The fact that every complete lattice can be represented as a hierarchy of concepts, which were conceived as sets of objects sharing a maximal set of attributes proved to be fruitful.

The main goal of FCA has been the support of rational communication and the representation and processing of knowledge based on the restructuring program (Wille 1996). Lattice theory is reworked in order to integrate and rationalize origins, connections to and interpretations in the real world.

FCA has capability of producing graphical visualizations of the inherent structures among data. FCA plays a prominent role in conceptual modeling by combining the ease of handling data base object that are defined through a list of properties to a mathematical model rooted in a formalization of logic by which reasoning is based on communicative rationality in the sense of pragmatism.

In FCA the concept understanding is considered as the basic unit of thought. A particular concept has both an extension and an intension.

FCA supposes that some relation between objects and properties is already established in the form of a context K = (G, M, I) where G is the set of objects, M is the set of properties or attributes and $I \subseteq G \times M$ is the incidence relation between objects and properties. A formal context K can best be represented by a table specifying which objects fall under which properties. This suggests that a context may be associated to classification and separation purposes.

The formal concepts of any formal context can be ordered in a hierarchy called more formally the context's concept lattice or Galois lattice.

Relational Concept Analysis RCA, was introduced as an extension of FCA for taking into account relations between objects. In this way, a concept is described with standard binary attributes but also with relational attributes (Bendaoud et al. 2008; Rouane et al. 2007, 2013). A relational attribute say r, describes the relation existing between objects that are instances of a concept say $c_1$, the domain of the r relation, with objects that are instances of another concept, say $c_2$, the range of relation r. RCA are organized within a relational context family composed of a set of contexts $K_i = (G_i, M_i, I_i)$ and a set of relations $r_k \subseteq G_i \times G_i$.

### 7.2.2 Multiple Separation Schemes

An example of FCA with a relation between multiple contexts is considered here (Iordache 2012, 2013).

It is a relation between properties or attributes.

**Table 7.2** Formal context for separations

| Compound | a | b | c | d |
|---|---|---|---|---|
| 1 | 1 | 1 | 0 | 1 |
| 2 | 0 | 1 | 1 | 0 |
| 3 | 1 | 0 | 0 | 0 |
| 4 | 0 | 0 | 1 | 0 |

**Table 7.3** Complementary formal context for separations

| Compound | α | β | γ | δ |
|---|---|---|---|---|
| 1 | 0 | 0 | 1 | 0 |
| 2 | 1 | 0 | 0 | 1 |
| 3 | 0 | 1 | 1 | 1 |
| 4 | 1 | 1 | 0 | 1 |

Separation operations transform a mixture of substances into distinct products. To allow separation, the components should differ in some properties, such as particle size, density, electric charge, solubility, volatility, substrate affinity, reactivity and so on.

An interesting case study corresponds to the separation of four compounds evaluated by four properties and by their complementary. This take into account that a compound separated by adsorption can be collected as adsorbed or as desorbed.

Table 7.2 shows a formal context for separations—4 compounds denoted 1, 2, 3 and 4 and 4 properties denoted a, b, c, d.

Table 7.3 shows the complementary formal context for separations—4 compounds 4 properties.

Table 7.3 shows the four complementary properties denoted α, β, γ, and δ.

If for instance, a, denotes adsorbability, then α denotes desorbability.

This corresponds to replacing of "1" by "0" and "0" by "1" in the tables of properties. The separation devices will change the light phase and heavy phase separation and reversely. In the case of absorption the separation may focus on non-absorbed or on absorbed compounds.

Figure 7.11 shows the concept lattice for separation—4 compounds 4 properties.

Figure 7.12 shows the concept lattice for complementary separation—4 compounds 4 properties.

### *7.2.3 Polytope for Lattices*

Figure 7.13 shows a polytope based on the example described by both Figs. 7.11 and 7.12.

Here S refers to the objects involved for instance the compounds to be classified or separated. K1 shows the information about objects contained by tables of properties.

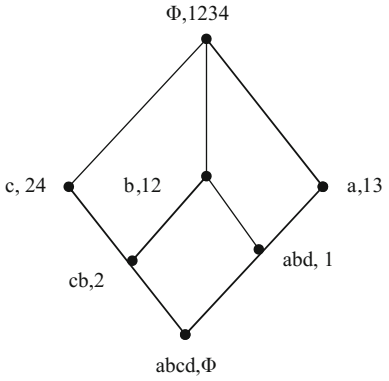


**Fig. 7.11** Concept lattice for separation—4 compounds 4 properties

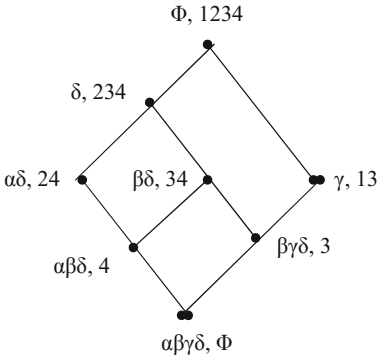


**Fig. 7.12** Concept lattice for complementary separation—4 compounds 4 properties

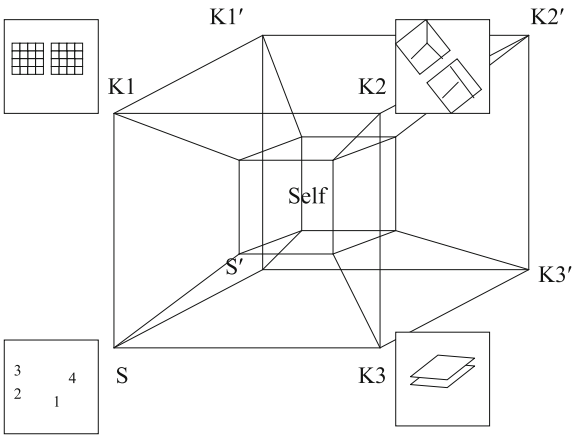


**Fig. 7.13** Polytope for formal concept analysis

There are two tables one for properties and the other for complementary properties.

K2 corresponds to FCA diagrams, the concept lattices.

K3 corresponds to the self-assembly of concept lattices.

We can identify:

- K0-Objects, Compounds
- K1-Objects with Properties
- K2-Lattices
- K3-Lattice of Lattices

The real separation process may switch for one to another of the concept lattices represented as superposed layers.

The multiplicity ensures the flexibility of the separation-integration network. Layered structures with reversible multiple linkages between layers allow self-evolvability.

Implementing the polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

The Self coordinated structures permit us to create a range of innovative potential combinations for schemas due to the interactions of layers.

Interactions of two lattices have been encountered in studies of knowledge discovery also (Joslyn et al. 2004). These imply to replace the poset by multi-posets.

A multi-poset is a union of partially ordered sets distinct two by two (Mao 2009).

Figure 7.14 illustrates the concept lattices interaction.

Transitions between lattices based on complementary properties are suggested. This means for separation case to shift the separation flow-sheet from heavy phase

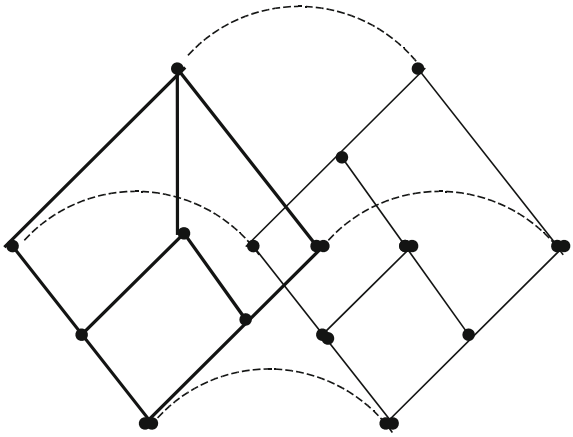

**Fig. 7.14** Concept lattices interaction

to light phase or reversely. The interface between separation lattices is where the most interesting interactions may take place. These are often the most valuable, diverse and productive elements

### 7.2.4 Meta-Meta-Modeling Approach

Falleri et al. (2007) show how to use Model Driven Engineering, MDE, in building generic FCA/RCA tools.

MDE is a software paradigm introduced to deal more with abstractions rather than code. In a MDE based development every produced or used artifact including code is a Model whose structure is defined by a Meta-Model. MDE assume the existence of a single Meta-Meta-Model which allows defining how a Meta-Model is structured.

Hinkelman et al. (2007) studied the relation between engineering design and Meta-Model architectures (Mellor 2004; OMG 2008).

The reality corresponds to S. The Model corresponds to K1.

The Model is a simplified representation of reality.

A Model is created with a modeling language. The modeling language specifies the building blocks or elements from which a Model can be made.

There can be different types of modeling languages depending on the kind of Model.

The main types of Models are:

- Graphical model
- Textual description
- Mathematical model
- Conceptual model
- Physical model

An example could be a table of objects and attributes a mathematical model as in FCA.

It defines for instance rules to combine object types and relations.

A Meta-Model defines the building blocks that can be used to make a model.

It defines:

- Object types that can be used to represent a model
- Relations between object types
- Attributes of the object types
- Rule to combine object types and relations

An example could be the concept lattice from FCA.

The Meta-Model is the abstract syntax while the modeling language is the concrete syntax.

A Meta-Meta-Model defines the language in which a Meta-Model can be expressed.

**Table 7.4** Meta-meta-model approach

| Layer | Description | Examples | FCA |
|---|---|---|---|
| Meta-meta-model K3 | Foundation for a meta-model<br>Architecture<br>Language to describe meta-models | Meta class<br>Meta attribute<br>Meta operation | Relational Concept Lattices |
| Meta-model K2 | An instance of a meta-meta model<br>Language to describe models | Class, attribute Operation | Concept Lattice |
| Model K1 | An instance of a meta-model<br>Language to describe information object domain | Product Details | Object Attribute Tables |
| Objects S | An instance of a model<br>Define specific information domain | Reality Objects | Reality |

Meta Object Facility, MOF is a common framework that is used to define other modeling frameworks within the OMG. MOF is itself a Meta-Meta-Model, a specification describing how one may build Meta-Models.

Thus for example MOF provides a specification for how to model the fact that an internet service has service endpoints. Table 7.4 summarizes information for 4 layer Meta-Model architectures.

Figure 7.15 shows the polytope projects associated to Meta-Meta-Model approach.

We can identify:

- S-Objects
- K1-Product Details
- K2-Class Attributes Operations
- K3-Meta Class Meta Attributes Meta Operations

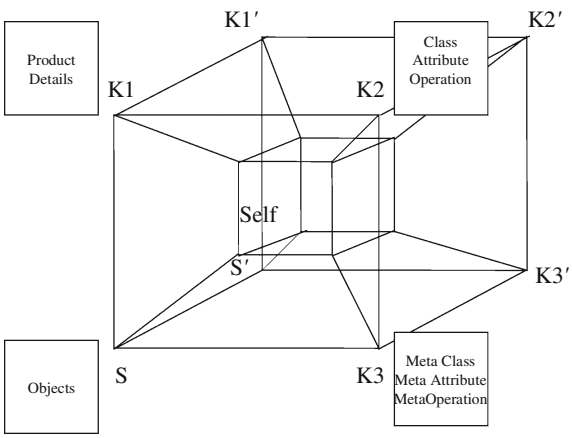


**Fig. 7.15** Meta-meta models approach

Implementing the polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complements this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$.

Modification of the direct sequence during reverse processing may occur.

Modeling from the direct sequence is replaced by de-modeling in the reverse sequence.

It is during these dual processes of modeling, de-modeling, followed by re-modeling that the variation allowing self-evolvability is generated.

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# Chapter 8
# Industrial Systems

## 8.1 Smart Manufacturing

### *8.1.1 Industry 4.0*

Industry 4.0 is a vision of integrated industry implemented by leveraging computing, software, and internet technologies. The label 4.0 refers to the vision of a fourth industrial revolution (Schwab 2016).

The 4.0 strategy emphasizes cooperation between industry and science to promote closer links between knowledge and skills. The reports of the industry 4.0 working groups, describe the using of Internet of Things technologies, communications, and web services in manufacturing. They create networks incorporating the entire manufacturing process that convert factories into smart factories (Zuehlke 2008; Kagermann et al. 2013). Linkages include smart machines, and production facilities that feature end-to-end integration, including logistic, production, marketing, and service. Industry 4.0 is projected to create closer cooperation between industry partners, suppliers and customers, and between employees, providing new opportunities for mutual benefit (Lee et al. 2015; Hermann et al. 2016; Hwang 2016).

The vision of industry 4.0 is significantly higher productivity, efficiency, and self-managing production processes where people, machines, equipment, logistics systems, and work-in-process components communicate and cooperate with each other directly.

A major goal is the application of mass production efficiencies to achieve make-to-order manufacturing of quantity one by leveraging embedded processing and communications. Production and logistics processes are integrated across company boundaries, creating a real-time lean manufacturing ecosystem that is more efficient and flexible. This facilitates smart value-creation chains that include all of the life-cycle phases of the product from the initial product idea, development, production, use, and maintenance to recycling.



O. Iordache, *Implementing Polytope Projects for Smart Systems*,
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Networking companies in the supply chain make it possible to optimize individual production steps and the entire value chain. For example, comprehensive real-time information enables companies to react during production to the availability of certain raw materials based on price, quality, and other factors for optimal efficiency. External linkages enable production processes to be controlled across company boundaries to save resources and energy.

The fabrication of physical or chemical objects is revolutionized by emerging materials science. Engineers may design and build from the molecular level, optimizing features and creating new materials, radically improving quality and reducing waste.

Devices and products are already appearing based on computationally engineered materials that literally did not exist a few years ago: novel metal alloys, graphene instead of silicon transistors and meta-materials that possess properties not possible in nature.

This era of new materials will be economically significant when combined with 3D printing, also known as direct-digital manufacturing-literally printing parts and devices using computational power, lasers and basic powdered metals and plastics. Already emerging are printed parts for high-value applications like patient-specific implants for hip joints or teeth, or lighter and stronger aircraft parts.

The digitization of industry is forecasted to foster new business models and present great opportunities for small-and medium-size enterprises. For example, to build low-volume metal parts, companies build virtual 3D models and use direct metal laser sintering, an additive process similar to 3D printing that deposits metal powder layers melted by laser, to create parts. These parts are fully dense metal with specified mechanical properties. Significantly, the 3D process can produce complex geometries that traditional machining processes are not capable of creating.

Conventional assembly manufacturing lines are synchronous, with predefined workflows based on production work orders running in enterprise business systems. Production steps are centrally communicated to each manufacturing station synchronized with the assembly line. In contrast, industry 4.0 is based on asynchronous manufacturing, with components in the production flow using self-identification technology to inform each machine and operator what needs to be done to produce the customized end product at each step of the production process. The use of new flexible machines that adapt to the requirements for the part being made is another capability of industry 4.0. This achieves a highly flexible, lean and agile production process enabling a variety of different products to be produced in the same production facility. Mass customization allows the production of small lots due to the ability to rapidly configure machines to adapt to customer-supplied specifications and additive manufacturing.

Industry 4.0 systems capture a wide range of data that can be used to improve performance and productivity with the application of analytics. Analytics are used in a number of ways, including real-time predictive maintenance, which helps manufacturing companies avoid interruption of production by unplanned machine failures on the factory floor-directly improving asset utilization. Another application

**Table 8.1** Digital manufacturing initiatives

| Country | Year | Name |
|---|---|---|
| Australia | 2013 | Next wave of manufacturing |
| Belgium | 2013 | Made different |
| Canada | 2015 | Smart manufacturing, industrie 4.0 |
| China | 2015 | Made in China 2025 |
| Denmark | 2012 | Made |
| France | 2015 | Industrie du futur |
| Germany | 2011 | Industrie 4.0 |
| India | 2014 | Make in India |
| Japan | 2015 | Industrial value chain initiative |
| Netherlands | 2014 | Smart industry |
| South Korea | 2015 | Manufacturing industry innovation |
| Sweden | 2014 | Produktion 2030 |
| UK | 2014 | High value manufacturing |
| USA | 2012 | Advanced manufacturing partnership |

of analytics is optimization of production operations, improving productivity and energy efficiency.

Industry 4.0 initiative is influencing thinking throughout the world, which in turn influences other initiatives and cooperative efforts.

The term Industrie 4.0 originated in Germany, but the concepts are in harmony with worldwide initiatives, including Advanced Manufacturing Partnership, Industrial Internet, smart manufacturing, and smart factories.

Table 8.1 shows the name of similar digital manufacturing initiative in different countries.

### *8.1.2 Smart Manufacturing Leadership Coalition*

The Smart Manufacturing Leadership Coalition (SMLC) was founded in the USA to overcome the costs and risks associated with the commercialization of smart manufacturing systems. The SMLC has not explicitly embraced Industry 4.0, but its vision and mission embrace many of similar concepts (Bryner 2012; Davis et al. 2012). The SMLC mission is to lead the industrial sector transformation into a networked, information-driven environment in which an open, smart manufacturing platform supports real-time, high-value applications for manufacturers. The mission is to optimize production systems and value chains, and radically improve sustainability, productivity, innovation, and customer service. SMLC intends to develop a cloud-based, open architecture manufacturing infrastructure and marketplace through the collaboration of manufacturing thought across industry, academia, consortia, and government.

SMLC goals include integrating plant-level systems and data, accelerating the development and deployment of reusable applications, providing an open and secure infrastructure accessible and affordable to all, and embracing evolving business needs and new market opportunities.

Greater manufacturing complexity, dynamics-based economics and radically different performance objectives requires the pervasive application of networked information-based technologies that transform a facilities focus to knowledge-embedded facilities, a reactive operational approach to one that is predictive, incident response to incident prevention, compliance to performance, and vertical decision making to local decision-making with global impact. Existing assets need to become globally competitive while the installed base of equipment runs its investment life cycle. Operating costs need to be lowered. Performance will need to be responsive to multi-faceted objectives. Advanced manufacturing and advanced networked information and computation technology will become significant.

The manufacturing workforce with advanced training and skills is the key competitive advantage as dynamic management and operation of demand-driven product profiles increase and as innovation and faster time-to-market for new products becomes a key economic driver. Small, medium and large manufacturers will depend on training and skills and the manufacturing workforce will distribute throughout the supply chain, advanced technology suppliers, innovation and start-up companies. Workforce training will no longer be about vertical factory operations but about dynamic interaction, innovation, rapid product changes, and new products to market all with sustainable operations spread across a widely distributed base of small and large companies. Not only will workforce training need to address a dramatically distributed manufacturing approach but also the technologies that support it. Smart manufacturing envisions the enterprise that integrates the intelligence of the customer, its partners and the public. It responds as a coordinated, performance-oriented enterprise, minimizing energy and material usage while maximizing environmental sustainability, health and safety and economic competitiveness. Business, operations, management, workforce and manufacturing process transformations are in response to new ways of reasoning about the manufacturing process. Smart manufacturing has been defined as the dramatically intensified application of manufacturing intelligence throughout the manufacturing and supply chain enterprise to both lead and respond to a dramatic and fundamental business transformation toward demand-dynamic economics, performance-based enterprises, demand-driven supply chain services and broad-based workforce involvement and innovation. This intensification of manufacturing intelligence comprises of the real-time understanding, reasoning, planning and management of all aspects of the enterprise manufacturing process and is facilitated by the pervasive use of advanced sensor-based data analytics, modeling, and simulation. SMLC is committed to a comprehensive vision in which technology and the business, operating and workforce models are transformed in concert to achieve a steep change in manufacturing productivity with respect to value add product economics. The deployment of smart manufacturing involves complex on-the-ground detail, difficult applications of technical and operational approaches,

difficult business models, the management of significant risk, and the need for research and development in new technologies, business models and organization engineering. The SMLC comes with a set of goals that no one company can accomplish alone:

- Integrate the intelligence of the customer, partner and public throughout the manufacturing supply chain
- Develop the collective capacity to respond as coordinated factory and supply chain enterprises
- Perform against new cross factory and supply chain key performance indicators that are radically different from traditional output/input metrics
- Increase the base of workforce innovation
- Increase productivity and quality by lowering the cost of IT infrastructure, sensing and the pervasive deployment of modeling and simulation
- Build equivalent capability across small, medium and large enterprises together
- Build a workforce that is trained in performance oriented decision making
- Define the technology research and development that is needed to achieve the full vision

### *8.1.3 Reference Architectures*

The Industrial Internet is an internet of things, machines, computers and people enabling intelligent industrial operations using advanced data analytics for transformational business outcomes, and the Industrial Internet Consortium (IIC) is devoted making the Industrial Internet a reality.

The reference architecture addresses the Industrial Internet problems by providing common and consistent definitions in the system of interest, decompositions, and design patterns, and provides a common terminology to discuss the specification of implementations so that options may be compared.

Industry 4.0 and related initiatives recognize that efficiently building self-managing production processes requires open software and communications standards that allow sensors, controllers, people, machines, equipment, logistics systems, and products to communicate and cooperate with each other directly. Future automation systems must adopt open source interoperability software application and communication standards similar to those that exist for computers, the internet, and cell phones.

Industry 4.0 demonstrations acknowledge this by leveraging existing standards, including the ISA-88 batch standards, ISA-95 enterprise-control systems integration standards, IEC 6-1131-3, and others.

The harmonization of standards worldwide took another step forward when providers of the Platform Industry 4.0 and the Industrial Internet Consortium (IIC) met to explore the potential alignment of their two architecture

efforts-respectively, the Reference Architecture Model for Industry 4.0 (RAMI4.0) and the Industrial Internet Reference Architecture (IIRA).

The OPC Foundation and Object Management Group (OMG) initiated a collaborative strategy for technical interoperability that encompasses the OPC Unified Architecture (OPC UA) and the OMG Data Distribution Service (DDS) standard.

These significant cooperative efforts recognize that manufacturing has worldwide interdependencies requiring common standards and interoperability (OMG 2008).

The Reference Architectural Model Industry 4.0, RAMI 4.0, consists of a three-dimensional coordinate system that describes all crucial aspects of industry 4.0. In this way, complex interrelations can be broken down into smaller and simpler clusters.

The Hierarchy Levels axis is based on the levels from IEC 62264, the international standards series for enterprise IT and control systems.

These hierarchy levels represent the different functionalities within factories or facilities.

In order to represent the industry 4.0 environment, these functionalities have been expanded to include work pieces, labeled Product, and the connection to the Internet of Things and Services, labeled Connected World.

The Life Cycle and Value Stream axis represents the life cycle of facilities and products, based on IEC 62890 for life-cycle management. Furthermore, a distinction is made between types and instances. A type becomes an instance when design and prototyping have been completed and the actual product is being manufactured.

RAMI 4.0 combine the basic elements of industry 4.0 in a three-dimensional layer model. Based on this framework, industry 4.0 technologies can be classified and further developed.

The Layers axis show six layers on the vertical axis and serve to describe the decomposition of a machine into its properties structured layer by layer, that is, the virtual mapping of a machine. Such representations originate from information and communication technology, where properties of complex systems are commonly broken down into layers.

These six layers are:

- Asset: representation of reality, such as a technical subject,
- Integration: providing computer processing information of assets,
- Communication: standardization of communication, using a unified data format,
- Information: software environment for event pre- processing,
- Functional: modeling environment for services that support business processes,
- Business: business models and the resulting business process

Within these three axes, all crucial aspects of industry 4.0 can be mapped, allowing objects such as machines to be classified according to the model.

Highly flexible industry 4.0 concepts can thus be described and implemented using RAMI 4.0. The reference architectural model allows for step-by step migration from the present industrial stage into the world of industry 4.0.

RAMI 4.0 integrate different user perspectives and provide a common understanding of industry 4.0 technologies. With RAMI 4.0, requirements of sectors—from manufacturing automation and mechanical engineering or chemical process engineering—can be addressed in standardization committees. Thus, RAMI 4.0 provide a common understanding for standards and use cases.

RAMI 4.0 can be regarded as a 3D map of industry 4.0 solutions. It provides an orientation for plotting the requirements of sectors together with national and international standards in order to define and further develop industry 4.0.

### *8.1.4 Generic Smart Grid Architecture Model*

The generic Smart Grid Architecture Model, SGAM, can act as a reference designation system in order to describe smart grid technical use cases as well as business cases.

The approach used in SGAM for reference designation proved its value, and it is necessary to follow basic guidelines for successful adoption of derived models for other domains (Fang et al. 2012; Uslar and Engel 2015).

One of the key challenges resulting from the Smart Grid vision is to handle complexity in the new distributed systems landscape. The Smart Grid, being a true system-of-systems is a prime example for the increasing complexity that emerges in any distributed system.

SGAM provides the means to express various domain-specific viewpoints on architecture models by the concepts of so called Domains, Zones and Layers.

Figure 8.1 shows the Layers for the original SGAM model for reference designation of standards.

The elements of the polytopic architecture from Fig. 8.1 have been identified as follows:

- S-Component
- K1-Communication
- K2-Information
- K3-Function

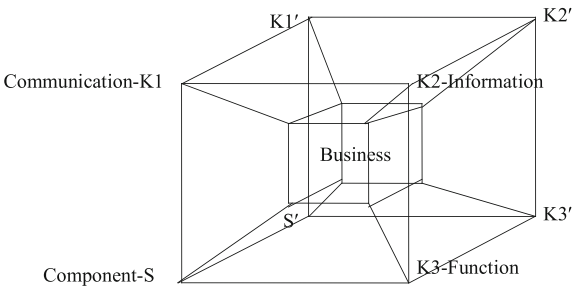


**Fig. 8.1** Layers for SGAM

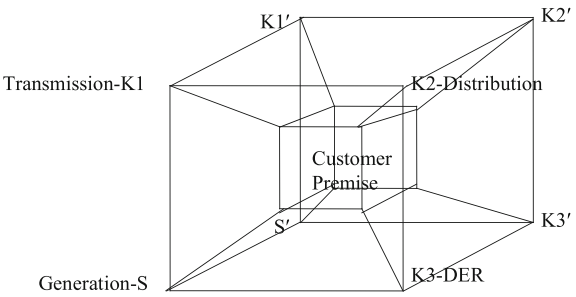


**Fig. 8.2** Domains for SGAM

- Self-Business

Business is identified as the Self of this polytope.

The Domains of SGAM regard the energy conversion chain and include: generation (conventional and renewable bulk generation capacities), transmission (infrastructure and organization for the transport of electricity), distribution (infrastructure and organization for the distribution of electricity), DER (distributed energy resources connected to the distribution grid) and customer premises (both end users and producers of electricity, including industrial, commercial, and home facilities as well as generation).

Figure 8.2 shows the Domains for the original SGAM.

The elements of the polytopic architecture are identified as follows:

- S-Generation
- K1-Transmission
- K2-Distribution
- K3-DER
- Self-Customer Premises

Customer Premises are identified as the Self of this polytope.

The hierarchy of power system management from the automation perspective is reflected within the SGAM by the following Zones: process (physical, chemical, biological or spatial transformations of energy and the physical equipment directly involved), field (equipment to protect, control and monitor the process of the power system), station (areal aggregation level for field level), operation control (power system control operation in the respective domain), enterprise (commercial and organizational processes, services and infrastructures for enterprises), and market (market operations possible along the energy conversion chain).

Figure 8.3 shows the Zones for the original SGAM.

The elements of the polytopic architecture are identified as follows:

- S-Process Field
- K1-Station
- K2-Operation Control
- K3-Enterprise
- Self-Market

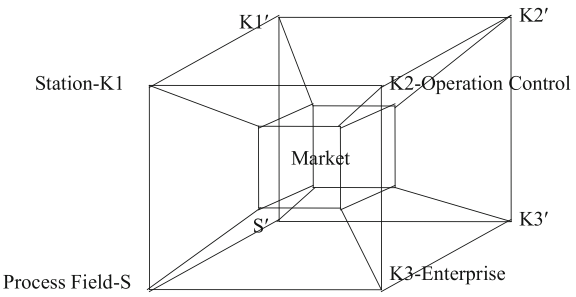


**Fig. 8.3** Zones for SGAM

Market is identified as the Self of this polytope.

SGAM may be represented using multi-level polytopes. Layers covers coarser granularity that Domains and these coarser granularity than Zones.

Reference architectures based on SGAM as generic reference architecture has been presented by Uslar and Engel (2015).

The Smart City Infrastructure Architecture Model (SCIAM) is one particular new derivative from the original SGAM model. The roadmap for Smart Cities is based on the original model of the SGAM. Instead of the business layer, an action layer was proposed.

As for Domains and Zones, new axes have been developed.

The Zones cover a mostly hierarchical way of structuring for physical locations. Market, Enterprise, Operation, Station and Field as well as Process, forms the Zones axis. This list can be considered a natural ordered list. In addition to this, the Domains consist of Supply/Waste Management, Water/Waste Water, Mobility and transport, Healthcare and Civil Security, Energy, Buildings as well as Industry.

The Electric Mobility Architecture Model (EMAM) is a particular architecture which is currently being developed in the context of the IT for electric vehicles programs.

It is a need for a consolidated use case collection and then deriving actors and technical requirements from them which will provide the basis of changing the granularity of the individual axis aspects. Re-using the SGAM in terms of modeling electric mobility is required.

The concept of the Home and Building Architecture Model (HBAM) has been developed to come up with a Standardization Roadmap on Smart Home and Building.

The Layers have been renamed to application, function, data model, interface and protocol and finally component.

The Zones axis contains the electronic health, building automation, physical security, consumer electronics and energy domain. Just like with the SCIAM more domains than one are addressed, but this time in the Zones area. The Domain axis has been structured with the lanes of devices, interfaces, control, accesses and data exchange.

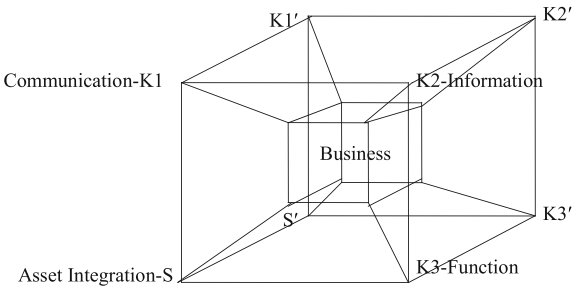


**Fig. 8.4** Layers for RAMI 4.0

The Reference Architecture Model for Industry 4.0 (RAMI 4.0) is an advanced derivative of SGAM (Uslar and Engel 2015). In addition to business, function, information, communication and asset representing component, a new layer called integration was introduced. The Domain and Zone axis are not custom taxonomies but are based on the IEC 62890 value stream chain or the IEC 62264/61512 hierarchical levels, respectively.

Figure 8.4 shows the Layers for RAMI 4.0.

The elements of the polytopic architecture are identified as follows:

- S-Asset Integration
- K1-Communication
- K2-Information
- K3-Function
- Self-Business

Business is identified as the Self of this polytope.

For this polytope presentation the asset and integration are considered as a single layer.

Figure 8.5 shows the Levels for RAMI 4.0.

The elements of the polytopic architecture from Fig. 8.5 are identified as follows:

- S-Product Field
- K1-Control Station
- K2-Work Unit

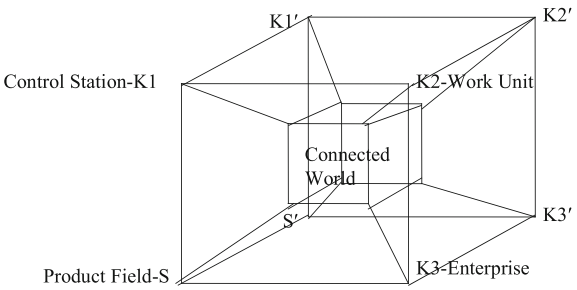


**Fig. 8.5** Levels for RAMI 4.0

- K3-Enterprise
- Self-Connected World

Connected world is identified as the Self of this polytope.

The model harmonizes different user perspectives on the overall topic and provides a common understanding of the relations between individual components for industry 4.0 solutions. Different industrial branches like automation, engineering and chemical process engineering have a common view on the overall systems landscape.

## 8.2 Systems Development

### *8.2.1 V-Model*

V-model is a general reference model for complex systems design and validation. A large number of different types of the V-models are used in industry (Estefan 2007; Strang and Anderl 2014).

V-model is suitable for presenting specification phases and associated validation test phases. The individual validation tests—acceptance tests, system tests and integration tests—are executed alongside the corresponding specification documents, user requirements and system specifications or technical specifications.

The V-model always offers a simplified and easily understandable presentation of the approach when validating is required between the specification and test phases.

The V-model was given its name from the presentation of the letter V in which the left-hand part represents the specification and design phases while the right-hand part the validation and test phases. The left side of the V-model represents the decomposition that is the refinement of design, while the right side describes the composition that is assembly or integration tasks.

Horizontal lines are drawn between the left- and right-hand parts of V-model. This illustrates that a dependency and a dialogue exists between the specification input, left-hand part, and the validation test phase output, right-hand part.

Figure 8.6 outlines the individual phases of the V-model.

The elements of the associated polytopic architecture from Fig. 8.6 are identified as follows:

- S-Detail Validation
- K1-Integration Validation
- K2-System Validation
- K3-User Acceptance Validation

Implementing polytope project starts from the direct sequence $S \rightarrow K1 \rightarrow K2 \rightarrow K3$ and complete this by the reverse sequence: $K3' \rightarrow K2' \rightarrow K1' \rightarrow S'$ (Iordache 2012, 2013).

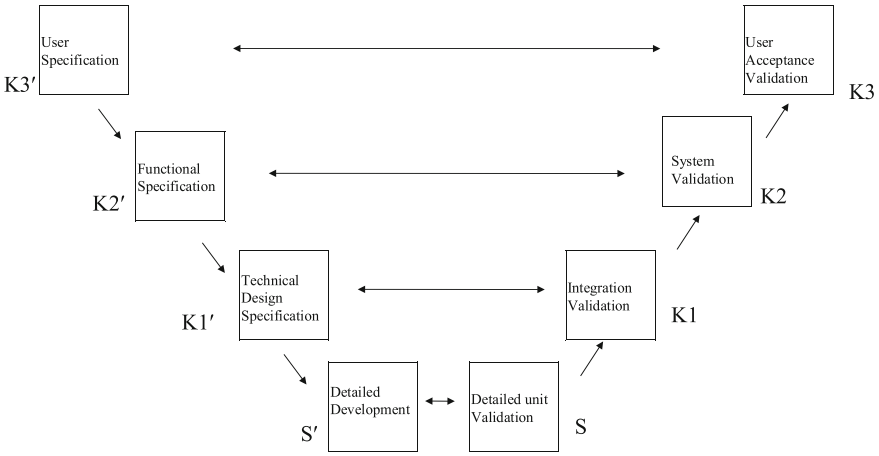


**Fig. 8.6** V-model

The right-hand side corresponds to the direct sequence while the left-hand side corresponds to the reverse sequence.

One could identify the levels in the reverse sequence shown in Fig. 8.6 as:

- K3′-User Specification
- K2′-Functional Specification
- K1′-Technical Design Specification
- S′-Detailed Development.

Figure 8.7 shows the polytope for V-model presented in Fig. 8.6.

The user requirement specification document contains either the process or the function-based requirements of the users and operators or the system owner.

The development and writing of requirements may vary in the context of the functional or process related basis. It is recommendable to write requirements on a process-based interpretation. In the functional specification the user requirements

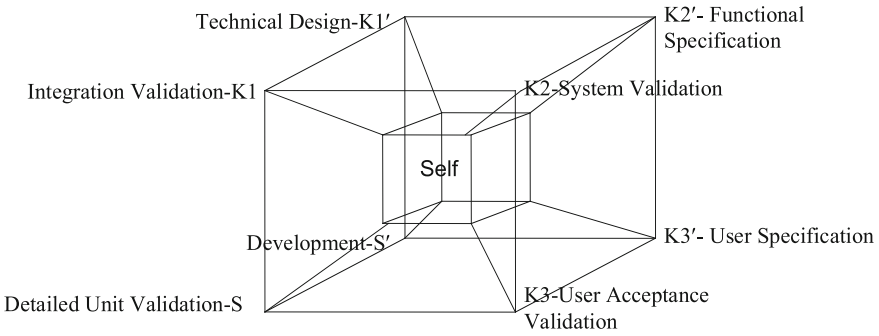


**Fig. 8.7** Polytope for V-model

are transformed further in functional terms for the purpose of the system implementation.

The technical specification design is an explanation for the programmer or the developer implementing the system function.

In program development, the technical specification is translated into an executable program. The technical design can also contain the specification of the required hardware and may comprise several parts. The unit validation test is related to the testing phase of the logical software modules or units.

The integration validation test is used for verifying the fulfillment of the technical specifications and the correct interactions between the different units or modules.

In the system validation the system is checked against the system specifications.

In the acceptance requirements the system is checked against the user requirements.

Currently, the development of mechatronic systems is often based on the V-model for the development of mechatronic systems according to guidelines which was derived from the original V-model for software development (Gausemeier and Möhringer 2003).

A case study, the template based V-model design analyzed by Kazenbach et al. (2007) is presented in Fig. 8.8.

The design process using templates follows a V-model as presented in Fig. 8.8.

The V-model starts from layout definition consisting of the basic structure, for instance body-in-white of a car (Kazenbach et al. 2007). It is then refined to provide details through the instantiation of templates, first assembly templates, then part templates and finally feature templates for the detailing phase. Then the various parts are assembled or integrated to reach the final design. During the V-model implementation, study templates are applied at several levels to evaluate the design.

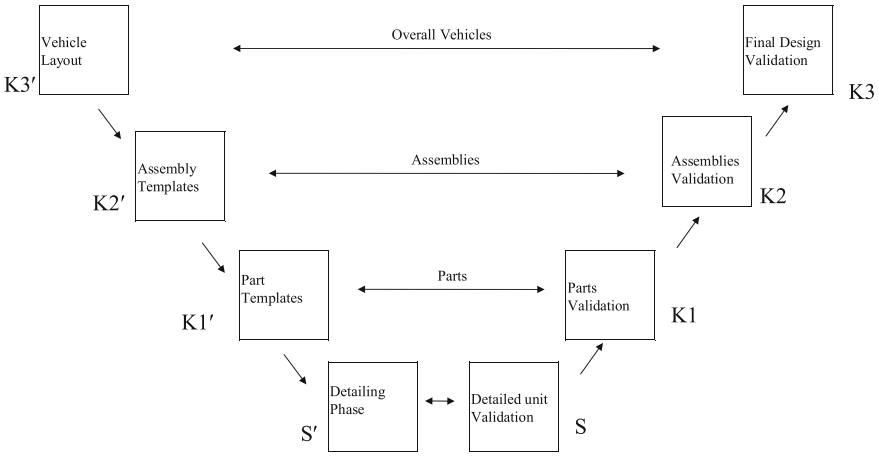


**Fig. 8.8** Template based V-model

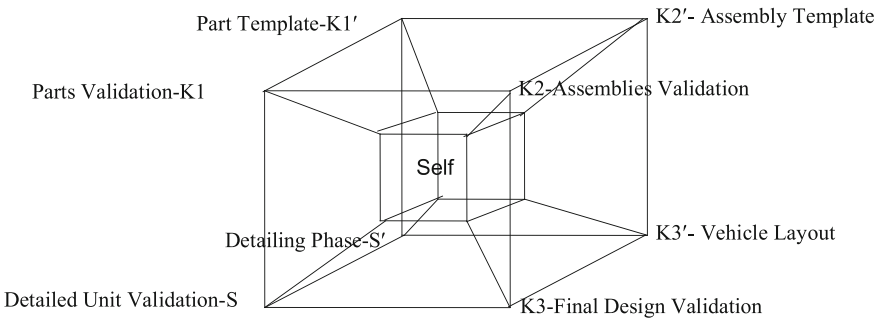


**Fig. 8.9** Polytope for template based V-model

Templates allow standardizing the design concepts and share them between several products. A study of the human factors regarding template use has been conducted. The objective was to evaluate the human factor in the adoption of templates aiming at the standardization of the process and to improve how templates are designed in order to facilitate its acceptance.

Figure 8.9 shows the polytope for template based V-model.

The elements of the polytopic architecture shown in Fig. 8.9 are identified as follows:

- S-Detailed Unit Validation
- K1-Parts Validation
- K2-Assemblies Validation
- K3-Final Design Validation

Implementing polytope project starts from the direct sequence S → K1 → K2 → K3 and complete this by the reverse sequence: K3′ → K2′ → K1′ → S′. One could identify the levels in the reverse sequence for instance:

- K3′-Vehicle Layout
- K2′-Assembly Template
- K1′-Part Template
- S′-Detailing Phase

## *8.2.2 Polytope Projects for Continuous Engineering*

Continuous engineering represents a new approach to systems engineering. It retains the overall systems focus, levels of abstraction, and core activities that form the basis of systems engineering but puts a new spin on how the activities are conducted. It also adds some fresh ingredients to pull in market and operational

knowledge from outside traditional processes and suggests ways to exploit strategic assets, such as engineering data and reusable code.

Figure 8.10 shows the V-model for continuous engineering approach.

In continuous engineering, the V no longer represents a sequential series of steps, as did the traditional V-model for systems engineering. Instead, it represents activities that are conducted iteratively and, to the greatest extent possible, in parallel, as needed throughout the product development process, relationships between activities, and linkages among engineering, operational, and market data.

So, for instance, requirements (left side of the V) are updated as changing or refined user needs are discovered from system verification or new operational data becomes available (right side of the V). Updated requirements in turn trigger changes in design, development, and testing. The middle of the V represents the ongoing interactions between left-side-of V activities and right-side-of V activities. This augments the relationships already spelled out by the shape of the V itself - requirements are related to designing, design is related to development, and so on, with the base of the V representing the implementation and embodiment of the requirements. The focus needs to be on actual running systems that may be virtual models, so teams can focus on executing system scenarios to manage risk and validation assumptions throughout the project life cycle.

Figure 8.11 shows the polytope project for continuous engineering approach.

The elements of the polytopic architecture are identified as follows:

- S-Detailed Validation
- K1-System Test
- K2-System Validation
- K3-Operation Maintenance Validation.

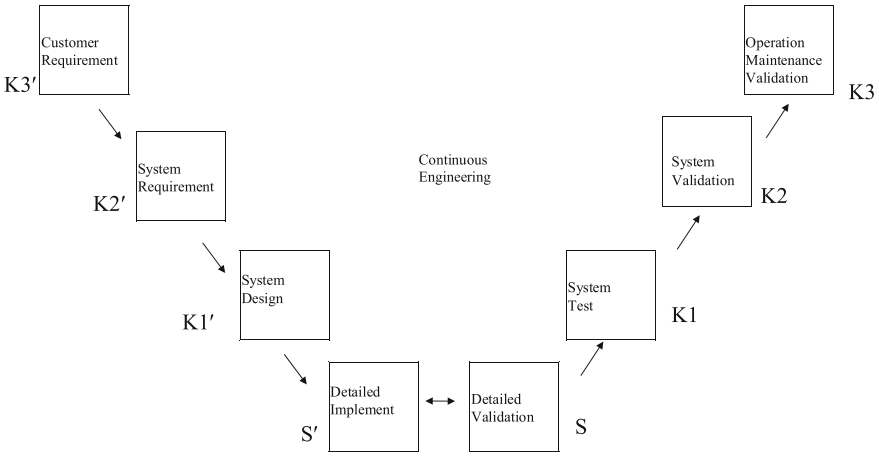


**Fig. 8.10** Continuous engineering V-model

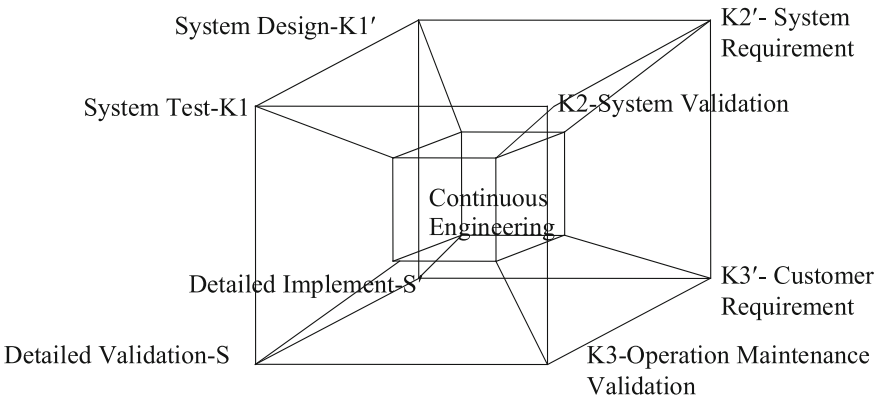


**Fig. 8.11** Polytope for continuous engineering

Implementing polytope project starts from the direct sequence S → K1 → K2 → K3 and complete this by the reverse sequence: K3′ → K2′ → K1′ → S′.

One could identify the levels in the reverse sequence for instance:

- K3′-Customer Requirement
- K2′-System Requirement
- K1′-System Design
- S′-Detailed Implement
- Self-Continuous Engineering

Continuous engineering from the middle of V-model is identified as the Self of this polytope project.

The basic levels are S, K1, K2 and K3 represented on the front face of the outer cube and S′, K1′, K2′ and K3′ represented on the back face of the outer cube of the polytope.

The dialogue between the two faces of the outer cube is mediated by the inner cube identified as the Self.

Figures 8.10 and 8.11 illustrate the importance of data relationships in an engineering context. Best practices in continuous engineering include sharing data across engineering disciplines, reusing design elements whenever possible, and incorporating market and operational data into product development activities.

Continuous engineering builds on the foundation of systems engineering practices by persistently applying engineering tools, methods, and techniques to address change and close gaps between current design plans and last requirements.

### 8.2.3 Logic and Hopf Algebras

The left side of the V-model represents the decomposition that is the refinement of design, while the right side describes the composition that is assembly or integration tasks. This suggests making use of Hopf algebras for V-model implementations (Sweedler 1969; Joni and Rota 1979; Blasiak 2010, Appendix B)

Combinatorial Hopf algebras emerged as the appropriate instrument in the study of composition and decomposition processes. The product or multiplication describes the assembly while the coproduct or comultiplication describes the disassembly.

A general problem for industrial systems development is that of specifying the utilized mathematical and logical models. The challenge is to describe the logic and the Hopf algebra behind the V-model or polytope project implementation. For instance, it would be of interest to identify the logic and the Hopf algebra behind the V-model design process at Daimler-AG (Katzenbach et al. 2007). The coproduct would describe the road from Vehicle Layout to Detailed Design while the product would describe the road from Detail Validation to Final Design Validation. The actual designs are a subset of what is logically possible.

Blute (1996) introduced Hopf algebras as a unifying framework for modeling several variants of multiplicative linear logic. By varying the Hopf algebra we are able to model the conventional commutative, non-commutative and cyclic linear logic. It is important to have a generic mathematical tool for modeling all these variants as this will allow direct comparison of the various theories and models. The structure of the variant we are modeling is reflected in the structure we require of the Hopf algebra. The particular Hopf algebra may be selected and will control the degree of symmetry of the model.

Benson (1989) introduced bialgebras as foundations for distributed and concurrent computation. Blute and Scott (1998) studied a Hopf algebra that is useful to describe concurrent processing. The key idea is the shuffle.

Consider a process containing many steps ordered by the logic of production.

Given two sequences a = x1x2 … xn and b = y1y2 … ym a shuffle is a permutation of the list x1x2, …, xn, y1, y2, …, ym such that the internal order of a and b is maintained in the result. Shuffle describes the switch between the sequences, a and b.

Let SH(a, b) denotes the set of all shuffles of a and b. The interleaving process naturally carries the structure of Hopf algebra.

It is an example of incidence Hopf algebra (Schmitt 1994).

Let X be a set and X* the free monoid generated by X. We denote the words that is the strings in X* by w, w′. The product is:

$$w \otimes w' \rightarrow w * w' = \sum_{u \in Sh(w,w')} u \tag{8.1}$$

Here Sh (w, w′) denotes the set of shuffled words of length |w| + |w′| obtained from w and w′. The coproduct is:

$$\Delta(w) = \sum_{w1w2=w} w1 \otimes w2 \tag{8.2}$$

Note that in the equation w1w2 = w we are using the original monoid multiplication of X*.

There exists also an antipode (Blute and Scott 1996).

Differential linear logic as introduced by Ehrhard and Regnier (2006) extends linear logic with an inference rule which is a version of differentiation. This may be correlated to decomposition task, that is, the refinement of design.

The corresponding structures called differential categories were studied by Blute et al. (2006, 2009). There is a natural transformation, called the deriving transform which models the differential inference rule. The relation with Faà di Bruno Hopf algebra is of interest for such studies (Figueroa et al. 2005).

The logical synthetic structure of integration was less studied than the differential logic.

It is an ongoing project to develop dual notions of integral linear logic and integral categories (Blute et al. 2010). Rota-Baxter Hopf algebras may be a source of inspiration for integral linear logic theory. Rota-Baxter algebras are associative Hopf algebras with an endomorphism which satisfies an abstraction of the integration by parts formula (Guo 2009). This algebra is appropriate for the study of compositions, that is, assembly or integration tasks.

Facing complexity is not only about differentiation bat also about integration and coordination.

The dual differential and integral linear logic may offer an answer to higher complexity problems as for instance modeling self-orientation for autonomous systems (Bartheye and Chaudron 2015).

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# Chapter 9
# Polytope Perspectives

## 9.1 Synopsis

### *9.1.1 Methodology*

Some of the basic steps of the polytope projects methodology are illustrated by examples and case studies in the following.

This helps in understanding where future studies heads and in implementing new polytope projects.

Consistent with Hartmann ontology, we refer to the four basic levels of reality: material, biological, cognitive and intelligent (Hartmann 1952). The associated abbreviations are: *Mat*, *Bio*, *Cog*, and *Intel.* Due to their specific role in this monograph, the mathematical objects pertaining to the intelligent level have been highlighted under the term *Math*. *Math* is included in *Intel.*

- Building blocks

  *Mat*: electrons, atoms, radicals, processes
  *Bio*: amino-acids, ribosome, cells, genes
  *Cog*: letters, words, records, signals, sensations, concepts, designs
  *Intel*: tools, devices, reactors, agents, programs, machines, manufacture, ideas, theories
  *Math*: lines, numbers, operations, graphs, propositions, equations, theorems

Polytope projects start by asserting a goal and this is significant for the selection of building elements. If a chemical reaction is studied we can start the study at the molecular level but if a chemical factory is studied we may start from devices or operations and evaluate their interactions.



O. Iordache, *Implementing Polytope Projects for Smart Systems*,
Studies in Systems, Decision and Control 92,
DOI 10.1007/978-3-319-52551-8_9

- Levels

  *Mat*: atoms-molecules-supramolecules-supra supramolecules (vesicles) (Lehn 2007); states- processes- processes of processes-processes of processes of processes (Iordache 2010)
  *Bio*: molec-organelles-cells-tissues-organs-organisms-populations-ecosystems
  *Cog*: words-propositions-phrases-texts; objects/properties-concepts-FCA/RCA (Ganter and Wille 1999)
  *Intel*: devices-structures-suprastructures-supra suprastructures; real systems-sensors-controls-actions; component-communication-information-function; texts-web 1.0-web 2.0-web-3.0 web 4.0; data-models-metamodels-meta meta-models (OMG 2008); manual-mechanical-electrical-electronic-digital industry
  *Math*: points-lines-polygons-polyhedrons-polytopes

It was observed that complex systems exhibit hierarchical self-organization in levels under selective constraints. Self-organization will occur when individual independent parts in a complex system interact in a jointly cooperative manner that is also individually appropriate, such as to generate a higher level organization.

Complex systems can be observed and described at different levels of investigation.

Levels may be decomposed in sub-levels, in sub-sub-levels and so on.

In some cases this decomposition shows self-similarity and reversibility by composition. Subject for debate are the relations between n-levels, n-categories and n-scales.

Reality levels have been associated to ontological categories (Poli 2001, 2007).

The ontological theory of levels considers a hierarchy of items structured on different levels of existence with the higher levels emerging from the lower but not reducible to the latter, as claimed by reductionism.

Poli has stressed the need for understanding causal and spatiotemporal phenomena formulated within a descriptive categorical context for theoretical levels of reality.

- Duality–Complementarity

  *Mat*: wave-particle, fission-fusion, composition-decomposition, oxidation-reduction, separation-integration, coagulation-dissolution, contraction-expansion, thermodynamics-kinetics
  *Bio*: anabolic (associative)-catabolic (dissociative), replication- metabolism, folding-unfolding, material-symbol, phenotype-genotype
  *Cog*: analysis-synthesis, coding-decoding, assimilation-accommodation, concept-knowledge, general-particular, extent-intent, explicit-implicit
  *Intel*: assembly-disassembly, design-verification, divergent-convergent, construction-deconstruction (Heidegger 1962), System 1-System 2 (Evans 2008), market-society
  *Math*: integration-differentiation, Hopf algebra (Sweedler 1969; Abe 1980), dual graded graphs (Fomin 1994), categorification-decategorification

Dual or complementary pairs are those things, events and processes in nature that may appear to be contraries but are mutually related and inextricably connected (Kelso and Engstrom 2006). Both aspect of a complementary pair are required for an exhaustive account of phenomena. Dual aspects are dynamic, contextual, dialogical and relational.

Complementarity manifests itself in the whole-part behavior of reality, in the energy-informational properties of reality.

Some modern ideas about brain organization have emerged that may provide support for dual representation of the cognitive and intelligent processes.

Complementarity approach finds a strong support in the studies of metastable coordination dynamics of the brain (Kelso 2002; Kelso and Tognoli 2009).

Metastability has been highlighted as a new principle of behavioral and brain function and may point the way to a truly complementary neuroscience. From elementary coordination dynamics it was shown explicitly that metastability is a result of a symmetry-breaking caused by the subtle interplay of two forces: the tendency of the components to couple together and the tendency of the components to express their intrinsic independent behavior. The metastable regime reconciles the well-known tendencies of specialized brain regions to express their autonomy, that is differentiation, and the tendencies for those regions to work together as a synergy, that is integration.

Cook (1986) model of the human brain provides a physiological basis for complementarity. Cook formulated the principle of dual control according to which systems pertaining to different levels of reality as the atom, the cell the brain and so on are isomorphic with respect to the duality of control mechanism. This isomorphism may be correlated to the search for the general reference architecture in polytope projects implementation.

Another step in this direction is the complementarist epistemology and ontology as developed by Ji (1995). Ji draws on the biology of the human brain, namely, the dual nature of its hemispheric specializations. The left and right hemispheres have relatively distinct cognitive functions, and the reality, as perceived and communicated by the human brain, is a complementary union of opposites (Ji 1995; Evans 2008).

Table 9.1 illustrates some of the hemispheric specialization of the human brain.

**Table 9.1** Hemispheric specialization

| | Right hemisphere | Left hemisphere |
|---|---|---|
| 1 | Synthetic | Analytic |
| 2 | Intuitive | Rational |
| 3 | Fast | Slow |
| 4 | Concrete | Abstract |
| 5 | Analogic | Digital |
| 6 | Associative | Dissociative |
| 7 | Specification | Generalization |
| 8 | Parallel | Sequential |
| 9 | System 1 | System 2 |

The dual aspects resulting from hemispheric specialization are significant. It suggests evaluating the correlation with dual graded graphs and Hopf algebras.

Generally speaking the Hopf algebra is both, the algebra and the dual of the algebra, the so-called coalgebra, which are compatible. There is a product rule which describes composing, associating or synthesis of the objects and a coproduct rule which describes decomposing, dissociating or analysis (Joni and Rota 1979).

The aspects recorded in first column in Table 9.1 are relatively close to the product rule (System 1) while the last column aspects are more close to the coproduct rule (System 2).

On a much finer-grained scale, Stephen Grossberg (2000) has drawn attention to the dual, nature of brain processes and explained how are the brain functionally organized to achieve self-adaptive behavior in a changing world. Grossberg (2000) presents one alternative to the computer metaphor suggesting that brains are organized into independent modules, into parallel processing streams with dual properties. Hierarchical interactions within each stream and parallel interactions between streams create coherent behavioral representations that overcome the complementary deficiencies of each stream and support unitary cognitive experiences.

Duality studies reveal upward and downward, forward and backward, divergence and convergence, composing and decomposing categorification and decategorification and other pairs of dual processes.

- Closure

  *Mat*: balance, conservation, molecular networks, reactions network, catalytic closure (Kauffman 1993, 2000), constitutional dynamic chemistry (Lehn 2007), algorithmic chemistry (Fontana 1991)
  *Bio*: homeostasis, cybernetics, hypercycle (Eigen and Schuster 1979), semantic closure (Pattee 1995, 2001), closure to efficient cause (Rosen 1991; Mossio et al. 2009), organizational closure (Maturana and Varela 1980), semantic biology (Barbieri 2003)
  *Cog*: Umwelt (von Uexküll 1973), circular schema (Piaget 1970, 1971)
  *Intel*: hermeneutic cycle (Heidegger 1962), operational closure (Luhmann 1995), embedded systems, cyber-physical systems, industrial internet
  *Math*: Axiomatic systems, circular-proofs (Blute 1996; Blute and Scott 1998)

Closure concepts play a prominent role in systems theory where may be used to identify the whole system in correlation with its environment and to define the autonomy of the systems. Different closure concepts are linked to different facets of complexity.

For example, a system is considered catalytically closed just in case every product of the system is also a catalyst in the system (Kauffman 1993, 2000). An autonomous agent must be an autocatalytic system able to reproduce and able to perform one or more thermodynamic cycles.

Constitutional dynamic chemistry is founded on a closure concept (Lehn 2007).

Supramolecular chemistry is intrinsically a dynamic chemistry in view of the fragility of the interactions connecting the molecular components of a supramolecular entity and the resulting ability of supramolecular species to exchange their constituents. The same holds for molecular chemistry when the molecular entity contains covalent bonds that may form and break reversibility, so as to allow a continuous change in constitution by reorganization and exchange of building blocks. These features define a Constitutional Dynamic Chemistry (CDC) on both the molecular and supramolecular levels. On the molecular level, CDC is expressed in dynamic combinatorial chemistry (DCC) an approach that uses self-assembly processes to generate libraries of chemical compounds. In contrast to classical combinatorial chemistry which is based on vast collections of prefabricated molecules, DCC implements dynamic libraries via the continuous inter-conversion between the library constituents by recombination of their building blocks. Spontaneous assembly-disassembly of the building blocks through reversible chemical reactions virtually encompasses all possible combinations, and allows the establishment of adaptive processes owing to the dynamic interchange of the library constituents. The merging of the features: information and programmability, dynamics and reversibility, constitution and structural diversity, points towards the emergence of self-adaptive and self-evolvable chemistry (Lehn 2007)

According to Pattee (1995, 2001) biological organization consists of the integration of two intertwined dimensions, which cannot be understood separately. On the one side, the organization realizes a dynamic and autopoietic network of mechanisms and processes, which defines itself as a topological unit, structurally coupled with the environment.

On the other side, it is shaped by the material unfolding of a set of symbolic instructions, stored and transmitted as genetic information.

The dynamic, that is, mechanistic and the informational dimensions realize a distinct form of closure between them, which Pattee labels semantic or semiotic closure. This concept refers to the fact that while symbolic information, must be interpreted by the dynamics and mechanisms that it constrains, the mechanisms in charge of the interpretation and the material translation require that information for their own production. Semantic closure, as an interweaving between dynamics and information, constitutes an additional dimension of organizational closure of biological systems, complementary to the operational or efficient one.

Autopoietic systems are also organizationally closed, that is they have a circular network of interactions, rather than a tree of hierarchically process (Maturana and Varela 1980).

The circularity and closure are correlated also to the "*Umwelt*" concept that was introduced by von Uexküll in theoretical biology to describe how cognitive organisms perceive and interpret their environments. The *Umwelt* was defined as the part of the environment that an organism selects with its specific sense organs according to its needs (von Uexküll 1973). *Umwelt* theory asserts that a complex system doesn't responds to its environment but rather to its perception of the environment. A complex system actively creates its *Umwelt*, through repeated

interactions with the environment. It simultaneously observes the world and changes it, the phenomenon which von Uexküll called a functional circle. The functional circle includes receptors and effectors. The sensory experience is based on interactions and these have specific purposes. The elementary unit of evolvable systems includes the functional circle of the following four parts: the environmental object, the receptors, the command generator and the effectors.

Circular reactions have been emphasized in the study of action schema done by Piaget (1970, 1971). Piaget called his general theoretical framework "genetic epistemology" because he was primarily interested in how knowledge develops in living organisms. Cognitive structures are patterns of physical or mental actions that underlie specific acts of intelligence and correspond to the stages of development.

The Piaget's action schema, which constitutes the foundation of his learning theory, is a cycle including three elements: a recognized situation, an activity that has been associated with this situation, and an expected result. The recognition of a situation involves assimilation, that is to say, the situation must manifest certain characteristics which the organism has abstracted in the course of prior experience. The recognition then triggers the associated activity. If the expected result does not occur, the organism's equilibrium is disturbed and an accommodation may occur, which may eventually lead to the formation of a new action scheme. Accommodation does not take place unless something unexpected happens.

Assimilation integrates new information in pre-existing structures while accommodation change and build new structure to understand information. The equilibration through assimilation and accommodation, takes into account three of the levels of the Hartman hierarchy, the material, the biologic level, more close to assimilation, and the cognitive level, more close to accommodation concept.

Piaget general equilibration theory offers a standpoint to consider the three level chains of interactions, namely biologic, cognitive and intelligent.

It can be observed that semantic closure, functional circle and circular reaction concepts have basic similarity despite the fact that they may refer to different levels of reality. They describe cycles or in other words loops of interaction between two or three successive levels or realms. Pattee focuses on two levels frameworks, the material versus biologic, or biologic versus cognitive, while von Uexküll and in part Piaget focuses on three level frameworks, material, biologic and cognitive level. It should be emphasized that some of the Piaget schemas embraces a four-level perspective including intelligence level (Piaget and Garcia 1989).

- Center-Self

  *Mat*: nucleus, catalyst, template, tile
  *Bio*: enzymes, ribosome, ribotype, cellular nucleus
  *Cog*: corpus callosum (Cook 1986), GW global workspace (Baars 2002), global landscape (Ehresmann 2012), rich club (Van Den Heuvel and Sporns 2011), dynamic core (Edelman 2003), post-formal stage (Piaget 1971)
  *Intel*: CE continuous engineering, cloud computing, market, business, web 4.0, Self

*Math*: Axioms, core arrays (Ceulemans et al. 2003), included middle (Lupasco 1947; Nicolescu 2002)

Centers are necessary to endorse the dialogue, coordination and coherence of the evolution on different levels. For polytope projects the Self focus and coordinates the multi-level self-evolvable frames.

The relation with concepts as "fold" (Deleuze 1988, 1993) "included middle" (Lupasco 1947; Nicolescu 2002) and "tilde" (Kelso and Engstrom 2006) is significant.

Following Lupasco, Nicolescu takes a transdisciplinary approach to nature and knowledge. Transdisciplinary knowledge, as based on the logic of the "included middle", necessarily leads to the inclusion of values and systemic understanding versus simple analytic reasoning. According to this logic, in every relation involving two separate levels of experience, there is a third level that belongs simultaneously to both. Complexity is the context in which this level of convergence takes place.

- Rhythms

  *Mat*: periodic chemical reactions, linear-cyclic processes, flow reversal
  *Bio*: hypercycle, biorhythms, meta-stability, chronotherapy, environmental rhythms
  *Cog*: cerebral, rhythms in problem solving, epistemology, circadian, development
  *Intel*: Pressure Switch Adsorption, Simulated Moving Beds, economical, social
  *Math*: Games, Process Semantics (Cockett 2006)

Modulated by the Self, the swinging rhythms "up" and "down", forward and backward, separating and integrating, composing and decomposing, constructing and deconstructing, dialoging between the two complementary or dual ways are crucial for polytope projects implementation.

### *9.1.2 General Theories*

*Mat*: Quantum theory, Self-organization theory
*Bio*: Hypercycle (Eigen and Schuster 1979), Complementarity (Kelso and Egstrom 2006), Cybernetics, Biosemiotics (Barbieri 2003)
*Cog*: Genetic Epistemology (Piaget 1971), Dual Process Theory, DPT (Evans 2008)
*Intel*: General System Theory, Ontology (Hartmann 1952), Epistemology of Deconstruction-Reconstruction (Heidegger 1962) Philosophical Categories (Peirce 1956)
Cyber-Semiotics (Brier 2008, 2009)
Reference Architectures in Industry 4.0: RAMI 4.0, IIRA, SGAM

*Math*: OMG: Data M0, Model M1, Meta-Model M2, Meta-Meta-Model M3 (OMG 2008)

Differential Linear Logic and Integral Linear Logic (Ehrhard and Regnier 2006; Blute et al. 2010), Hyperstructures (Baas 2009, 2015a, b), n-Categories.

In the domain of sciences of mater there exists a highly developed theory, the quantum chemistry allowing the successful classification of the elements in the chemical periodic table. The theoretical explanation of the chemical classification, by Schrödinger's wave equation and Pauli's exclusion principle, is a success of physics and chemistry in the 20th century. One can look at this theory from very diverse points of view that follow closely the above presented methodology. The building blocks are the electrons. The levels refer to discretization of the energy of oscillators and the discretization of angular momentum.

De Broglie and Schrödinger approaches, emphasized the wave-matter duality. Finally, these diverse points of view are all corollaries of that of Heisenberg statement: physical quantities are governed by non-commutative algebra.

Chemists working at the material level of reality make use of theoretical tools as the periodic table for classification, the balance equations describing transfer phenomena in engineering and models as the wave equation from quantum chemistry. Also the chemists have many devices and technologies to combine substances and afterwards to decompose and separate them.

The challenge for researchers focusing on other levels of reality, biological, cognitive, industrial, socio-economical, logical and mathematical systems is to develop analogous methods, techniques and models for coding and classifying, devices for composing and decomposing specific building blocks and components.

Self-organization is a core concept of systems science. It refers to the ability of a class of systems, the self-organizing systems, to change their internal structure and their function in response to external circumstances. Some elements of self-organizing systems are able to manipulate or organize other elements of the same system in a way that stabilizes either structure or function of the whole against external fluctuations. The process of self-organization is often achieved by growing the internal space-time complexity of a system and results in layered or hierarchical structures or behaviors. This process is understood not to be directed from outside the system and is therefore called self-organized.

Modern ideas about self-organization start with the foundation of cybernetics in the 1940s. Later, the concept was adopted in physics and nowadays pervades most of natural sciences. Some theories focused the processes of self-organization in systems far from equilibrium (Nicolis and Prigogine 1977; Haken 2000).

Chaos theory (Mandelbrot 1982) was a line of inquiry into nonlinear systems in mathematics. Autopoiesis and self-maintenance were at center stage in biology (Eigen and Schuster 1979). The theory of autocatalytic hypercycles supposes that organisms consist of functionally related self-replicative units formed into multiple feedback loops.

Self-organizing systems have assumed center stage in the cognitive science (Maturana and Varela 1980) and social sciences (Luhmann 1995).

Engineering is beginning to see the usability of the concept of self-organization in connection with the approach of nanotechnology applications and the growing complexity of human artifacts (Brueckner et al. 2006). Self-reconfiguring automata, is a recent domain of research for engineers (Yim et al. 2007).

In *On a New List of Categories*, Peirce formulates a theory of categories that can demonstrate what the universal conceptions of reality and of thought are (Pierce 1956).

Peirce's categories are meant to provide a basis for an exploration of a large variety of phenomena, including natural, biological, reasoning and technological.

Peirce proposed an initial list of five philosophical categories: *substance*, *quality*, *relation*, *representation* and *being*.

Later, Peirce discarded substance and being from his initial list of five categories and focused mainly on quality, relation and representation which he called in his technical terms *firstness*, *secondness* and *thirdness*, respectively. These have been associated to 1-level, 2-level and 3-level systems (Iordache 2012).

Taking inspiration from Peirce's philosophy, Brier formulated a transdisciplinary theory of information, semiotics, consciousness and cultural social communication illustrated by the four fold cybersemiotic star (Brier 2008).

The four folds of the star correspond to the four main areas of knowledge that is: Material, Living, Consciousness and Mentality. A comparison with the Hartmann's ontological hierarchy is of interest (Hartmann 1952).

The center of the cybersemiotic star was related by Brier to semiotic mind. It may be considered as a meta-representation of the four fold star and it is linked to self-evolvability.

The polytope projects have been proposed as general theories, basic guides, for problems understanding and solving, for designing, building and managing self-evolvable systems (Iordache 2012, 2013).

The polytope projects start from a biologically inspired general architecture, useful for artifacts building, information representation, design, operation and calculus.

Highlighting different aspects, material, technological, scientific and socio-economical, the resulting architectures will be also interesting in themselves as geometrical objects like lattices, hypercubes and other polytopes.

The issues raised by implementing polytope projects concern the hardware and software, the foundational brain-like machine structure, the engineering methods and so on.

The polytope projects are based on findings from material science and electronics, biology, psychology and informatics and it is expected to provide a general framework for higher level innovative quantitative and theoretical research in these domains.

The polytope projects follow a natural trend to unify and standardize the research discovery, design and control methods (Langley et al. 1987; Langley 2006).

## 9.2 Perspectives

### *9.2.1 Leading Projects*

*Mat*: Quantum Computer, Living Technologies, Self-fabrication
*Bio*: Genome Coding, Bio-Molecular Computer, Artificial Life
*Cog*: Neural Coding, Neural Computer, Artificial Brain
*Intel*: Intelligence Coding, Autonomous Experiments, Artificial Intelligence, Smart Systems, Industry 4.0, Sustainable industry, Ecology
*Math*: Mathematical Coding, Artificial Mathematics

The highlighted future leading technological and scientific projects require coding exploration and target artificial living-like systems. This refers to periodic table of elements, Human Genome project and to BRAIN initiative (Jorgenson et al. 2015).

Living technologies, artificial life (von Kiedrowski et al. 2010), artificial brain, artificial intelligence are future leading scientific and technological projects.

Living technology is very promising because it shares the fundamental properties of living systems (Bedau et al. 2010). These include self-assembly, self-organization, growth and division, purposeful action, adaptive complexity, evolution, and intelligence. Existing technologies are becoming increasingly life-like, and powerful. Examples of living technology projects are synthetic biology attempts to make living systems from scratch in the laboratory, systems exhibiting collective and swarm intelligence distributed across the world wide web, self-reconfiguring robots, and others.

Quantitative, predictive understanding of complex systems requires comprehensive information. High-throughput methods and laboratory automation technology have the potential to deliver the necessary data. To harvest this potential, experimental design has to become evolvable and autonomous.

Autonomous experimentation systems are computational systems capable of autonomously investigating large experimental parameter space (Matsumaru et al. 2004; Lovel and Zauner 2009).

Such systems should develop hypotheses, plan experiments and perform experiments in a closed loop manner without human interaction.

In this new approach, artificial intelligence techniques are employed to carry out the entire cycle of cognition including the elaboration of hypothesis to explain observations, the design of experiments to test these hypotheses and the physical implementation of the experiments using laboratory automats to falsify hypotheses.

In the coming decades a confluence of wireless networks and lab-on-chip sensor technology with application in health monitoring is expected. In such lab-on chip network each sensor node is endowed with a limited supply of chemicals. The network will collectively or via the self-evolution level decide how the drug resources will be spent. Environmental monitoring and improving, new drugs and new material discoveries may be performed by similar autonomous experimentation architectures.

### 9.2.2 Society 4.0

The digital revolution is not limited to industry but is changing all aspects of the human activity (Helbing 2014, 2015; Scharmer 2009; Scharmer and Kaufer 2013; Schwab 2016). The invention of the coal powered steam engines turned agricultural society ("society 1.0") into industrial society ("society 2.0"), and wide-spread education turned it into service society ("society 3.0"). The Internet, the World Wide Web, and Social Media are transforming service societies into digital societies ("society 4.0").

With computers reaching the level of human brainpower, with intelligent service robots, and the Big Data advent, the majority of jobs in the industrial and service sectors will be modified within the next years. Most of our current institutions will fundamentally change: the way we educate (Massively Open On-line Courses and personalized education), the way we do research (Big Data analytics), the transportation way (self-driving Google cars and drones), the way of shopping (Amazon and eBay), the way of producing (3D and 4D printers), but also our health system (personalized medicine), and most likely politics (participation of citizens) and the entire economy as well (the emerging sharing economy, and co-producing consumers). Financial business, which used to be the domain of banks, is increasingly replaced by algorithmic trading. How will this change the society is a challenging problem for complexity science.

Industry 4.0 must be understood as a future concept for society as a whole, the so-called "society 4.0" in which people, more than ever, are at the forefront. The increasing diversity of products with short delivery cycles and simultaneously decreasing numbers of personnel available can present an additional challenge for many companies. It is also important that the urban production of the future is moving closer to people.

This will require different logistics concepts for production supply and disposal. People are not being disregarded, quite the opposite in fact. Their requirements must be taken into account to a much greater extent in corporate planning in the future.

The industry 4.0 eco-system consists of smart factories and intelligent products with a memory that control production. It is a question of allowing people to perform high quality and creative work and giving them the opportunity to achieve a work/life balance—with just as much flexibility as the production systems of the future that will be controlled by people (Schwab 2016).

The U-cycle theory introduced by Scharmer (2009) in the study of "society 4.0" may be presented as an implementable polytope project.

Figure 9.1 shows the U-cycle construction and deconstruction.

Here we identified:

- S-Downloading
- K1-Sensing
- K2-Crystallizing
- K3-Performing

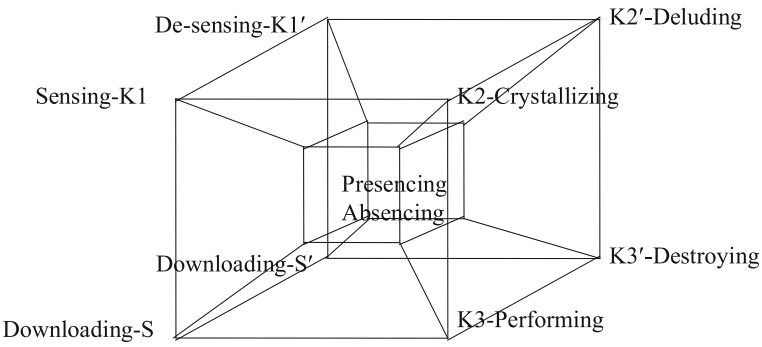


**Fig. 9.1** U-cycle construction and deconstruction

Implementing polytope project starts from the direct sequence S → K1 → K2 → K3 and complete this by the reverse sequence: K3′ → K2′ → K1′ → S′. One could identify for instance:

- K3′-Destroying
- K2′-Deluding
- K1′-De-sensing
- S′-New Downloading
- Self-Presencing Absencing

The Self is in this case the pair: Presencing, Absencing.

The basic levels are S, K1, K2 and K3 represented on the front face of the outer cube and S′, K1′, K2′ and K3′ represented on the back face of the outer cube of the polytope.

The swinging between the two faces of the outer cube is mediated by the inner cube, the Self.

Implementing a polytope project onto conventional systems is expected to be an important and useful instrument in creating significantly new capabilities and structures.

Table 9.2 conceptualizes the levels in evolution of different domains and allows putting them in parallel with polytope projects architecture (Scharmer and Kaufer 2013).

Notice that 0.0, 1.0. 2.0. 3.0, 4.0 may be assimilated to S(K0), K1, K2, K3 and Self in the polytope projects frame.

We identify:

- S-0.0
- K1-1.0
- K2-2.0
- K3-3.0
- Self-4.0

**Table 9.2** Society 4.0

| | Agriculture | Capital | Computing technology | Consummation |
|---|---|---|---|---|
| 0.0 | Natural | Natural | Human | Survival |
| 1.0 | Subsistence | Human | Main frames | Traditional needs driven |
| 2.0 | Industrial | Industrial | PC | Consumerism mass consume |
| 3.0 | Selective cultures | Financial | Internet, IoT | Selective conscious |
| 4.0 | Collaborative conscious | Cultural creation serving | Self-learning robots | Collaborative conscious |

| | Coordination | Defense | Design | Economy |
|---|---|---|---|---|
| 0.0 | Community | Individual | Individual | Tradition |
| 1.0 | Hierarchy control | Weapons | Traditional artifacts | Agriculture |
| 2.0 | Market competition | Machines | Products services | Industrial |
| 3.0 | Networks negotiation | Systems automation | Organizational transformation | Service |
| 4.0 | Awareness collective action | Unmanned self-organizing robots drones | Social transformation | Digital |

| Level | Education learning | Energy | Food | Health |
|---|---|---|---|---|
| 0.0 | Tradition | Natural | Natural | Tradition |
| 1.0 | Memorization | Utilities | Cultivation | Examination dialogue |
| 2.0 | Open access library internet | Personal driven | Mechanization manufacturing | Open access internet |
| 3.0 | Knowledge producing | Renewable | Processing genetics | Semantic personalized |
| 4.0 | Innovation producing | Smart grids self-organized | Collaborative integrative | Symbiotic conscious |

| | Industry | Labor work | Leadership | Marketing |
|---|---|---|---|---|
| 0.0 | Manual | Self sufficiency | Community | Individual |
| 1.0 | Mechanic | Slave | Authority | Product centric |
| 2.0 | Electric | Labor commodity | Incentives | Customer centric |
| 3.0 | Electronic automation | Labor regulated commodity | Participative | Human centric |
| 4.0 | Internet digital informational self-organized | Social business entrepreneur | Co-creative participation | Self-actualization |

| | Mobility | Nature | Organization | Ownership |
|---|---|---|---|---|
| 0.0 | Individual | Mother nature | Community | Communities |
| 1.0 | Public | Resources | Entrepreneur | State |
| 2.0 | Private cars | Commodity land materials | Professional | Private |

(continued)

**Table 9.2** (continued)

| | Mobility | Nature | Organization | Ownership |
|---|---|---|---|---|
| 3.0 | Driver-less vehicles | Regulated commodity | Shared values | Mixed public/private |
| 4.0 | Autonomous transport systems | Eco-system commons | Project product facing-strategy | Shared common |

| | Social Stage | Technology | Web internet | Work security |
|---|---|---|---|---|
| 0.0 | Communal | Indigenous | Human direct | Individual |
| 1.0 | State centric | Tools mechanical | Read | Protect worker |
| 2.0 | Free market ego-centric | Machines industry | Social read/write | Social security |
| 3.0 | Social market regulated | System centric automation | Semantic read/write/execute | Social market security |
| 4.0 | Co-creative eco-centric | Human centric information | Symbiotic: read/write execute/concurrency | Self-organized supply market |

Each column of Table 9.2 indicates the critical factors in each developmental stage (Scharmer and Kaufer 2013).

If we refer to coordination the community coordination 0.0, turned into hierarchical control 1.0, this into market competition 2.0, this into networks negotiation 3.0, and this will evolve into awareness based followed by collective actions 4.0.

If we refer to economy, the traditional primitive economy 0.0, turned into agricultural economy 1.0, this into industrial economy 2.0, this into service economy 3.0, and this will evolve into digital economy 4.0.

If we refer to education, the traditions learning 0.0, turned into memorization 1.0, this into open access to libraries and education 2.0, this into knowledge production learning 3.0, and this will evolve into innovation production learning 4.0.

If we refer to industry we may associate industry 0.0 to manual energy, industry 1.0 to mechanical energy, industry 2.0 to electricity, industry 3.0 to electronics and automation and industry 4.0 to digitalization.

If we refer to web internet we may associate web 0.0 to texts and human direct interactions, web 1.0 to read capability, social web 2.0 to read/write, semantic web 3.0 to read/write/execute and symbiotic web 4.0 to read/write/execute/concurrency capability (Choudhury 2014).

In the 0.0 stages nature is frequently emphasized, indicating that this is the critical factor for the production function. Then, at stage 1.0, dependent labor became the critical developmental factor. The production function changes from one factor (nature) to two factors (nature, labor). In stage 2.0, when economies move from state-centered societies to market economies, industrial capital becomes the critical developmental factor. Capital allows the new players in the market economy to be productive, and as a result the production function of the economic system now has three factors (nature, labor, capital).

In the stage 3.0, technology emerges as a critical factor, and with that the factors of production evolve to four (nature, labor, capital, technology).

Finally, in the currently emerging stage 4.0, all of the factors may turn out to be bottlenecks, or critical factors, in the economy:

The stage 4.0 highlights the role of self-organization, cooperation, collaboration and connectivity. This stage is identified as Self in polytope project implementations.

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# Appendix A
# Dual Graded Graphs

A significant generalization of the concept of differential posets (Stanley, R.: Differential posets, J. Amer. Math. Soc. **1**:919–961, 1988) is that of dual graded graphs, DGG (Fomin, S.: Duality of graded graphs, J. Algebraic Combin **3**,357–404, 1994).

A graph is said to be graded if its vertices are divided into levels numbered by integers, so that the endpoints of any edge lie on consecutive levels.

A graded graph is a triple G = (P, ρ, E) where:

- P is a discrete set of vertices
- ρ: P → Z is a rank function
- E is a multiset of arcs (x, y) where ρ (y) = ρ(x) + 1.

The set $P_n$={x: ρ(x) = n ∈ Z} are called levels of G.

G can be regarded either as oriented or as non-oriented graph. The accessibility relation in an oriented graph defines a partial order on P. If there are no multiple arcs, G is the Hasse diagram of this poset. The paths in non-oriented graphs are the Hasse walks.

As for the differential posets the "down" D and "up" U operators can be defined.

Let G= (P, ρ, E) be a graded graph. Linear operators U and D are defined by:

$$Ux = \sum_{(x,y)\in E} m(x,y)y; \quad Dy = \sum_{(x,y)\in E} m(x,y)x \tag{A.1}$$

Here m (x, y) is the multiplicity of the edge (x, y) in E.

The main idea of Fomin (1994) was to consider the pairs of dual graded graphs $G_1$ = (P, ρ, $E_1$) and $G_2$ = (P, ρ, $E_2$) with a common set of vertices and a common rank function.

The oriented graded graph G = ($G_1$, $G_2$) = (P, ρ, $E_1$, $E_2$) is then the directed graded graph on P with edge in $E_1$ directed upwards, and edges in $E_2$ directed downwards.



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The "up" U and "down" D operators associated with the graph G = ($G_1$, $G_2$) are defined by:

$$Ux = \sum_{(x,y)\in E_1} m_1(x,y)y; \quad Dy = \sum_{(x,y)\in E_2} m_2(x,y)x \tag{A.2}$$

Here $m_i(x, y)$ denotes the multiplicity of (x, y) in $E_i$.

Let ($G_1$, $G_2$) be an oriented graded graph such that:

- It has a zero, $\hat{0}$
- Each rank has a finite number of elements

The graphs $G_1$ and $G_2$ are said to be dual as operators in G= ($G_1$, $G_2$) if:

$$D_{i+1}U_i - U_{i-1}D_i = r_iI_i \tag{A.3}$$

Here $U_i$ (respectively $D_i$) denote the restriction of the operator U (respectively D) to the i-th level of the graph, $I_i$ denote the identical operator at the same level and $r_i$ are positive integers. If $r_i$ = r, $G_1$, and $G_2$ are r-dual graphs and we call the pair ($G_1$, $G_2$) an r-dual graded graph.

The 1-dual graphs satisfy the relation:

$$DU - UD = I \tag{A.4}$$

The quantum dual graphs satisfy the relation:

$$DU - qUD = I \tag{A.5}$$

They have been introduced by Lam (Lam, T.: Quantized dual graded graphs. Electron. J. Combin. **17**(1), Research Paper 88, 2010)

The dual filtered graphs satisfy the relation:

$$DU - UD = D + I \tag{A.6}$$

They have been introduced by Patrias and Pylyavskyy (Patrias, R., Pylyavskyy, P.: Dual Filtered Graphs. arXiv preprint arXiv:1410.7683, 2014).

# Appendix B
# Hopf Algebras

The aim of this appendix is to introduce basic concepts of the bialgebra and Hopf algebra (Sweedler, M. E.: Hopf algebras, Mathematics Lecture Note Series, W. A. Benjamin, Inc., NY, 1969; Abe, E.: Hopf algebras, Cambridge University Press, Cambridge, 1980).

Let $k$ be a commutative ring, one calls algebra over $k$, or also $k$-algebra, a module A together with a linear mapping: $A \otimes A \rightarrow A$.

Let A be an algebra over $k$.

The algebra A is of finite dimension over $k$ if it is a finite dimensional as a vector space.

The algebra A is associative if the inner product is so.

A is an algebra with unit if the inner product has a neutral element.

Let A be an associative algebra A with unit. An element of A is invertible if it is invertible under the ring structure.

The algebra A is commutative if the inner product is so.

One defines an associative algebra with unit as follows: an associative algebra over $k$ is a triple $(A, \nabla, \eta)$, where A is a $k$-module, $\nabla: A \otimes A \rightarrow A$ and $\eta: k \rightarrow A$ are morphisms of $k$-vector spaces such that: $\nabla \bigcirc (\eta \otimes id_A)$ and $\nabla \bigcirc (id_A \otimes \eta)$ are scalar multiplication.

Coalgebras are structures that are dual to unital associative algebras.

The axioms of unital associative algebras can be formulated in terms of commutative diagrams. Turning all arrows round, one obtains the axioms of coalgebras.

Every coalgebra, by duality, gives rise to an algebra, but not in general the other way.

In finite dimension, this duality goes in both directions.

Formally, a coalgebra over a field $k$ is a vector space C over $k$ together with $k$-linear maps $\Delta: C \rightarrow C \otimes_k C$ and $\varepsilon: C \rightarrow K$ such that:

1. $(id_C \otimes \Delta) \bigcirc \Delta = (\Delta \otimes id_C) \bigcirc \Delta$
2. $(id_C \otimes \varepsilon) \bigcirc \Delta = id_C = (\varepsilon \otimes id_C) \bigcirc \Delta$

A bialgebra over a field $k$ is a vector space over $k$ which is both a unital associative algebra and coalgebras, such that these structures are compatible.



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(B, ∇, η, Δ, ε) is a bialgebra over $k$ if it has the following properties:

1. B is a vector space over $k$
2. There are $k$-linear maps (multiplication or product) $\nabla : B \otimes B \to B$ and unit $\eta: k \to B$, such that (B, ∇, η) is a unital associative algebra
3. There are $k$-linear maps (comultiplication or coproduct) $\Delta: B \to B \otimes B$ and counit $\varepsilon : B \to k$, such that (B, Δ, ε) is a (counital coassociative) coalgebra
4. Compatibility conditions are expressed by the following commutative diagrams:

Figure B.1 refers to product and coproduct

Figure B.2 refers to product and counit, coproduct and unit, unit and counit

Here $\tau : B \otimes B \to B \otimes B$ is the linear mapping defined by $\tau(x \otimes y) = y \otimes x$ for all $x, y \in B$.

The diagrams (∇, Δ) and (∇, ε) express that the multiplication ∇ is a morphism of coalgebras. The diagrams (Δ, η) and (η, ε) express that the unit η is a morphism of coalgebras. The diagrams (∇, Δ) and (Δ, η) express that the comultiplication Δ is a morphism of algebras. The diagrams (Δ, ε) and (η, ε) express that the counit ε is a morphism of algebras.

A bialgebra is a $k$-vector space B, endowed with an algebra structure (B, ∇, η), and with a coalgebra structure (B, Δ, ε) such that ∇ and η are morphism of coalgebras; equivalently, it follows that Δ and ε are morphism of algebras.

A Hopf algebra is a (associative and coassociative) bialgebra H over a field $k$ together with a $k$-linear mapping $\chi : H \to H$, called the antipode, such that the diagram from Fig. B.3 commutes.

Figure B.3 shows the Hopf algebra diagram.

The antipode χ sometimes required to have a $k$-linear inverse, which is automatic in the finite-dimensional case, or if H is commutative or cocommutative (or more generally quasi-triangular). If $\chi 2 = \mathrm{id}_H$ then the Hopf algebra is said to be involutive.

If H is finite-dimensional semisimple over a field of characteristic zero, commutative, or cocommutative, then it is involutive. If a bialgebra B admits an antipode χ it is unique. The antipode can be equivalently defined as the inverse of $\mathrm{id}_H$ for the associative convolution product.

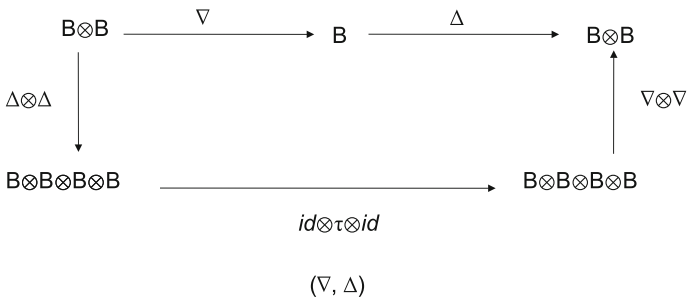


**Fig. B.1** Product and coproduct

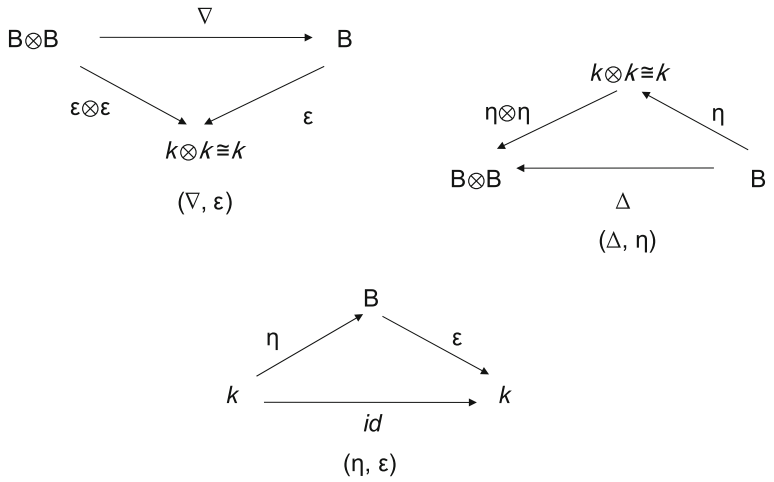


**Fig. B.2** Product and counit, coproduct and unit, unit and counit

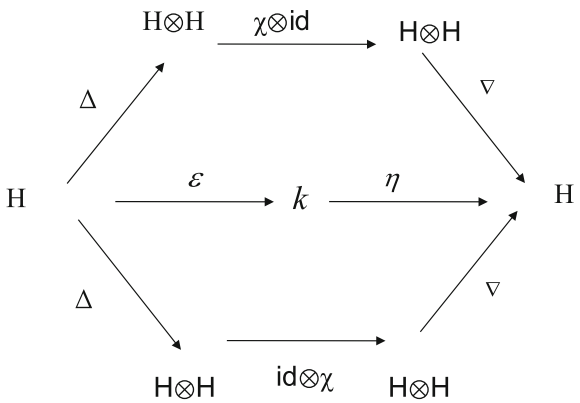


**Fig. B.3** Hopf algebra diagram

# Implementing Polytope Projects for Smart Systems

Octavian Iordache

The book is devoted to a domain of highest industrial and scientific interest, the study of smart systems and structures. Such systems contain multifunctional parts that can perform sensing, control, and actuation. Smart systems should be implemented in industry giving that devices, tools, methodologies or organizations based on electronics and information technology for automation, specific to third industrial revolution reached or will reach their limits soon. Polytope projects are comprehensive physical and cognitive architectures allowing the investigation,

fabrication and utilization of smart systems and structures as key elements of the fourth industrial revolution.

The book begins with the presentation in Chap. 1 of polytope projects as reference architecture for cyber-physical systems and smart systems. Chapter 2 focuses on industrial processes synthesis. Flow-sheet trees, cyclic separations and smart configurations for multi-component separations are discussed here. Periodic features for drug delivery systems and networks of chemical reactions are presented in Chap. 3. Conditioned random walks characteristic packing problems to polymers and smart materials structure are studied in Chap. 4. Chapter 5 examines self-assembling and self-reconfiguring at different scales from molecular to micro systems. Smart devices and technologies represent the subject of the Chap. 6. Modular micro reactor systems and timed automata are the presented case studies. Chapter 7 focuses on inferential engineering designs, concept-knowledge, relational concept analysis and model driven architecture. Smart manufacturing, industry 4.0, reference architectures and models for new product development and testing are presented in Chap. 8. Chapter 9 highlights the polytope projects methodology and the perspectives for smart systems and structures. Focusing on process engineering and mathematical modeling for the fourth industrial revolution the book will be useful to engineers, scientists and entrepreneurs working in chemical, biochemical, pharmaceutical industries, material science or systems chemistry, to students in different domains of production and engineering and to applied mathematicians.

**Keywords**
Assembling · Chronotherapy · Closure · Composition · Concept analysis · Cyclic separation · Decomposition · Disassembly · Drug delivery systems · Dual graded graphs · Flexible flow-sheeting · Hopf algebra · Industrial internet · Industry 4.0 · Inferential design · Meta-meta models · Microreactors · N-levels · Packing · Programmable matter · Reaction networks · Reconfiguring · Reference architecture models · Smart manufacturing · Smart materials · Self-evolvable · Verification and validation models

# Index





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