Report on the Trimester Program Mathematics for Complex Materials

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Topics

"*Complex materials*" have extraordinary features and capabilities that have been intensively exploited technologically including many of the most impressive technological applications of our modern living.

Despite outstanding physical achievements, the rigorous mathematical foundations of understanding the complex materials still pose substantial challenges and give rise to paradigmatic mathematical problems. On the one hand, these difficulties already arise with the modelling aspect: Due to the complexity of the relevant materials, in various cases (such as for newer types of liquid crystals like twist-bend nematics, chromonics, blue phases or for various types of mixtures like elastomers, polymer stabilized nematics, colloids) the models are still debated in the respective communities. Often such models are generated on a phenomenological and rather ad hoc basis, in many cases lacking first principles derivations. Here a mathematical approach based on rigorous tools such as the identification of relevant limiting regimes or the derivation of simpler models e.g. by dimension reduction and Γ convergence arguments is of central importance. It could provide a rigorous basis for the various models, highlighting unifying structures and principles.

On the other hand, also for more established complex materials and models (such as the Oseen-Frank, Leslie-Ericksen, which are to some extent simpler versions of Landau de Gennes theory for liquid crystals or the Landau-Lifschitz theory for micromagnetics) many open problems remain unsolved. In fact, for many of these models it is known that they give rise to notoriously difficult mathematical problems involving uniqueness and more generally well-posedness, sometimes even predicting unexpected and/or unphysical behaviour. Prototypical analytical challenges which arise in this context often stem from

- the multi-scale nature of the description of the materials and their pattern formation,
- the non-standard interactions between topological features related to long-range correlations,
- geometrical aspects describing local interactions and constraints,
- algebraic aspects, encoding the local symmetry of the material.

Goals

The main aims of the programme were:

- to address key challenges related to partial regularity, symmetry and solution multiplicity in existing models of complex materials, in particular through interactions of the participants and building on their diverse and complementary expertise;
- to attract new talent to the area, in particular from the next generation of mathematicians, contributing to create a critical mass of mathematicians knowledgeable in the advanced mathematical tools necessary for the study of complex materials, in particular through a school-type conference;
- to explore the applicability of existing tools to the development and understanding of recently discovered materials, thus identifying the mathematical developments necessary for making these tools relevant to the study of the emerging materials;
- to identify the physically relevant analytical challenges and problems that are common to a large class of complex materials and provide basic steps for addressing them. This in turn will contribute to providing a basis for generating a mathematically unifying approach to the study of new materials that balances modelling constraints with fundamental analytical issues, such as well-posedness, regularity and symmetries of solutions.

To this end we focused on problems relevant to key classes of materials and models, specifically but not limited to: alloys, magnetic materials, liquid crystals, nonlinear elastic materials (elastomers), colloids, topological materials. From a mathematical perspective we concentrated on the following core topics:

- Differential inclusions between rigidity and flexibility,
- Topological defects and phase transitions,
- Renormalized energies,
- Symmetries.

Organization

Central activities of the trimester programme consisted of

- a spring school "Recent trends in the mathematics of complex materials" (March 20 24, 2023),
- two workshops on "Current challenges in complex materials: modelling and analysis" (January 9 - 13, 2023) and on "Topological and geometrical aspects in complex materials" (March, 27 - 31, 2023),
- a joint workshop with the PP 2256 on "Variational methods for complex phenomena in solids" (February 21 24, 2023),
- a weekly seminar series,
- a weekly reading course.

Spring School

The main objectives of the spring school were three-fold:

- to give an overview on recent advances in the field of mathematics for complex materials,
- to introduce and attract early career researchers to the field,
- to facilitate more advanced researchers aiming to enter a new field of study.

To this end, five experts provided introductions into their research areas:

- Valeria Banica (Sorbonne): "Singular dynamics for the Schrödinger maps",
- Radu Ignat (Toulouse) and Arghir Zarnescu (BCAM): "Analysis of point defects in nematic liquid crystal",
- Richard James (University of Minnesota): "Origami and Materials Science",
- Lucia Scardia (Heriot Watt, Edinburgh): "Minimisers of nonlocal energies: The effect of anisotropy".

Workshops

An essential and inspiring part of the trimester were the three workshops in which senior and junior scientists presented their research. All workshops took place fully in presence.

In an opening workshop in the first week of the trimester, leading researchers from engineering and mathematics presented some of their most recent results on modelling and analysis. The topics covered included, for instance, Oseen-Frank and Landau-de Gennes models for liquid crystals, Landau-Lifschitz models for magnetic materials, models for polycrystaline shape-memory alloys, the discussion of homogenization as well as defects and grain boundaries in solids. This very international workshop provided a very inspiring start into the trimester programme.

The second workshop of the trimester programme focused on variational methods for complex phenomena in solids. It brought together experts in this field and provided a platform enhancing the interaction between the researchers from the Germany-based Priority Programme 2256 and the trimester programme. Some topics of this very stimulating workshop consisted of the study of dislocations, plasticity, fracture and damage, the folding of paper, isometric immersions in kirigami, the static and dynamic pattern formation in magnetism and compliance minimization, homogenization, the study of minimizers of anisotropic nonlocal energies, of metamaterials, viscoelastic fluid models and Cosserat shell models as well as wave propagation and Korn-Maxwell-Sobolev inequalities.

The final workshop shortly before the end of the trimester programme concentrated in topological and geometrical aspects in complex materials. It offered a showcase of important recent developments in the field. Topics of discussion included vortices and boundary vortices in different (competing and non-competing) theories, the interplay of geometry/topology and physics in different theories, Ginzburg-Landau theory, the Aviles-Giga functional, the Gross-Clark system, the Gross-Pitaevskii equation, Landau-de Gennes theory, the Landau-Lipschitz-Gilbert equation, the eikonal equation, harmonic map equations, the isoperimetric problem, the stability problem in ferromagnetic nano wires, topological singularities in magnetic skyrmions, microstructures in shape-memory alloys, rigidity, flexibility and scaling laws in differential inclusions.

Reading course and seminar series

A weekly seminar series took place during the whole programme, with usually one, and up to three, talks per week. Most talks were recorded and are available online. They provided a beautiful collection of recent results by some of the long-term guests, and an excellent catalyzer of discussions and interactions between participants.

We also encouraged the organisation of specialized reading courses held and followed by small groups of interested guests. The following topics were studied: a recent construction, by Colombo and Tione, of wild solutions to the *p*-Laplace equation with convex integration methods; estimates of Bourgain and Brezis for Helmholtz-Hodge decompositions and their applications to geometric rigidity statements.

Results

The trimester programme lead to many new interactions and cooperations. At the point of writing the report already 22 articles or preprints had appeared by participants of the TP.

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