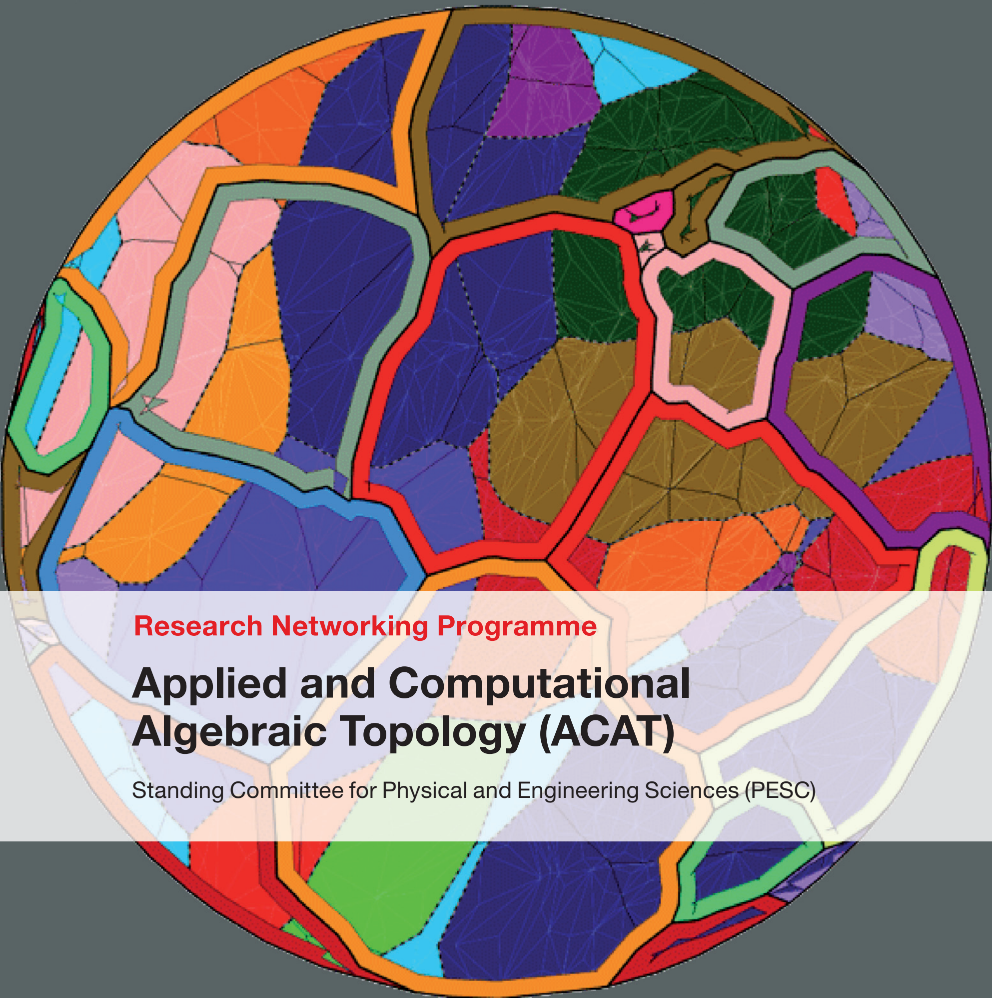


Research Networking Programme

Applied and Computational Algebraic Topology (ACAT)

Standing Committee for Physical and Engineering Sciences (PESC)

The revolutionary growth of experimental data in the sciences and the availability of unprecedented computing power pose many challenges to contemporary mathematics. This ESF Research Networking Programme on applied and computational algebraic topology (ACAT) combines efforts of researchers throughout Europe developing mathematical tools for the following broad research themes:

- the topological and statistical analysis of shapes, images, and high-dimensional data sets;
- algorithms for motion planning and the study of configuration spaces of mechanical systems;
- stochastic topology and the study of large growing systems;
- the theory of concurrent computation and computer networks.

Research on these themes is currently carried out in small groups spread over several European countries. The Network facilitates intensified interactions and cross-fertilisation, which we predict will lead to new results and entire new research directions as well as to commercial applications. The Network organises summer schools and conferences to support the formation of an integrated research community in applied and computational algebraic topology and to attract an increasing number of students to the field. Research visits to departments in European countries may be facilitated by short visit and exchange grants. The Network actively collaborates with experts outside Europe.

The running period of the ESF ACAT Research Networking Programme is for four years, from July 2011 to July 2015.

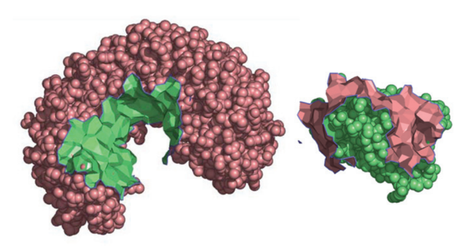


Figure 1.
Two interacting proteins taken apart after computing the interface surface of the complexed form.

The front cover shows a two-dimensional rendering of a protein–protein interface. After constructing the interface (see Figure above), it is flattened and deformed into a round disk. Since the interface separates two proteins, the disk is coloured on both sides, each colour indicating the neighbouring amino acid type. One side is rendered transparent, indicating the coloured regions with narrow strips outlining the boundary. We see clearly which amino acids of the two proteins interact. (Courtesy of work by Andrew Ban, Herbert Edelsbrunner and Johannes Rudolph as part of the biogeometry project funded by NSF, 2001-2006.)

A particularly delicate step is the selection of the finite portion of the infinite surface that separates two proteins sitting in three-dimensional space. All neighbourhood information of the amino acids is already contained in that surface, but flattening it and colouring the regions as shown makes the result much more compelling and easier to comprehend. The neighbourhood information is topological and may be represented by weighted networks of amino acids and/or proteins. It is still not known how to predict the interaction given the structural knowledge of the two proteins in space individually, but not put together forming the complex. The computational problem of this prediction is known as the protein–protein docking problem.

Scientific Background

The mathematical discipline of *algebraic topology* forms the background for several areas of application-oriented mathematical research. The aim is to develop new theoretical instruments and algorithms connecting topological methods with applications. The last two decades have shown that this is both possible and mutually beneficial. The growing number of such connections has given rise to the emerging field of *applied and computational algebraic topology* (ACAT), which includes the following areas:

- computational algebraic topology;
- topological robotics;
- stochastic topology;
- combinatorial algebraic topology and concurrency.

We give a brief description of the background and the main aims for each of these research areas. ACAT facilitates research within each of these areas and enhances collaboration between researchers in different areas.

Computational Algebraic Topology

This area deals with the analysis of shapes, images, and high-dimensional data sets. It is often based on a filtration that represents the space across scale levels, from fine to coarse. Combinatorial complexes can be constructed to represent the data at a given level, and topological invariants of those (e.g. ranks of homology groups) can be determined. The interest is in *persistence*, i.e. the length of the activity interval of such an invariant along the filtration. *Persistence diagrams* in the plane are combinatorial representations of the homological information contained in the filtration. They form an invariant of the filtration and are stable under perturbations. This paves the way for the use of homology in a wide range of applications in mathematics and computing but also in the sciences and engineering (for an introduction, see

Computational Topology, an Introduction, by H. Edelsbrunner & J.L Harer, American Mathematical Society, 2010).

The development underpins the need for fast algorithms to compute homology for data sets of a few million elements or more, which arise in diverse areas such as image analysis, dynamical systems, robotics, electromagnetic engineering, and material science. Similar methods are applied in the classification of shapes and their retrieval from databases. An essential ingredient in this undertaking is a measure of dissimilarity between shapes. If we enhance shapes by functions on them, we can use the pseudo-distance that can be approximated by persistent homology. We continue by listing a few of the questions to be investigated by members of this project:

• *Well modules* have recently been introduced to measure the robustness of intersections and to prove the stability of contours of mappings. They can also be used to formulate a notion of robustness for fixed points of mappings. Can these ideas be further developed to obtain a notion of persistence for dynamical systems? On a related note, we need a notion of persistent homology for maps, and fast algorithms.

• Image processing raises a number of challenges to our understanding of our topological tools. How do we use persistent homology under partial information, such as partially occluded shapes?

• Filtrations are generated by real-valued functions on the space. Replacing the functions by *vector-valued* mappings gives multi-parameter filtrations. A deeper understanding of the rank invariant of these more general filtrations is important for applications in shape analysis and retrieval.

• Homology algorithms can be extended to computing *cohomology*, which is particularly important in electromagnetic engineering. The running time characteristics of the cohomology variants are likely to be different from the homology algorithms, and this difference needs to be explored.

• *Matrix reduction algorithms* lend themselves to implementations on parallel computer architectures, which promise a further increase in efficiency. We need to understand which reduction algorithms are best suited for this effort.

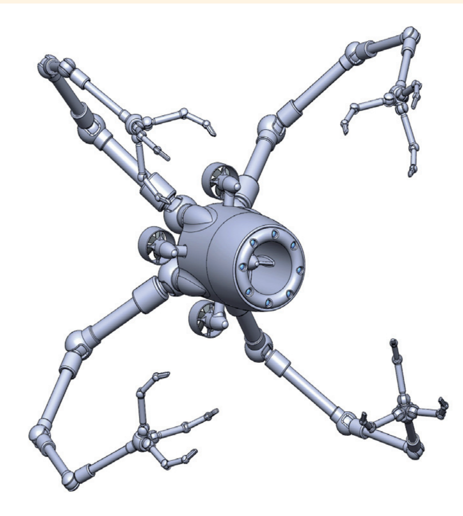
Topological Robotics

This mathematical discipline studies topological problems relevant to practical applications in modern robotics, engineering and computer science. With any mechanical system, one associates the configuration space, which encodes all admissible configurations of the system. Many important engineering questions about the system reduce to geometric questions about the configuration space. For instance, the connectivity of the configuration space means that the mechanical system is fully controllable. In other words, we can bring the system from any initial state to any desired state by a continuous motion. Curiously, the interaction between topology and mechanical engineering is bi-directional because any smooth manifold can be realised as configuration space of a mechanical system. We continue by outlining a few broad topics within the area.

• Configuration spaces of simple *linkages* represent an interesting class of closed smooth manifolds. These remarkable spaces are also known as polygon spaces because they parameterise the space of all n-sided polygons with given side lengths. In the last few years significant progress has been made in classification of configuration spaces of linkages leading to a solution of the Walker conjecture, which is a question about the invertibility of the mapping from a linking to its configuration space.

• The *motion planning problem* plays a prominent role in modern robotics. An autonomous mechanical system must be able to select a motion once the current and the desired states are given; such a selection is made by a motion planning algorithm. Continuous motion planning algorithms rarely exist, which explains why decisions are often discontinuous as functions of the input data. The notion of *topological complexity* measures these discontinuities numerically. Many properties of this notion are known, but its computation in general is quite difficult; a situation similar to the related Lusternik-Schnirelmann category.

• We plan to apply the theory of motion planning algorithms in the context of *directed* topological spaces when only directed paths between the source and the target are allowed. This theory would then be applicable to problems of concurrent computation, as discussed below. We also plan to create appropriate cohomological tools for estimating the sectional category of fibrations. This will involve strengthening and generalising the technique of category weight of cohomology classes and using cohomology operations, as suggested by Fadell and Husseini in the context of the Lusternik-Schnirelmann category.



Stochastic Topology

In applications with large mechanical systems, the traditional concept of a configuration space is unfortunately inadequate. For a mechanical system of great complexity, it is unrealistic to assume that its configuration space can be fully known or completely described. It is more reasonable to assume that the space of all possible states of such a system can be understood only approximately, or that it is described using probabilistic methods. Similar problems arise in modeling of large financial, biological and ecological systems. This motivates the study of random manifolds and random simplicial complexes as models for large systems. We continue with a number of specialised topics in the area:

• Recent results about topology of linkages with *random* length parameters show that despite limited information one may predict the outcome topology, say, the Betti numbers, with surprising precision. This happens in situations when the system depends on many independent random parameters, similar to the classical central limit theorem.

• We plan to study models that produce high-dimensional random complexes (generalising the well-developed theory of random graphs) and investigate their applications in engineering and computer science. This includes the *Linial-Meshulam model* which has been studied extensively in recent years.

Figure 2. Underwater robot with sense of touch.
© DFKI Bremen

• A recent and dynamic branch of combinatorial algebraic topology also brings probability aspects into play. There have been several developments studying probability spaces arising naturally in topology, and establishing *thresholds* for non-triviality of various algebraic invariants. The idea is to incorporate into the computational model not just the final data sample, but the sampling process itself. These methods give global quality assessment invariants for specific computations in terms of tools of probability theory.

• One hopes that it will be possible to answer some famous outstanding open problems about two-dimensional complexes, such as the *Whitehead* or the *Eilenberg-Ganea conjectures* using probabilistic tools. The methods involving probability were successfully used in the past in other areas of mathematics to construct objects with curious combinations of properties.

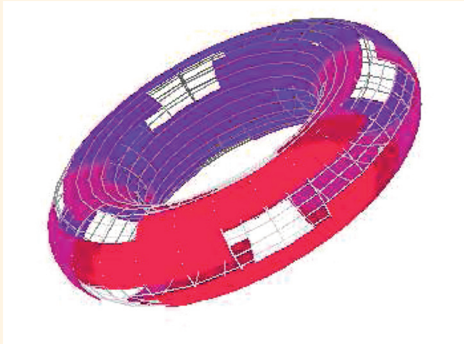


Figure 3.
State space in the form of a torus with rectangular holes. © CEA-LIST.

Combinatorial Algebraic Topology and Concurrency Theory

The idea of combinatorial algebraic topology is to form complexes that represent collections of configurations, for example the set of all colourings of a graph, or the set of all executions of a protocol. The complexes are typically high-dimensional and have a high degree of symmetry. These are expressed via actions of the symmetric group or of a group composed of subgroups of symmetric or related groups. Effective computations of algebraic invariants exploiting these symmetries are still a challenge that will be pursued within this project. There has already been some work exploiting tools from the combinatorial context, such as discrete Morse theory, to the calculation of persistent homology, as well as of some related invariants. Possibilities for further connections in this direction are much greater than has been explored until now. Equivariant methods have been useful in connecting combinatorial algebraic topology with applications in computer science, in particular the feasibility of distributed systems. This topic is embedded in the larger field of *concurrency theory* within theoretical computer science. This field investigates the challenges represented by parallel architectures within an individual computer or within computer networks; in particular for the assessment of the correctness and safety of non-sequential distributed algorithms.

A particular concurrency model, the *higher-dimensional automata*, can be described by pre-cubical complexes with a direction reflecting the time flow. For a mathematical analysis of these models, one has to incorporate direction into tools and methods from algebraic topology. This is the topic of *directed algebraic topology*, which uses fast homology algorithms to analyse the large models arising in practical applications. In a directed topological space, a subcategory of the path category is singled out as the (allowable) directed paths. It is important to note that these are most often not invertible. For applications, the topological state space reflects coordination constraints between individual processes, and directedness is a property of the time flow. The main aim is to understand the properties of (directed) path spaces associated to a well-structured directed topological space, to perform calculations of standard invariants, and to investigate the sensitivity of these invariants with respect to the chosen end points. Directed paths in the same component model computation schedules that will always yield the same result. We mention a few particular questions in the area.

- For geometric models of computation, abstract homotopy theory tools yield models for associated spaces of directed paths in a combinatorial form, i.e. as simplicial complexes. Ongoing work aims to develop this theoretical method into algorithms for applications allowing machine calculations of their homology groups.
- It is desirable to decompose a given directed space into *components* such that the homotopy types of path spaces only depend on the components of start and end point. If finitely (or countably) many such components suffice, it is possible to describe coarser models that can be used by a machine. The existing theory and algorithmic methods apply only to a restricted class of model spaces and should be extended to more general and realistic settings. A related question is the application of persistence to possibly understand the hierarchical structure of such decompositions.
- The literature contains a variety of suggestions for a directed replacement of the notion homotopy equivalence. We will investigate their properties and single out which of them are most suitable in theory and in applications.

Funding

ESF Research Networking Programmes are principally funded by the Foundation's Member Organisations on an *à la carte* basis. ACAT is supported by:

- **Fonds zur Förderung der wissenschaftlichen Forschung in Österreich (FWF)**
  Austrian Science Fund, Austria
- **Det Frie Forskningsråd (DFF)**
  The Danish Council for Independent Research, Denmark
- **Aalborg Universitet,** Denmark
- **Deutsche Forschungsgemeinschaft (DFG)**
  German Research Foundation, Germany
- **Centre National de la Recherche Scientifique (CNRS)**
  National Centre for Scientific Research, France
- **Commissariat à l'Énergie Atomique – Institut LIST (CEA LIST)**
  Atomic Energy Commission – LIST Institute, France
- **National University of Ireland,**
  Galway, Ireland
- **University of Bologna – Centro di Ricerca Avanzato sui Sistemi Elettronici,** Italy
- **University of Warsaw,** Poland
- **Jagiellonian University,** Poland
- **Wyzsza Szkola Biznesu – National Louis University,** Poland
- **Nicolaus Copernicus University,** Poland
- **Centro de Matematica da Universidade do Minho,** Portugal
- **Javna agencija za raziskovalno dejavnost Republike Slovenije (ARRS)**
  Slovenian Research Agency, Slovenia
- **University of Ljubljana,** Slovenia
- **Universidad de Malaga,** Spain
- **Schweizerischer Nationalfonds (SNF)**
  Swiss National Science Foundation, Switzerland
- **University of Warwick,** United Kingdom

ACAT Steering Committee

- **Professor Martin Raussen** (Chair)
  Department of Mathematical Sciences,
  Aalborg University, Aalborg • Denmark
  Email: raussen@math.aau.dk
- **Professor Herbert Edelsbrunner**
  Institute of Science & Technology Austria,
  Klosterneuburg • Austria
  Email: herbert.edelsbrunner@ist.ac.at
- **Professor Graham Ellis**
  Department of Mathematics, National
  University of Ireland, Galway • Ireland
  Email: graham.ellis@nuigalway.ie
- **Professor Michael Farber**
  Mathematics Institute, University
  of Warwick, Coventry • United Kingdom
  Email: michaelsfarber@googlemail.com
- **Professor Dmitry Feichtner-Kozlov**
  FB3 Mathematik, University Bremen,
  Bremen • Germany
  Email: dfk@informatik.uni-bremen.de
- **Professor Massimo Ferri**
  Department of Mathematics,
  University of Bologna, Bologna • Italy
  Email: massimo.ferri@unibo.it
- **Professor Eric Goubault**
  CEA and École Polytechnique,
  Gif-sur-Yvette • France
  Email: eric.goubault@cea.fr
- **Professor Thomas Kappeler**
  Institute of Mathematics, University
  of Zurich, Zurich • Switzerland
  Email: thomas.kappeler@math.unizh.ch
- **Professor Neza Mramor Kosta**
  Faculty of Computer and Information
  Science, University of Ljubljana,
  Ljubljana • Slovenia
  Email: neza.mramor@fri.uni-lj.si
- **Professor Marian Mrozek**
  Department of Computational
  Mathematics, Jagiellonian University,
  Krakow • Poland and WSB-NLU,
  Nowy Sacz • Poland
  Email: Marian.Mrozek@ii.uj.edu.pl
- **Professor Aniceto Murillo**
  Dept. Algebra Geometria y Topologia,
  Universidad de Malaga, Malaga • Spain
  Email: Aniceto@uma.es
- **Professor Lucile Vandembroucq**
  Centro de Matematica, Universidad
  de Minho, Braga • Portugal
  Email: lucile@math.uminho.pt

Observer

- **Professor Roy Meshulam**
  Department of Mathematics, Technion –
  Israel Institute of Technology, Haifa • Israel
  Email: meshulam@tx.technion.ac.il

ESF Liaison

Dr Thibaut Lery
Science
Ms Catherine Werner
Administration

Physical, Engineering and
Space Sciences Unit
European Science Foundation
1 quai Lezay-Marnésia • BP 90015
67080 Strasbourg cedex • France
Tel: +33 (0)3 88 76 71 28
Fax: +33 (0)3 88 37 05 32
Email: cwerner@esf.org

For the latest information on this Research Networking Programme consult the ACAT websites: **www.esf.org/acat** and **acat.lix.polytechnique.fr** or contact Lisbeth Grubbe Nielsen at **grubbe@math.aau.dk**

The European Science Foundation (ESF) was established in 1974 to provide a common platform for its Member Organisations to advance European research collaboration and explore new directions for research. It is an independent organisation, owned by 72 Member Organisations, which are research funding organisations and research performing organisations, academies and learned societies from 30 countries. ESF promotes collaboration in research itself, in funding of research and in science policy activities at the European level.

European Science Foundation
www.esf.org

January 2012 – Print run: 1000