Soft packings, nested clusters, and condensed matter

organized by
Karoly Bezdek, Nikolai Dolbilin, Egon Schulte, and Marjorie Senechal

Workshop Summary

This Workshop brought together a diverse range of researchers from throughout mathematics and other sciences, to explore new ways of modeling the geometry of condensed matter and study the underlying mathematical concepts. The primary focus was on "soft packing" and "nested clustering" phenomena in discrete geometric structures and their applications to understanding the internal atomic structure of solids and fluids.

The Workshop closely followed the AIM format. The Monday and Tuesday morning lectures were given by the organizers. Marjorie Senechal started off the week with an "umbrella talk" addressing the goals and setting the overall context for the meeting. The morning speakers on Wednesday were Jean Taylor and Oleg Musin, and on Thursday, Sergey Krivovichev and Woden Kusner. There were three shorter talks on Friday morning, by Laurant Betermin, Pablo Damasceno and Nikolay Erokhovets. The afternoon working groups assembled along three broad topics: soft packing, modeling of aperiodic structures, and Delaunay sets.

Soft Packing Group

Group members: Laurent Betermin, Karoly Bezdek, Alexey Garber, Alexey Glazyrin, Zsolt Langi, Woden Kusner and Oleg Musin.

In [2], the notion of a packing of congruent soft balls has been introduced as follows: a soft ball in Euclidean d-space $\mathbb{E}^d$ is a pair of concentric balls such that the smaller ball has radius 1 and the larger ball has radius $1 + \lambda$, with $\lambda > 0$. A packing by a given soft ball is simply an arrangement of congruent copies of it in $\mathbb{E}^d$ such that the corresponding unit balls have pairwise disjoint interiors. In particular, the density of this soft ball packing in $\mathbb{E}^d$ is the fraction of space covered by the (possible overlapping) balls of radius $1 + \lambda$. Thus, finding the densest packing of congruent soft balls means finding the largest density of packings of congruent soft balls for given λ and d.

In [2], the authors prove an analogue, for soft ball packings in $\mathbb{E}^d$, of Rogers' density upper bound for hard ball packings. This estimate is sharp for $d = 2$ but is not for $d = 3$. Thus, as a long term goal it is natural to ask for soft analogues of the Kepler conjecture at least for sufficiently small $\lambda > 0$ in Euclidean 3-space.

In particular, an easier but still challenging problem is the classification of the densest lattice packings of soft balls for values of λ with $1 < 1 + \lambda < \sqrt{5/3}$, where $\sqrt{5/3}$ is the simultaneous packing and covering constant of the unit ball in Euclidean 3-space [3]. In connection with the local version of the latter problem the Group proved the following statement (with no immediate restriction on the dimension): if Λ is a locally optimal lattice packing of the hard unit ball such that the symmetry group of Λ acts transitively on the facets of the Voronoi cell of Λ, then Λ is locally optimal for lattice packings of soft balls as well for all $\lambda > 0$.

The Group had highly interesting discussions on further related problems as well, including the following: phase transition for densest soft ball lattice packings; finding upper bounds for the density of soft ball packings in spherical (resp., hyperbolic) spaces; the Tammes problem for soft caps; potentials for soft ball packings; soft ball packings with different radii; and contact numbers for finite soft ball packings.

Clusters Group

Group members: Pablo Damasceno, Yaov Kallus, Marjorie Senechal, Jean Taylor and Erin Teich.

The Group self-assembled to study models of "exotic" order in condensed matter (large unit cell crystals and quasicrystals) for clues to their nucleation and growth. This is timely because the 200-year old "building block" model of crystal structure is fast yielding to one in which nested atomic clusters link and apparently overlap, yet cluster models are still undeveloped geometrically, and poorly understood physically.

The Group decided to study the clusters in two specific aperiodic crystals, one experimental and one simulated (Pablo was an author of the simulations paper [6]). Though their geometric descriptions in the literature are quite different, reexamining the data the Group found common features that their descriptions had obscured. The Group members different backgrounds resulted in discovering some exciting connections. For example, Erin noted that these same key features had appeared in her simulations of dense-packing various solids, including unit balls, in large spheres [7]. This suggests that geometry may play a larger role in the growth of these curious structures than had been thought and will help explain the growth and form of aperiodic crystals more generally.

Five days wasn't enough time to resolve all the questions, but it was long enough to persuade the members that they are fundamental, and that they as a Group are well prepared to address them. The Group hopes to continue to work together, and has applied to the AIM SQuaREs program to that end.

Delaunay Sets Group

Group members: Igor Baburin, Mikhail Bouniaev, Nikolay Dolbilin, Nikolay Erokhovets, Sergey Krivovichev and Egon Schulte.

The Group's activity focused on the local theory of regular systems (orbits of crystallographic groups) in Euclidean d-space. Two new results on the regularity radius and the stabilization radius of Delaunay sets were established and are described below.

The local theory of regular systems, initiated by Delaunay in the 1970's [4], aims at providing a rigorous explanation for the occurrence of global order in a crystalline structure based on the occurrence of congruent patterns. Mathematically, the analysis is carried out in terms of what nowadays are called Delaunay sets X of type (r, R), and of ρ-clusters of Delaunay sets X (the set of points in X at distance at most ρ from a given point). A main goal is to find small positive numbers ρ with the property that each Delaunay set X of type (r, R) with mutually congruent ρ-clusters must be a regular system. The smallest such number ρ, denoted R_d, is called the regularity radius and apriori depends on d, r and R.

Two further problems related to the Local Criterion for Regular Sets of Points were also discussed [4]. They both are relevant for estimates of the regularity radius.

Problem 1 (Group Order Problem): Given a dimension d find an upper bound $C(d)$ for the order of the symmetry group $S(2R)$ of the 2R-clusters of d-dimensional Delaunay sets of type (r, R) with mutually congruent $2R$-clusters. A sharp upper bound is known for $d = 2$ and $d = 3$, namely $C(2) = 12$ and $C(3) = 48$. A conjecture about the sharp upper bound in any dimension d was discussed.

The second problem concerns the symmetry groups $S_x(\rho)$ of ρ-clusters centered at x in a Delaunay set X of type (r, R). It can be shown that if, for some radius ρ of clusters, $S_x(\rho) = S_x(\rho + 2R)$ for each point x of X, then $S_x(\rho') = S_x(\rho)$ for each $\rho' > \rho$ and each point x in X. The smallest such number ρ is called the stabilization radius and is denoted by ρ_s. The Local Criterion for Regular Sets of Points implies that $R_d \leq \rho_s + 2R$.

Problem 2 (Group Stabilization Problem): Estimate from above the stabilization radius ρ_s for Delaunay sets of type (r, R) with congruent $2R$-clusters.

The Group's discussions of these problems resulted in proofs of the following two new results. First, the regularity radius R_d is bounded from below by $2dR$; and second, the stabilization radius ρ_s is bounded from below by $2(d-1)R$.

Further problems discussed include the local theory of t-bonded sets [1], a generalization of Delaunay sets; the dimension problem and its connection with the Voronoi conjecture [5]; and a local approach to characterization of vertex-transitivity of graphs.

There was a good dynamic within the Group that lead to very constructive discussions and remarkably positive outcomes in the short period of time. The Group intends to publish its new findings and hopes to continue to work together on fundamental questions about Delaunay sets. Some members of the Group are planning to submit an application to AIM's SQuaRE program.

In conclusion, the Workshop was a great success! The AIM workshop style with its focus on small working groups fostered both stimulating discussions about general directions of the field as well as hands-on work on specific research problems. We greatly appreciated the opportunity to meet at AIM.

References

[1] M. Bouniaev and N. Dolbilin: Local theory of t-bonded sets, arXiv:1609.02050.

[2] K. Bezdek and Zs. Langi, Density bounds for outer parallel domains of unit ball packings, Proc. Steklow Inst. Math. 288 (2015), 209–225.

[3] K. Böröczky, Closest packing and loosest covering of the space with balls, Studia Sci. Math. Hungar. 21/1-2 (1986), 79–89.

[4] B.N. Delone, N.P. Dolbilin, M.I. Stogrin, R.V. Galiulin: Local Criterion for Regular Sets of Points, Soviet Math.Dokl., 17, 1976, 319–322.

[5] N. P. Dolbilin, Parallelohedra: Retrospective and Recent Results, Trans. Moscow Math. Soc., 2012, 207–220.

[6] M. Engel, P.F. Damasceno , C.L. Phillips and S.C. Glotzer: Computational self-assembly

of a one-component icosahedral quasicrystal, Nature Materials 14 (1), 109–116.
[7] E.G. Teich, G. van Anders, D. Klotsa, J. Dshemuchadse and S.C. Glotzer: Clusters of polyhedra in spherical confinement, Proc. Natl. Acad. Sci. USA 113, E669 (2016).