

# Preface

This book comprises a collection of papers presented in the THALES workshop “Algebraic modeling of topological and computational structures and applications”, that took place at the National Technical University of Athens (NTUA), 1–3 July 2015. This workshop disseminated the results of the research project THALES MIS 380154 with the same title, which was implemented from October 2011 until December 2015. The project has been co-financed by the European Union (European Social Fund—ESF) and Greek National Funds through the Operational Program “Education and Lifelong Learning” of the National Strategic Reference Framework (NSRF)—Research Funding Program: THALES: Reinforcement of the interdisciplinary and/or interinstitutional research and innovation.

The research project THALES was concerned with the study of topological and computational structures and applications, mainly with the use of algebra and especially with braid groups. Braids can be viewed as algebraic as well as topological objects and they play a crucial role in knot theory and in low-dimensional topology, in the study of homotopy groups, in reflection groups and  $C^*$ -algebras, in statistical mechanics, in cryptography, and in Galois theory. The project consisted in three research programs (RP), corresponding to the three research groups involved:

RP1 “Algebraic modeling of topological structures”

RP2 “Algebraic modeling of applications”

RP3 “Algebraic modeling of computational structures”

RP1 aimed at the study of topological structures, such as knots, links, 3-manifolds and classical homotopy groups, using braid groups, classical and generalized, and their representations. Knot theory is the area of low-dimensional topology that deals with the problem of classification of embeddings of a circle or collections of circles into three-dimensional space. This problem is tackled by the construction of knot invariants. Within this project, new skein link invariants were extracted from the Yokonuma-Hecke algebras and other new (framization) knot algebras, via the celebrated method of V.F.R. Jones, which uses braid groups and the Alexander and Markov theorems. Another subproject was about the study of the mixed braid groups related to knots and links in specific 3-manifolds, and the construction of quotient

algebras of the mixed braid groups. Further, the HOMFLYPT skein module of the lens spaces was investigated via the Artin braid groups of B-type. The study of the knot theory of a 3-manifold renders information about the topological structure of the manifold, while the use of braids in the study provides more structure and more control on the moves for topological equivalence. Powerful algebraic and computational tools can then be employed. Our next focus was on special decomposable groups. In particular, the linearity of groups that fit into a short exact sequence with kernel a free group and cokernel a linear group was studied. Finally, the connections between modular invariant theory and certain unstable coalgebras over the mod  $p$  Steenrod algebra were investigated. This problem is related to the stable homotopy groups of spheres.

RP2 was concerned with the study of some novel application areas. One of them was the development of new measures of polymer entanglements. Polymer chains are long flexible molecules that impose topological constraints on each other, called entanglements, which affect the physical properties of the polymer. The Gauss linking number was extended to open polymeric chains in 1, 2 and 3 Periodic Boundary Conditions (PBC) and the simulation of polymeric chains through braid groups was proposed. Also, Fourier braids were introduced and PBC were represented by algebraic conditions. Furthermore, Turaev's knotoids were retaken, which are ideal for modeling, abstractly, polymers and biopolymers. The knotoids are a new chapter in classical knot theory that is worth studying for its own sake and that allows topological modeling of open-ended arcs in three-dimensional space (such as long chain molecules, proteins, DNA). Another application area was the molecular simulation of ionic liquids and their mixtures. Molecular simulation is a powerful tool for the study of physical systems, based on fundamental principles of statistical mechanics. This simulation manages to predict various properties of materials through the connection of their microscopic structure and their macroscopic properties. It can efficiently contribute to the production of new materials with desired properties. The modeling of many natural processes via topological surgery in 1, 2, and 3 dimensions was another application of the project. Topological surgery is a mathematical technique used for creating new manifolds out of known ones and, as we observed, it appears in nature in numerous, diverse processes of various scales as, for example, in the reconnection of cosmic magnetic lines, in DNA recombination, in the formation of tornadoes and of Falaco solitons, in drop coalescence, in cell mitosis, and in the formation of black holes. Inspired by such phenomena new theoretical concepts were introduced, which enhance topological surgery with the observed dynamics, and a connection with a 3D Lotka–Volterra dynamical system was also pinned down.

RP3 was concerned with the algebraic modeling of computational structures and applications. A subproject was about the unification of the well-known algebraic specification language CafeOBJ with the strong theorem prover Athena within a common interface. Other outputs included the development of novel techniques for system modeling and verification, as well as applications on the modeling of video and of musical structure. Algebraic modeling techniques were also applied in the geometry of curves over finite fields and applications to cryptography and coding

theory were investigated. The aim was the study of open problems referring to zeta functions of certain algebraic curves aiming to calculate the number of rational elements. Finally, another application was in the field of medical imaging, where a new medical PET (Positron Emission Tomography) data reconstruction algorithm was proposed for reconstructing sinograms to tomographic images. Also, various deformable methods for optic disk extraction in retinal images were studied and evaluated.

The research team of the project THALES comprised 56 researchers from universities and research institutions from all over the world. The Scientific Coordinator of the project and coordinator of the first RP was Professor Sofia Lambropoulou of the NTUA. Professor Doros Theodorou of the NTUA was the coordinator of the second RP and Assistant Professor Petros Stefaneas of the NTUA was the coordinator of the third RP. Finally, Professor Louis H. Kauffman of the University of Illinois at Chicago was the Invited Researcher of the project.

The THALES workshop was attended by more than 100 researchers. In total, 37 research talks and 17 posters were presented. The present book contains 23 chapters, arranged into three parts that correspond to the three RPs of the project.

### **Part I: Algebraic Modeling of Topological Structures**

A knot algebra is an algebra obtained as a quotient of the group algebra of a braid group and endowed with a Markov trace; it can be thus used for the definition of knot invariants. Framization is a mechanism proposed recently by Juyumaya and Lambropoulou which consists of constructing a nontrivial extension of a knot algebra for the definition of framed knot invariants. The inspiring example of framization is the Yokonuma-Hecke algebra of type A, introduced by Yokonuma in the context of finite reductive groups as a generalization of the Iwahori-Hecke algebra of type A. The first five chapters of Part I are concerned with framizations of known knot algebras.

In Chap. 1 by Konstantinos Karvounis and Sofia Lambropoulou, the families of framed, classical, singular, and transverse link invariants defined via the Yokonuma-Hecke algebras of type A are presented. The Yokonuma-Hecke algebras comprise a family of algebras that generalize the classical Iwahori-Hecke algebra and that also support Markov traces that give rise to those families of link invariants. The family of classical link invariants is of special interest, since it contains the HOMFLYPT polynomial  $P$  and, moreover, it extends to a three-variable skein link invariant generalizing  $P$  and which is stronger than  $P$ .

Chapter 2 by Dimos Goundaroulis is a brief and comprehensive review of the construction of the framization of the Temperley-Lieb algebra of type A and its derived invariants for framed and classical links. Key elements of the representation theory of the involved quotient algebras are also included. The invariants for classical links are compared to the Jones polynomial and then they are generalized to a two-variable invariant that is stronger than the Jones polynomial.

In Chap. 3, Maria Chlouveraki studies the algebraic structure and the representation theory of the Yokonuma-Hecke algebra of type A, as well as of some

similar framizations of the affine Hecke algebra of type A, the Ariki-Koike algebra, and the Temperley–Lieb algebra.

Furthermore, in Chap. 4, Loïc Poulain d’Andecy studies the affine Yokonuma-Hecke algebra, seeing it as a quotient of a certain braid group. A large family of Markov traces is constructed and, using well-known relations between braids and links, this way invariants for classical links and for links in the solid torus are produced. The study uses extensively a purely algebraic result, namely an isomorphism theorem relating affine Yokonuma-Hecke algebras with the usual affine Hecke algebras, which moreover allows one to deduce naturally some properties of the invariants.

In Chap. 5, Marcelo Flores gives a review about two framizations of the Hecke algebra of type B, and the results related to each of these. He begins by presenting the cyclotomic Yokonuma-Hecke algebra introduced by Chlouveraki and Poulain d’Andecy, which provides one of such framizations. Next, Flores focuses on a new framization defined recently by himself together with Juyumaya and Lambropoulou, and on the results obtained for this new algebra. The author concludes with a preliminary comparison between the isotopy invariants derived by both framizations.

In order to have a good understanding of knot theory in 3-manifolds, one should be able to visualize and understand link diagrams in these manifolds. In Chap. 6, Bostjan Gabrovsek and Maciej Mroczkowski present a survey of the so-called arrow diagrams, which are used for representing links in Seifert fibered spaces, a large class of 3-manifolds. Moreover, they show how to pass between some of the different types of diagrams found in the literature. Using arrow diagrams, the authors express the basis of the Kauffman bracket skein module and the HOMFLYPT skein module of some 3-manifolds and they present new bases for these skein modules for the solid torus and lens spaces.

In Chap. 7, Ioannis Diamantis and Sofia Lambropoulou present recent results toward the computation of the HOMFLYPT skein module of the lens spaces  $L(p, 1)$ ,  $\mathcal{S}(L(p, 1))$ , using the braid approach. They describe first the HOMFLYPT skein module of the solid torus  $ST$ ,  $\mathcal{S}(ST)$ , using the mixed braid group  $B_{1,n}$ , which is the Artin braid group of type B, and they present a new basis,  $\mathcal{A}$ , for it, through which the braid band moves are naturally described. The authors then derive the relation between  $\mathcal{S}(ST)$  and  $\mathcal{S}(L(p, 1))$  and show that in order to compute  $\mathcal{S}(L(p, 1))$  one needs to solve a controlled infinite system of equations obtained by performing all possible braid band moves on elements in the basis  $\mathcal{A}$ .

In Chap. 8, Dimitrios Kodokostas and Sofia Lambropoulou define a tower of Hecke-type quotient algebras of the mixed braid group with two fixed strands,  $B_{2,n}$ . The groups  $B_{2,n}$  are related to the knot theory of the handlebody of genus two, the complement of the 2-unlink in  $S^3$  and the connected sums of two lens spaces. The authors focus on the algebras  $H_{2,n}(q)$ ,  $n \in \mathbb{N}$  and review their work on extracting inductive spanning sets for these algebras, appropriate for constructing Markov traces. They also provide corresponding spanning sets for the other algebras defined in the paper and they conjecture all spanning sets to be linear bases for the algebras defined.

In Chap. 9, Valerij Bardakov proves that the kernel of the map from the braid group in the handlebody,  $B_{g,n}$ , to the classical braid group is a semi-direct product of free groups. Also, he introduces an analogue of the Hecke algebra for the braid group in the handlebody and formulates a conjecture on the basis of this algebra.

In Chap. 10, the research is twofold. First, Nondas Kechagias gives an invariant theoretic description for the *modp* cohomology of the stabilization functor on the basepoint of the zero sphere previously described by D. Quillen and M. Barratt—S. Priddy independently. Second, the author compares the *modp* Dyer-Lashof algebra with a co-free Steenrod coalgebra and he provides cogenerators along with corelations. His approach is connected with the Peterson conjecture relating the Dickson algebra with a quotient of a free unstable Steenrod algebra.

## Part II: Algebraic Modeling of Applications

In Chap. 11, Eleni Panagiotou and Ken Millett extend the topological Gauss linking number to open chains in systems employing one-dimensional periodic boundary conditions to define periodic linking and periodic self-linking numbers. These give rise to a periodic linking matrix and associated eigenvalues that are applied to Olympic gels and tubular filamental structures.

The theory of knotoids, that was introduced in 2012 by Vladimir Turaev, was proposed as a new diagrammatic approach to classical knot theory and also as a generalization of classical knot theory. The notion of knotoids extends the notion of 1-1-tangles or long knots by having two distinct endpoints that may lie in any region of knotoid diagrams. This makes knotoids a natural domain for understanding physicality and topology of open-ended space curves and also for a transition and relationships with virtual knot theory. The height of a knotoid, that measures the distance between the endpoints of a knotoid, is an efficient tool for the classification of knotoids. In Chap. 12, Neslihan Gügümcü and Louis H. Kauffman review their results on the estimation of the height of a knotoid given by the affine index and the arrow polynomials. These polynomials, first defined in virtual knot theory, are here given definitions in the category of knotoids.

In Chap. 13, Stephan Klaus constructs braids by folding periodic complex valued functions. The method of finite Fourier approximation shows that braids are given by certain finite Laurent polynomials  $g(z)$  such that an associated algebraic discriminant has no root on the unit circle. This condition is studied from the algebraic and topological viewpoint. Algebraic transformations of  $g(z)$  correspond to geometric operations of the braid, for example, a Dehn twist. Moreover, this algebraic method allows one to construct braids in a thickened torus or in other spaces.

Chapter 14 is devoted to the computational study of ionic liquids at the molecular level. Ionic liquids are organic salts that are in the liquid state at room temperature and exhibit a fascinating combination of properties due to their dual ionic and organic nature that renders them ideal for use in a wide range of state-of-the-art applications. Niki Vergadou applies molecular simulation methods for the investigation of the microscopic phenomena that determine macroscopic properties of ionic liquids and for the study of their complex dynamics and structure.

In Chap. 15, Stathis Antoniou and Sofia Lambropoulou show that topological surgery happens in natural phenomena at various scales and analyze the common features of their underlying processes. These features are captured by schematic models and new definitions which provide the theoretical setting for describing the topological changes that occur. We believe that the understanding of their underpinning topology will lead to the better understanding of the phenomena themselves, as well as to new mathematical notions, which will in turn lead to new physical implications.

### Part III: Algebraic Modeling of Computational Structures

Chapter 16 is a survey on the theory of curves with automorphisms. Several bounds on the order of the automorphism group curve are discussed, mostly related to the research of the authors, Jannis Antoniadis and Aristides Kontogeorgis. The authors' point of view is to relate the theory of (modular) representations of automorphism groups acting on natural objects related to the curve, such as (co)homology spaces and spaces of holomorphic (poly)differentials. The chapter concludes with applications to deformation theory of curves, liftings to characteristic zero and moduli problems.

Chapter 17 by Nicola Angius, Maria Dimarogkona, and Petros Stefaneas provides a first attempt at constructing semantic theories over institutions and examines the logical relations holding between different such theories. The results show that this approach can be very useful for theoretical computer science and may also contribute to the current philosophical debate regarding the semantic and the syntactic presentation of scientific theories.

Chapter 18 is a survey of results related to generic constructions and generic limits for semantic and syntactic cases. The authors Sergey Sudoplatov, Yiannis Kiouvrekis, and Petros Stefaneas consider both the pure model theory approach and the institutional approach.

Chapter 19 by Katerina Ksystra, Nikos Triantafyllou, and Petros Stefaneas contains some steps towards a verification framework based on the combination of the CafeOBJ algebraic specification language with the interactive theorem proving system Athena. The proposed framework combines two different specification and theorem proving systems, in order to facilitate the modeling and analysis of critical software systems.

Chapter 20 by Theodoros Mitsikas, Petros Stefaneas, and Iakovos Ouranos demonstrates the design of an innovative rule based approach for the Air Traffic Control regulations during the takeoff and landing phases, covering both current and future separation standards of ICAO and FAA. The rule base consists of the rules implementing the air traffic control regulations, and a database containing characteristics of airports and aircraft. The proposed rule base constitutes a flexible tool for the computation of the aircraft separation according to current and future regulations, useful in the fields of conflict detection, conflict avoidance, and scheduling aircraft landings. A further application will be for a decision support tool in real-time environments, guaranteeing the enforcement of all the separation standards.

In Chap. 21, Marianthi Bozapidou demonstrates that every commutative affine musical contour actually simulates the classical one. Affine contours may be viewed as an abstraction of the notion of musical intervals and are closely related to sequential machines. Sequential machines are mathematical tools that can be depicted by finite directed graphs and are suitable to describe and represent various phenomena in music.

In Chap. 22, Antonios Kalambakas, Nikolaos Triantafyllou, Katerina Ksystra, and Petros Stefaneas indicate how hyperoperation can be utilized in order to formally represent and compare video content using algebraic semiotics. In this setup, pictures are defined as a specific type of rectangular graphs and the picture hyperoperation is given by virtue of the notion of the path inside such a picture.

Finally, in Chap. 23 Evi Karali presents and evaluates a new iterative algorithm for medical image reconstruction, under the name Image Space Weighted Least Squares (ISWLS). She then compares various snake or deformable methods, towards a modified self-affine mapping system technique, more suitable for weak edge detection. All methods were applied to glaucomatic retinal images with the purpose of segmenting the optical disk.

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