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MS11: Mathematics for Materials Science

Organisers:	**Pawel Dlotko (Polish Academy of Sciences)**
	Vitaliy Kurlin (Liverpool)
Venue:	**Bute 5**

- 09:00-09:20 **Pawel Dlotko (Polish Academy of Sciences)**
  Computational topology tools in material science
- 09:20-09:40 **Vitaliy Kurlin (Liverpool)**
  Introduction to Periodic Geometry for materials applications
- 09:40-10:00 **Matthew Bright (Liverpool)**
  Introduction to Periodic Topology for Textiles and Crystals
- 10:00-10:20 **Frank Lutz (TU Berlin)**
  Reconstructing metallic foams from tomography data
- 10.20-10:40 **Mark Haw (Strathclyde)**
  From clusters to chains and labyrinths: Structure and kinetics in systems of particles with competing interactions
- 10:40-11:00 **Teresa Heiss (IST Austria)**
  A Topological Fingerprint for Periodic Crystals

Minisymposium: **MS 11 Mathematics for Materials Science**

Organiser: **Pawel Dlotko** (Polish Academy of Sciences)

Vitaliy Kurlin (University of Liverpool)

Timeslot: Friday

Venue: Bute 5

Titles/Abstracts are listed in MS running order.

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Pawel Dlotko (Polish Academy of Sciences)

Computational topology tools in material science

Both topology and material science uses a lot a concept of shape. In this talk I will present computational tools from Topological Data Analysis that can be used in the context of material science.

Vitaliy Kurlin (Liverpool)

Introduction to Periodic Geometry for materials applications

The Crystal Structure Prediction (CSP) aims to discover new solid crystalline materials (crystals) with desired properties for a given chemical composition. The typical approach to CSP is an almost random initial sampling of simulated crystals and their subsequent time-consuming optimization by supercomputers. The resulting CSP landscapes are unstructured plots of thousands or even millions of (often nearly identical) approximations to local minima. The main bottleneck in the CSP is the ambiguity challenge meaning that a real object such as a crystal can be represented in infinitely many different ways. Hence many similar crystals are treated as different and even more resources are wasted on running predictions of physical properties for near duplicate crystals. We introduce key concepts and first results in the new area of Periodic Geometry, which will enable a guided exploration in the space of all potential materials instead of the current random sampling.

Matthew Bright (Liverpool)

Introduction to Periodic Topology for Textiles and Crystals

A structure embedded in n-dimensional space is k-periodic if it maps to itself under k independent translations. This is a property of interest to materials scientists - textiles form 2-periodic structures, crystals are in general 3-periodic. Topological invariants of k-periodic structures are therefore of interest as a means of investigating and classifying materials, and potentially designing new ones.

We can consider k-periodic structures as the cover of some finite object - such as an embedding in the flat torus (1) or as a labelled graph (2). In all cases this involves selecting a fundamental repeating unit of the structure - a unit cell. Since there is no unique selection of unit cell, the appropriate equivalence relation in this context is periodic isotopy, which encompasses isotopic deformations of the object itself and all possible unit cell selections.

Our recent work has developed and refined tools for investigating periodic isotopy. We have used the presentation of textiles embedded in a thickened torus in to extend a knot representation - the Gauss code (3) - to the 2-periodic setting. This can be used as input to an efficient algorithm for determining the realisability of an arbitrary code as a textile structure (4) In the 3-periodic context we have developed a closed form for the periodic linking number (5) that allows it to be quickly computed for a crystal structure considered as a spatially embedded graph (6).

References

(1) Grishanov, S. et al. Textile Research Journal 79(8):702-713 (2009)
(2) Eon, J-G. Act. Cryst. A. 72: 268-293 (2015)

(3) Kurlin, V. Math. Proc. Cambridge Phil. Soc. 145: 129-140 (2008)
(4) Bright, M. et al. Computers and Graphics 90: 51=61 (2020)
(5) Panagiotou, E. J. Computational Physics 300: 533-573 (2020)
(6) Bright, M. et al. arXiv:2011.04631v2 (2020)

Frank Lutz (TU Berlin)

Reconstructing metallic foams from tomography data

Simple foams respect Plateau's rules combinatorially in the sense that every cell edge is contained in exactly three cells and every vertex is contained in exactly four cells. Though simple foams can be reconstructed from their adjacency graphs, in practice, the registration process of adjacency graphs from tomography greyscale image data of metallic foams comes along with errors. We discuss heuristics for the correction of the registration errors as a preprocessing step for the combinatorial analysis and roundness computation of the resulting foam structures. (Joint work with Ihab Sabik and Paul H. Kamm.)

Mark Haw (Strathclyde)

From clusters to chains and labyrinths: Structure and kinetics in systems of particles with competing interactions

Even simple interactions in systems of particles—colloids, nanoparticles, proteins—can create surprisingly complex structures and kinetics, with implications for a wide range of applications (eg nanoporous materials, foods, coatings, drug delivery, membranes) as well as fundamental scientific insight (eg the physics of biological systems such as cell membranes). Moreover while the equilibrium state is related to the interaction potential through thermodynamics, many useful systems are not at equilibrium, for example, metastable mixtures of oils and water in foods and personal care products: thus the structures created on the system's "journey" toward equilibrium, often different to those found at equilibrium, and how that journey can be interrupted, sometimes on very long timescales, i.e., the kinetics of structural change, are important factors. These kinetic aspects are even less straightforward to predict from the interaction potential.

Here, using computer simulation, we explore structures and kinetics in two-dimensional systems of colloids with an arguably 'simplest case' complex interaction: a combination of short-range attractive and long-range repulsive potentials. The interaction leads to a range of structural outcomes, such as compact clustering, chain 'labyrinths', and coexisting clusters and chains. We explore how different structural measures can lead to useful insight, description and categorisation of the possible structures and how they evolve. Cooperative effects mean the attractive potential, despite being very short-ranged compared to the repulsion, can have significant sometimes counter-intuitive effects on large-scale structure. Kinetics of structural change can also be very sensitive to interactions: for example in some regimes small changes in repulsion range and/or particle area fraction can change timescales of structural evolution by many orders of magnitude.

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Teresa Heiss (IST Austria)

A Topological Fingerprint for Periodic Crystals

As the atoms in periodic crystals are arranged periodically, such a crystal can be modeled by a periodic point set, i.e. by the union of several translates of a lattice. Two periodic point sets are considered equivalent if there is a rigid motion from one to the other. A periodic point set can be represented by a finite cutout s.t. copying this cutout infinitely often in all directions yields the periodic point set. The fact that these cutouts are not unique creates problems when working with them. Therefore, material scientists would like to work with a complete, continuous invariant instead. We conjecture that a tool from topological data analysis, namely the sequence of order k persistence diagrams for all positive integers k, is such a complete, continuous invariant of equivalence classes of periodic point sets.