Topological Crystallography

Toshikazu SUNADA *Mathematical Analysis Group Leader*

Position Title,Affiliated Department	：Fellow, MIMS; Professor, School of Science and Technology, Meiji University
Specialized Field, Academic Degree	：Discrete Geometrical Analysis, Ph.D., The University of Tokyo
Research Description	：Analysis of Network System

Research Outline

It is said that geometry in ancient Greece started from the curiosity of mathematicians about the shapes of crystals. Indeed their curiosity culminated in the classification of regular convex polyhedra which is addressed in the final volume of Euclid's Element. Since then, geometry had taken its own path, and the study of crystals had not been the central theme in mathematics (an exception is the work of Johannes Kepler on snowflake). It is only in the 19th century that mathematics began to play a role in crystallography; that is, group theory became matured enough to be applied to the morphology of crystals. Crystallographic groups introduced to describe macroscopic symmetry of crystals have been a basic tool in classical crystallography even after Raue's discovery of crystal structures by the diffraction of X-rays.

This study follows the Greek tradition in the sense that we seek beautiful shapes like regular convex polyhedra. Our primary aim was to use algebraic topology to explore the rich world of crystal structures. More specifically, we employ graph theory, homology theory and the theory of covering maps to introduce the notion of topological crystal which retains, in an abstract way, all the information on the connectivity of atoms in the crystal. This explains the reason why this study is entitled ‘’Topological Crystallography’’.

Topological crystals are "living in the logical world, not in space". This leads us to the issue on how to place (realize) them "canonically" in space. We proposed the notion of standard realizations of topological crystals in space which are characterized by a certain minimal principle, and include, as typical examples, the crystal structures of Diamond and Lonsdaleite. Standard realizations are the most symmetric placements so that, if we take for granted the belief that beauty is bound up with symmetry, then the standard realizations may deserve to be called most beautiful.

We also gave a mathematical view to the standard realizations by relating them to asymptotic behaviors of random walks and harmonic maps. Furthermore, we observed that a discrete analogue of algebraic geometry is linked to the standard realizations.

Applications of our discussion include not only a systematic enumeration of crystal structures, an area of considerable scientific interest for many years, but also the architectural design of lightweight rigid structure.

Model-aided Understanding of Self-Organized Patterns in Biological and Chemical Systems

Masayasu MIMURA *Leader of all research projects*

Position Title,Affiliated Department ：Director, MIMS; Professor, School of Science and Technology, Meiji University

Specialized Field, Academic Degree ：Mathematical Modeling and Analysis (MMA), Ph.D., Kyoto University

Research Description ：MMA of Nonlinear Non-equilibrium Phenomena

Research Outline

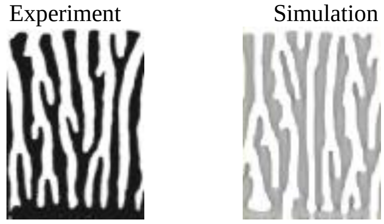
The following paragraphs are the two main achievements obtained for the research theme during the current fiscal year:

1) Diversity of combustion patterns in smoldering combustion in microgravity environments

The US National Aeronautics and Space Administration (NASA) has been conducting combustion experiments in microgravity (μg) environments in space. Of particular interest is their 1998 report discussing an unpredictable complex combustion propagation when a filter paper is gradually burned from one point ignition in a microgravity environment, which completely differs from the one under normal gravity (1g). We address the question, “can combustion propagation in a microgravity environment be predicted from the perspective of mathematical modeling and analysis?” and propose a PDE Model by simplifying the smoldering combustion process as a slowly progressing exothermic reaction. From the various results obtained, we have found that complex combustion propagation patterns appear as a nonlinear, non-equilibrium state, due to the balance between the supply and consumption (combustion) of combustible substances, and that the diversity of the patterns is due to the self-organizing mechanism seen in the phenomena[3].

Smoldering combustion pattern in paper under microgravity environment ([3])

Experiment Simulation

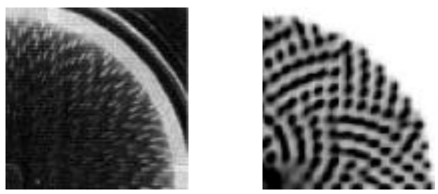


2) Complex patterns in chemotactic E. coli colonies

The July 1995 cover of Nature magazine was a mysterious and beautiful pattern that looked like a flower, and surprisingly the pattern was actually a colony made by the growth and division of E. coli. The question is, “is the formation based on the top-down process of gene regulation, or the bottom-up process of self-organization?” The possibility of the former was experimentally rejected, but the explanation why the latter was the reason was unclear. From our model and simulation analyses, we suggested that it is due to the self-organization mechanism[4].

Spot pattern in chemotactic *E. coli* colonies ([4])

Experiment Simulation



Papers presented in 2010

[1] J. Zu, M. Mimura and J. Y. Wakano: The evolution of phenotypic traits in a predator-prey system subject to Allee effect. , J. Theor. Biol. 262, 528-543 (2010)

[2] M. Bertsch, R. Dal Passo and M. Mimura: A free boundary problem arising in a simplified tumour growth model of contact inhibition, Interfaces and Free Boundaries, 12, 235-250 (2010)

[3] A. Fasano, M. Mimura and M. Primicerio: Modeling a slow smoldering combustion process, Math. Meth. Appl. Sci., 33, 1211-1220 (2010)

[4] A. Aotani, M. Mimura and T. Mollee: A model aided understanding of spot pattern formation in chemotactic E. coli colonies, Japan J. Industrial and Applied Mathematics, 27, 5-22 (2010)

Theoretical Foundation of Combinatorial Optimization and Application to Mathematical Sciences Based on Modeling and Analysis

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Position Title,Affiliated Department : Fellow, MIMS; Professor, School of Science and Technology, Meiji University
Specialized Field, Academic Degree : Theory of Computation, Ph.D., University of Tronto
Research Description : Computation and Theory of Algorisms

Research Outline

Our studies on combinatorial optimization ranged from the theoretical foundation to applications.

For the theoretical approaches, we focused on the problem of determining the directed pathwidth of directed graphs and obtained successful results. The directed pathwidth of a directed graph G is the minimum k that is larger than the indegree of the set of vertices belonging to any prefix of any row of all vertices of G.

No existing studies have reported on polynomial time algorithms to determine whether the given directed pathwidth of a directed graph is below k, even if k is a constant. In this study, we developed such an algorithm for the first time. In particular, assuming that the number of vertices of G is n and that the number of edges is m, then the execution time of the algorithm would be expressed as $O(mn^{k+1})$. The problem of determining the directed pathwidth of directed graphs includes that of undirected graphs as a special case. The developed algorithm also serves as an excellent algorithm for determining the pathwidth of undirected graphs. The best theoretical algorithm for this problem was developed by Bodlaender. Although it is linear with reference to n, it is exponentially related to k3. Our algorithm is therefore faster, depending on the values of n and k. In addition, Bodlaender's algorithm is said to be very complex and difficult to implement, whereas ours is very simple and easy to implement. The study discussing the results was accepted for presentation at the Workshop on Graph-Theoretic Concepts in Computer Science (WG2011).

The problem of determining the directed pathwidth of directed graphs was raised for the issue of identifying attractors in the Boolean network, which was presented in our research outline in last year's annual report. We demonstrated that for Boolean networks with a small directed pathwidth, using a directed path partition enables high-speed identification of all attractors, as compared to simple methods. We carried out even more precise experiments on this application and presented the results as a paper at the IISCIT2010 (International Symposium on Communication and Information Technologies).

The outline of our study in the last annual report discussed the relation between the bandwidth of a planar graph and the size of the largest grid minor, namely, the theory that "if the bandwidth of a graph G is expressed as bw(G) and the maximum value of g when G has a $g \times g$ grid as the minor gm(G), the equation of $bw(G) \leq 3gm(G) + 1$ is established for planar graphs." We revised our paper detailing this theory by correcting the errors and differences in detail and successfully eliminated the +1 term on the right-hand side of the inequality. This was a joint study conducted with Professor Qian-Ping Gu at the Simon Fraser University.

Separately, we considered the problem of deciding whether a given graph does have a k-cyclic orientation. The results showed that this problem is NP-complete for every fixed $k \geq 3$ for general graphs and for every fixed $k \geq 4$ for planar graphs; however, a polynomial time algorithm was established if $k = 3$. This was a joint research carried out with Yasuaki Kobayashi, our graduate student.

Mathematical Expressions of Nonlinear Structures and Patterns

Hirokazu NINOMIYA

Position Title, Affiliated Department : Fellow, MIMS; Associate Professor, School of Science and Technology, Meiji University

Specialized Field, Academic Degree : Nonlinear Partial Differential Equations, Ph.D. (Science), Kyoto University

Research Description : Mathematical science of diffusion and propagation phenomena and pattern structures

Research Outline

Many phenomena in the natural world are often described using partial differential equations that depend on both time and space. Of a range of partial differential equations available, reaction-diffusion equations are applied to most natural phenomena including chemical reactions, physiological phenomena, mathematical ecology, and mathematical biology. Reaction-diffusion equations take the following form and are made up of only diffusion and reaction:

$$u_{j,t} = d_j \Delta u_j + f_j(u_1, \cdots, u_m) \qquad (j = 1, \cdots, m)$$

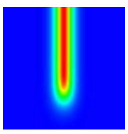
In other words, they correspond to phenomena described by the particle moving according to random walk and the reaction at the point.

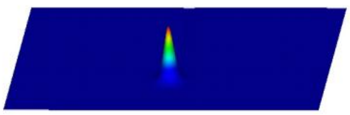
Diffusion in the multiparticle system can sometimes bring about effects that differ from the diffusion of a single particle system. One notable example is diffusion-induced instability discovered by Alan Turing. It is a phenomenon in which periodic patterns are produced by the effect of special uniformity, or diffusion. In collaboration with Associate Professor Noriko Mizoguchi and Professor Eiji Yanagida, we expanded the theory and discovered diffusion-induced explosion. The expanded theory produced an example of explosion* caused by applying diffusion effects even in stable systems where the solutions converge at one point. It also demonstrated that on the contrary, explosions can be inhibited by diffusion in some types of equations. This is called the inhibition of diffusion-induced explosion.

The scope of our research also includes diffusion-induced extinction in models on competition among living things where an inferior species may defeat a stronger species, thereby causing the stronger species to become extinct. We are currently investigating this area focusing on the role of diffusion in reaction-diffusion systems.

The quality of diffusion changes as the type of particles increases. By demonstrating that the combination of reaction and diffusion can produce nonlinear diffusion effects, which has not been understood, our mathematical approach contributes to the present study of modeling.

The diffusion also seems to affect the formation of shapes and patterns, as illustrated by diffusion-induced instability proposed by Alan Turing. In this area, we are studying the relation between nonlinearity and pattern in the formation of V shapes, localization patterns, and finger-like patterns.





*Infinite divergence in limited time