1 Excellence

1.1 Quality and pertinence of the project's research and innovation objectives (and the extent to which they are ambitious, and go beyond the state of the art)

Motivation

There are fundamental differences between the standard scientific method and the method of mathematical research. Generally speaking, the scientific method is based on observations of natural phenomena and measurement of physical quantities. These are then used to pose hypotheses, which are then tested against cleverly designed experiments. In this way, many false hypotheses can be quickly rejected, while those that survive these tests are eventually recognised as laws of nature.

On the other hand, in theoretical mathematics we are often faced with a lack of initial data upon which we can formulate hypotheses. The process of mathematical research thus usually starts with an abstract idea, sometimes based on intuition and hopefully a handful of examples. These ideas eventually evolve to conjectures. However, unlike in natural sciences, in many branches of mathematics the notion of experiment is non existent making it very difficult to test these conjectures against experimental data. As we all know too well, this often results in hours spent on attempts of proving false conjectures, hours that could be spent on proving theorems instead.

Mathematicians are so used to this way of conducting research that the possibility of using experimental data is often overlooked even when available or not too difficult to obtain. In the last few years, with the development of computers, running experiments and computing large datasets of mathematical objects has opened up new opportunities in mathematical research. Very broadly speaking, the aim of the proposed project PolyData is to use this opportunity in an area of mathematics where such data-driven approach is feasible.

The main objective of PolyData is to develop datasets and computational tools for highly symmetrical discrete objects, in particular abstract polytopes, maps and maniplexes. More precisely, the main research goals for PolyDataare *building complete, accessible, useful and reliable datasets of abstract polytopes* (see RO1 and RO3) and *developing new theoretical tools for constructing abstract polytopes, maps and maniplexes* (see RO2). Finally, we shall encourage the mathematical community to adopt PolyData as a standard for creating, storing and presenting datasets of combinatorial objects (see RO4).

The nature of PolyDatainvolves a two-way flow of knowledge: With the aim of generating new datasets of highly symmetric polytopes and related objects, we will develop new theoretical results and methods, enabling us to devise new algorithms and combinatorial representation for constructing highly symmetric abstract polytopes. The algorithms will then be carefully implemented and executed. The obtained datasets will then be analysed with the aim of finding interesting patterns, suggesting new conjectures and proposing new directions for further research .

As a result of the success of our research we will develop a family of repositories, datasets and software packages that allow both researchers and students to experiment, to identify patterns and to formulate conjectures on abstract polytopes. To achieve this objective, the project will bring together a researcher with expertise on construction of abstract polytopes with prescribed combinatorial conditions with a supervisor with large experience on datasets of discrete objects, in particular of highly symmetric graphs and maps.

Research objectives

Abstract polytopes (AP) are combinatorial objects that generalise (the face lattice) of convex polytopes. Enumeration and classification of highly symmetric convex polytopes goes all the way to the Greeks and the classical problem of classifying what today we know as *Platonic Solids* to the beginning of last century when the classification of higher dimensional convex polytopes was achieved. By considering combinatorial objects and hence removing the geometric constraints, often imposed by the ambient space, opens the possibilities for abstract polytopes and turns the complete classification problem into a series of enumerating families with particular characteristics.

The degree of symmetry of a polytope can be measured by the number of orbits of its automorphism group on certain substructures called *flags*. This combinatorial way of measuring symmetry agrees with the classical geometrical notion. *Regular polytopes* are those that are flag-transitive, meaning they have exactly 1 flag-orbit. This *symmetry type* of polytopes has been traditionally the most studied one and includes classical examples as Platonic solids and regular tilings of Euclidean and Hyperbolic spaces. A slightly less symmetric class of polytopes is that of 2-*orbit polytopes* and among those, *chiral polytopes* are the most studied. The notion of chirality is a classical one in other natural sciences, notably in Chemistry. However, in the context of AP a chiral polytope is one that admit maximal degree of combinatorial rotations but that do not admit mirror reflections. As I will described in detail below, the classes of regular and chiral polytopes are by far the most studied symmetry types of AP. This has led to the constructions of some datasets of highly symmetric polytopes, which shall be described in detail below.

Chiral polytopes are just one of $2^n - 1$ possible symmetry types of 2-orbit n-polytopes. Classical examples of some of the other classes of the 2-orbit polytopes are known. However, the general problem of determining if for

Dataset	Rank 3	Rank 4	Rank $\geqslant 5$
Hartley - Regular	64.55%	31.61%	3.84%
Hartley - Chiral	85.71%	14.29%	0.00%
Conder - Regular	61.51%	34.70%	3.79%
Conder - Chiral	87.01%	12.87%	0.12%
Leemans - Regular	95.35%	4.37%	0.30%
Leemans - Chiral	87.82%	11.97%	0.21%

Table 1: Percentages of examples according to rank

every pair (n, T) with $n > 3$ and T a 2-orbit symmetry type exists an n-polytope of symmetry type T remains open. Some examples of maniplexes (a slightly more general class of objects) were build very recently[1], but whether or not they are polytopal remains unknown. Constructing and classifying n-polytopes with k-orbits and given symmetry type is still a widely open problem[2] and it is one of the main motivations for the development of PolyData.

These existing datasets of polytopes suffer of the following restrictions

(i) They are mainly focused on regular or chiral polytopes.

(ii) The size of the examples is very restrictive.

(iii) They often exhibit numerous examples of rank 3 but the amount of examples of rank higher than 4 drops dramatically.

(iv) They are not very user-friendly, either because they exist only as raw data or because the are specific-programming language oriented.

In Table 1 we show the proportion of examples according to ranks on the existing datasets of polytopes with examples of rank higher than 3.

There are two obvious gaps that need to be pushed forward, not necessarily in an independent way, on the process of building new datasets of abstract polytopes: finding examples of higher ranks and building sets that consider different types of symmetries (besides chiral or regular). With the emerging development of theoretical results for less symmetric polytopes and the need to identify patterns and to find new constructions to attack the numerous open problems related to the existence of polytopes, it is clear that building new datasets of polytopes that overturn the restrictions mentioned above would not only be beneficial but it is almost necessary.

The problematic expressed above outlines our first objective.

RO1 *Extend the existing and build new datasets of abstract polytopes and related structures with particular focus on*

(i) Building examples on ranks higher than 3

(ii) Exploring different symmetry types.

RO1 is of course very general but also very ambitious and should be interpreted as the general research line of PolyData. Any contribution to this objective is a good way of measuring the overall success of PolyData.

Many of the first data sets of abstract polytopes are based on the (small) size of the objects. Either by taking advantage of previously computed objects (such as the library `SmallGrp`) or by using computational routines that, because of their own nature are limited by the size of the input (such as the `LowIndexNormalSubgroups`). However, it has been shown that the size of the smallest regular polytope of rank n grows exponentially with n[3], while the size of the smallest chiral n-polytope is at least of factorial growth with respect to n[4]. This explains why the amount of examples of higher rank polytopes drops dramatically in the current available datasets.

There is a natural theoretical counterpart to RO1, which outlines RO2: The lack of datasets AP including other symmetry classes mostly caused by the lack of examples and theoretical constructions of such objects. Hence, parallel to RO1 we shall develop the following RO.

RO2 *Develop new constructions of highly symmetric polytopes. In particular, focus on the constructions of abstract regular polytopes with given symmetry type to eventually build the corresponding datasets.*

RO2 by itself represents an extremely ambitious and it goes beyond any two year project. Any theoretical contribution is already of great interest to the community. However, we strongly believe that in order to really cause

[1] D. Pellicer, P. Potočnik, and M. Toledo. "An existence result on two-orbit maniplexes". In: *J. Combin. Theory Ser. A* 166 (Aug. 2019).
[2] G. Cunningham and D. Pellicer. "Open problems on k-orbit polytopes". In: *Discrete Math.* 341.6 (2018).
[3] M. Conder. "The smallest regular polytopes of given rank". en. In: *Adv Math* 236 (Mar. 2013).
[4] G. Cunningham. "Non-flat regular polytopes and restrictions on chiral polytopes". In: *Electron. J. Combin.* 24.3 (2017).

an impact on the workflow of research on abstract polytopes all theoretical contributions should be accompanied by its computational analogue. As mentioned before, this RO should go parallel to RO1, meaning that those theoretical construction should allow us to build new datasets and by exploring those datasets we should be able to identify pattern, formulate conjectures and develop new theoretical constructions.

Another pressing issue to address is that the existent datasets of highly symmetric maps and polytopes are not only limited on size, rank and symmetry type, but they are practically not used. One of the reasons behind it is that the information in most of these data sets is not very user-friendly. Even the small amount of existing datasets have been developed by several people, mostly in an independent way, using different notation and different computer algebra systems. Moreover, many of these datasets exist only as raw text which is not always easy to consult. This motivates our next RO.

RO3 *Develop standards and a platform for storing and presenting the datasets of abstract polytopes (both new and existing) in a unified and user-friendly way, complying with the FAIR principles. In particular:*

(i) Survey the existing datasets of AP and related objects, with the emphases on the ways in which they are stored, documented and presented.

(ii) Identify the strengths and weaknesses of the existing datasets and propose unified standards for presentation, management and stewardship of the datasets of AP, following FAIR guideline principles.

(iii) Build a web-based and user-friendly interface to datasets of abstract polytopes stored in accordance with the proposed standards.

RO3 is very concrete and very easy to verify. It will very easily show progress on PolyDatawhile at the same time will set a good and concrete step towards our ambitious general objective.

Of course, PolyDatais aimed to become a long term and eventually permanent resource for the community doing research on symmetries of maps and abstract polytopes. This will not be achievable without the involvement of such community.

RO4 *Encourage and motivate both well-established and young researchers to use and contribute to PolyDataso that it eventually becomes the standard way to explore, experiment and publish data sets, routines and computational tools for the development of the research of abstract polytopes.*

RO4 is very ambitious and we acknowledge that it depends on the community more that on ourselves, but we strongly believe that our approach and the the current status of the could fit together to fill a gap that has been present for many years now. We shall achieve this objective by actively consulting an *external committee* of leading experts on the community.

State of the art

Enumeration and classification of mathematical objects is a natural way of conducting research. The discrete nature of combinatorial objects turn them into natural candidates to not only classify families of interesting objects but to enumerate and explicitly list the elements of such families. This research approach has resulted in the development of interesting data sets of combinatorial objects. Highly symmetric graphs is arguably the most studied family of combinatorial objects from the approach of building datasets of objects. It is believed that empirical study of symmetric graphs of small valence started in 1930s, when R.M. Foster began collecting examples of interesting graphs that could serve as models for electrical networks[5].

The development of the theory, together with more powerful computers, resulted in a breakthrough of datasets of highly symmetric graphs constructions. Using the classification of automorphism groups of 3-valent arc-transitive[6] and bitransitive[7] graphs, together with new methods for finding normal subgroups of finite index in a finitely presented group allowed a construction of complete list of all 3-valent arc-transitive graphs[8][9] of order up to 10000 vertices, and a list of all 3-valent bitransitive graph on up to 768 vertices[10]. Based on their deep theoretical result on the order of automorphism groups[11], Spiga, Verret and Potočnik compiled a complete list[12] of all trivalent

[5] R. M. Foster. "Geometrical Circuits of Electrical Networks". In: *Transactions of the American Institute of Electrical Engineers* 51.2 (June 1932).

[6] D. Ž. Djoković and G. L. Miller. "Regular groups of automorphisms of cubic graphs". In: *J. Combin. Theory Ser. B* 29.2 (1980).

[7] D. M. Goldschmidt. "Automorphisms of trivalent graphs". In: *Ann. of Math. (2)* 111.2 (1980).

[8] M. Conder and P. Dobcsányi. "Trivalent symmetric graphs on up to 768 vertices". In: *J. Combin. Math. Combin. Comput.* 40 (2002).

[9] M. Conder. *Trivalent (cubic) symmetric graphs on up to 10000 vertices*. https://www.math.auckland.ac.nz/~conder/symmcubic10000list.txt, Accessed online January 7th 2022.

[10] M. Conder et al. "A census of semisymmetric cubic graphs on up to 768 vertices". In: *J. Algebraic Combin.* 23.3 (2006).

[11] P. Potočnik, P. Spiga, and G. Verret. "Bounding the order of the vertex-stabiliser in 3-valent vertex-transitive and 4-valent arc-transitive graphs". en. In: *J. Combin. Theory Ser. B* 111 (Mar. 2015).

[12] P. Potočnik, P. Spiga, and G. Verret. "A census of 4-valent half-arc-transitive graphs and arc-transitive digraphs of valence two". In: *Ars Math. Contemp.* 8.1 (2015).

vertex-transitive graphs of order at most 1280. Very recently, using the database of vertex-transitive groups of small degree, Conder and Verret have compiled a complete list of all edge-transitive graphs (of arbitrary valence) up to order 63[13], while Holt and Royle have extended their census of all vertex-transitive graphs up to order 48[14].

The problem of enumerating and classifying regular polyhedra in the Euclidean space is as old as formal mathematics themselves. The enumeration and classification of the five Platonic Solids is one the most antique classification problems. For many years it was considered a complete classification problem (and it was) but later it was shown that by relaxing geometrical constraints we could generalise platonic solids to stellated polyhedra[15 16 17], *infinite skew polyhedra*[18] and finally to *Grünbaum-Dress polyhedra*[19 20 21], which is what today is accepted as the complete classification of regular polyhedra in the Euclidean space[22].

B.Grünbaum was one of the firsts that formally treated geometrical polyhedra-like objects as purely combinatorial objects by introducing the notion of the notion *polystroma*[23]. This notion eventually evolved to what we know today as *abstract polytopes*, introduced in the early 80's[24]

The theory of highly symmetric abstract polytopes nourishes from several branches of mathematics, including group theory, topology and geometry. Coxeter is also attributed to classify the groups generated by hyperplane reflections, leading to what we today know as *Coxeter groups*. They of course, appear as the symmetry groups of regular polytopes and tessellations of the Euclidean and Hyperbolic spaces[25], but they have made their way to Tits geometries[26], computational Lie group theory, Hecke algebras[27], just to mention some.

In 1978 G. Jones and D. Singerman published his classical manuscript[28] which settle the necessary theory to identify maps on orientable surfaces with what in modern terminology we called its *monodromy group*. The ideas behind this paper show important equivalences between topological maps (embedding of graphs on orientable surfaces), certain quotients triangular groups (Coxeter groups of rank 3), maps on Riemann surfaces and certain permutations on the darts of the map. These equivalences are a combinatorial/discrete version of the classical Uniformization theorem[29] for Riemann surfaces. The work of Jones and Singerman was an important contribution on the theory of discrete group actions on Riemann surfaces and it was eventually connected the theory Grothendieck's *Dessins d'enfant*[30].

Abstract polytopes include many of the object mentioned above. Regular abstract polytopes, those with larger degree of symmetry are by far the most studied class of abstract polytopes. Most of this early theory can be found in the very dense and comprehensive monograph written by Schulte a McMullen[31]. Of our particular interest is the problem of building regular polytopes, for which numerous publications exists. We should mention that there exist

[13]M. D. E. Conder and G. Verret. "Edge-transitive graphs of small order and the answer to a 1967 question by Folkman". In: *Algebr. Comb.* 2.6 (2019).
[14]D. Holt and G. Royle. "A census of small transitive groups and vertex-transitive graphs". In: *J. Symbolic Comput.* 101 (2020).
[15]J. Kepler. *Harmonia Mundi in Opera Omnia, Editor: Frisch CH, Heyder & Zimmer, Frankfurt, Vol.* 1864.
[16]L. Poinsot. *Mémoire sur les polygones et sur les polyèdres*. 1810.
[17]A. Cauchy. "AL Cauchy, Recherche sur les polydres-premier mémoire". In: *Journal de l'Ecole Polytechnique* 9 (1813).
[18]H. S. M. Coxeter. "Regular Skew Polyhedra in Three and Four Dimension, and their Topological Analogues". In: *Proc. London Math. Soc.* S2-43.1 (1937).
[19]B. Grünbaum. "Regular polyhedra—old and new". In: *Aequationes Math.* 16.1-2 (1977).
[20]A. W. M. Dress. "A combinatorial theory of Grünbaum's new regular polyhedra. I. Grünbaum's new regular polyhedra and their automorphism group". In: *Aequationes Math.* 23.2-3 (1981).
[21]A. W. M. Dress. "A combinatorial theory of Grünbaum's new regular polyhedra. II. Complete enumeration". In: *Aequationes Math.* 29.2-3 (1985).
[22]P. McMullen and E. Schulte. "Regular polytopes in ordinary space". In: *Discrete Comput. Geom.* 17.4 (1997). Dedicated to Jörg M. Wills.
[23]B. Grünbaum. "Regularity of graphs, complexes and designs". In: *Problèmes combinatoires et théorie des graphes (Colloq. Internat. CNRS, Univ. Orsay, Orsay, 1976)*. Vol. 260. Colloq. Internat. CNRS. CNRS, Paris, 1978.
[24]E. Schulte. "Reguläre Inzidenzkomplexe". PhD thesis. University of Dortmund, 1980.
[25]J. E. Humphreys. *Reflection Groups and Coxeter Groups*. Vol. 29. Cambridge Studies in Advanced Mathematics. Cambridge University Press, June 1990.
[26]J. Tits. *Buildings of spherical type and finite BN-pairs*. Lecture Notes in Mathematics, Vol. 386. Springer-Verlag, Berlin-New York, 1974.
[27]A. M. Cohen. "Coxeter Groups and three Related Topics". en. In: ed. by A. Barlotti et al. NATO ASI Series. Dordrecht: Springer Netherlands, 1991.
[28]G. A. Jones and D. Singerman. "Theory of maps on orientable surfaces". In: *Proc. London Math. Soc. (3)* 37.2 (1978).
[29]W. Abikoff. "The Uniformization Theorem". In: *Amer. Math. Monthly* 88.8 (Oct. 1981).
[30]G. A. Jones and J. Wolfart. *Dessins d'Enfants on Riemann Surfaces*. Springer London, Limited, 2016.
[31]P. McMullen and E. Schulte. *Abstract regular polytopes*. Vol. 92. Encyclopedia of Mathematics and its Applications. Cambridge University Press, Cambridge, 2002.

universal constructions[32 33], constructions prescribing local combinatorics[34 35] and constructions fixing interesting families of groups as automorphism groups[36 37 38 39] .

The second most studied symmetry class of polytopes is that of *chiral polytopes*. They were introduced by Schulte and Weiss in 1990[40] as a natural generalization of *chiral maps*, which have been part of the classical theory of maps from it begging and numerous examples exist[41 42 43] . However, the problem of constructing chiral polytopes of higher ranks has proved to be much harder to that of constructing regular polytopes. Some rank 4 examples were constructed as quotients of hyperbolic tilings[44 45 46 47] . A universal construction[48] was used to produce the first (infinite) example of a rank-5 chiral polytope. However, the first finite rank 5 polytopes were constructed by Conder et al. in 2008[49]. It was until 2010 that Pellicer showed[50] the existence of chiral polytopes of rank n for ever $n \geqslant 4$; The result by Pellicer, although constructive, is not very practical. The size of his examples grow as a tower of exponential functions with length depending on n. Later on examples of new chiral polytopes have been constructed from previously known ones[51 52 53 54] .

The problem of classifying and enumerating highly symmetric polytopes has been part of the theory from the beginning. These has lead to the construction of some datasets of highly symmetric polytopes, which we review below.

Conder - Regular orientable maps by genus Computed by M. Conder it originally contained all (3378) regular maps on orientable surfaces of genus 2 to 101 up to isomorphism an duality. It was later extended to include genus up to 301 for a total of 15824 maps. Computed with the help of `LowIndexNormalSubgroups`routine of MAGMAand published as raw text.

Conder - Regular non-orientable maps by genus Every map on a non-orientable surface admits an orientable double cover. Conder used this fact to originally compute all (862) non-orientable regular maps of genus 2 to 202 and then extended to genus up to 602 for a total of 3260 maps. Computed with the help of `LowIndexNormalSubgroups`routine of MAGMAand published as raw text.

Conder - Chiral maps by genus Census containing all (594) chiral maps on orientable surfaces of genus 2 to 101. This census was later extended to genus up to 301 for a total of 3870. Computed with the help of `LowIndexNormalSubgroups`routine of MAGMAand published as raw text.

Conder - Rotary maps by size This census contains all rotary (that is regular or chiral) maps whose rotation group has less than 2000 elements (equivalently, such that the map has less than 1000 edges). Computed with the help of `LowIndexNormalSubgroups`routine of MAGMAand published as raw text. There exist versions of this census containing only regular and only chiral maps.

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32 E. Schulte. "On arranging regular incidence-complexes as faces of higher-dimensional ones". In: *European J. Combin.* 4.4 (1983).
33 E. Schulte. "Extensions of regular complexes". In: *Finite geometries (Winnipeg, Man., 1984)*. Vol. 103. Lecture Notes in Pure and Appl. Math. Dekker, New York, 1985.
34 L. Danzer. "Regular incidence-complexes and dimensionally unbounded sequences of such. I". in: *Convexity and graph theory (Jerusalem, 1981)*. Vol. 87. North-Holland Math. Stud. North-Holland, Amsterdam, 1984.
35 D. Pellicer. "Extensions of regular polytopes with preassigned Schläfli symbol". In: *J. Combin. Theory Ser. A* 116.2 (2009).
36 P. J. Cameron et al. "Highest rank of a polytope for A_n". In: *Proc. Lond. Math. Soc. (3)* 115.1 (2017).
37 M. E. Fernandes and D. Leemans. "C-groups of high rank for the symmetric groups". In: *J Algebra* 508 (2018).
38 D. Leemans, J. Moerenhout, and E. O'Reilly-Regueiro. "Projective linear groups as automorphism groups of chiral polytopes". In: *J. Geom.* 108.2 (2017).
39 D. Pellicer. "CPR graphs and regular polytopes". In: *European J. Combin.* 29.1 (2008).
40 E. Schulte and A. I. Weiss. "Chiral polytopes". In: *Applied geometry and discrete mathematics*. Vol. 4. DIMACS Ser. Discrete Math. Theoret. Comput. Sci. Amer. Math. Soc., Providence, RI, 1991.
41 H. S. M. Coxeter and W. O. J. Moser. *Generators and relations for discrete groups*. Third. Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 14. Springer-Verlag, New York-Heidelberg, 1972.
42 M. Conder and P. Dobcsányi. "Determination of all regular maps of small genus". In: *J. Combin. Theory Ser. B* 81.2 (2001).
43 F. A. Sherk. "A family of regular maps of type $\{6,6\}$". In: *Canad. Math. Bull.* 5 (1962).
44 B. Nostrand, E. Schulte, and A. I. Weiss. "Constructions of chiral polytopes". In: *Proceedings of the Twenty-fourth Southeastern International Conference on Combinatorics, Graph Theory, and Computing (Boca Raton, FL, 1993)*. Vol. 97. 1993.
45 E. Schulte and A. I. Weiss. "Chirality and projective linear groups". In: *Discrete Math.* 131.1-3 (1994).
46 B. Nostrand. "Ring extensions and chiral polytopes". In: *Proceedings of the Twenty-fifth Southeastern International Conference on Combinatorics, Graph Theory and Computing (Boca Raton, FL, 1994)*. Vol. 102. 1994.
47 B. Nostrand and E. Schulte. "Chiral polytopes from hyperbolic honeycombs". In: *Discrete Comput. Geom.* 13.1 (1995).
48 E. Schulte and A. I. Weiss. "Free extensions of chiral polytopes". In: *Canad. J. Math.* 47.3 (1995).
49 M. Conder, I. Hubard, and T. Pisanski. "Constructions for chiral polytopes". In: *J. Lond. Math. Soc. (2)* 77.1 (2008).
50 D. Pellicer. "A construction of higher rank chiral polytopes". In: *Discrete Math.* 310.6-7 (2010).
51 G. Cunningham and D. Pellicer. "Chiral extensions of chiral polytopes". In: *Discrete Math.* 330 (2014).
52 M. D. E. Conder and W.-J. Zhang. "Abelian covers of chiral polytopes". In: *J. Algebra* 478 (2017).
53 A. Montero. "Chiral extensions of toroids". PhD thesis. National University of Mexico, 2019.
54 A. Montero. "On the Schläfli symbol of chiral extensions of polytopes". en. In: *Discrete Math* 344.11 (Nov. 2021).

Potocnik - Regular maps by size An improvement on Conder's census containing all (255, 980) regular maps whose automorphism group is of order less than 6, 000 for orientable maps and 3, 000 for non-orientable maps. Published as MAGMAfiles available to download with a CVS-file of precomputed information.

Potocnik - Chiral maps by size An analogous to the one above but for chiral maps. It contains a total of 122, 092 chiral maps whose automorphism group has order less than 6, 000.

Hartley - The Atlas of Small Regular Polytopes It was build using `SmallGrp` routine of GAP and contains all regular polytopes with at most 2000 flags, except those of size 1024 and 1536. It contains 9212 examples. They are presented in a nice web interface and the code is available to download.

Hartley - The Atlas of Small Chiral Polytopes Every chiral polytope admits a minimal regular cover. Hartley used this fact to compute the first atlas of chiral polytopes. This dataset consists of all chiral polytopes whose minimal regular cover belongs to the Atlas of Small Regular Polytopes. This gave a total of 48 chiral polytopes of rank 3 and 8 polytopes of rank 4.

Conder - Regular polytopes up to 2,000 flags A dataset containing, up to duality, all (5809) regular polytopes with at most 2000 flags (which is the same as the order of the automorphism group).

Conder - Chiral polytopes up to 2,000 flags A dataset containing, up to duality, all (839) chiral polytopes with at most 2000 flags (which is the twice the order of the automorphism group).

Leemans et al. - An Atlas of polytopes for small simple groups This is an ongoing atlas that contains regular polytopes whose automorphism group is an almost simple group. It currently contains 55, 575 regular polytopes. The atlas is presented on a website with downloadable data.

Leemans et al. - An Atlas of chiral polytopes for small simple groups It is the analogous to the one above but for chiral polytopes. It currently contains a total of 19, 964 polytopes.

1.2 Soundness of the proposed methodology

Overall methodology

Symmetries of abstract polytopes lie in the intersection of several mathematical disciplines: *combinatorics, group theory, geometry* and *topology*. On the other hand, construction of datasets of mathematical objects calls for the expertise in *computer science* and the emerging field of *mathematical knowledge management*.

The central objectives of the proposed research are of course RO1 and RO2 (construction of datasets and infinite families of highly symmetrical abstract polytopes). In order to achieve these objectives, a variety of techniques drawing ideas from all of the above mathematical areas will need to be used. Below, we give a short overview of some of the techniques we plan to use.

In parallel to objectives RO1 and RO2, a major emphasis will be given to RO3 (development of standards for management and stewardship of datasets of abstract polytopes and a web-based platform). Here, the general FAIR-principles will be carefully implemented on existing and constructed datasets of abstract polytopes.

Finally, to achieve RO4 of inviting the community to adopt PolyData as a standard we shall follow strategies such as *show by the example*: exhibit how well-documented and well-presented datasets can be useful in theoretical research. Initiate and carry out some theoretical research based on the data obtained in the datasets. *Present the results*: use forums such as large conferences to present our results, methodology and how PolyData can be actively used in mathematical research. *Organise workshops* where issues regarding the presentation and stewardship of data in mathematics are discussed and *actively solicit suggestions and contributions* to PolyData by a larger mathematical community.

In order to build new datasets of AP (and develop RO1 and RO2) we need both, theoretical techniques and computationally efficient ways to represent and compute data. These two paths will grow in parallel: we shall implement theoretical constructions into datasets and from analysing those datasets we will identify patterns, formulate new conjectures and eventually develop new theoretical constructions. To achieve this goals, we introduce come methods of constructing and representing AP that we can use from the beginning of PolyData. However, we should keep in mind that part of our proposed research is to find and develop new methods and techniques to build AP.

Constructing abstract polytopes from groups. Given a group G and a family of generators satisfying certain group-theoretical conditions it is possible to build an abstract polytope with G as its automorphism group. These conditions for regular and chiral polytopes have been known and exploring known databases of groups have been the main tool used to build the existing datasets of polytopes. For different symmetry types, other than regular and chiral, those conditions were recently characterised by Mochán[55]. The fact that these conditions were not fully understood

[55] E. Mochán. "Abstract polytopes from their symmetry type graph". PhD thesis. National University of Mexico, 2021.

before is most likely the reason why there are no datasets of non regular or chiral polytopes. Using these novel results I shall explore known libraries of groups to build abstract polytopes from groups with different symmetry types (besides regular and chiral). Even though this is a very naive approach, it should be a first approach towards RO1.

Schreier coset graphs and permutation groups. The previous method of constructing polytopes is limited by the size of the group on existing databases of groups, a slightly different approach is to build such groups in an efficient way. Schreier coset graphs are a classical tool to represent a permutation groups. Large groups can be represented with relative small graphs; for example, the symmetric group S_n with $n!$ elements admits a representation on a graph with n vertices. Schreier coset graphs allows us to build (the automorphism group of) new abstract polytopes from previously existing ones. We are going to use this method as follows: take a Schreier coset graph of a known existing polytope, then we shall use classical graph operations such as *covers* or *voltage assignments* to build a new graph and then determine whether or not this a a Schreier coset graph of a polytope.

This tool allows us not only to build new abstract polytopes but also to find a computationally efficient way of storing the automorphism group of an abstract polytope.

It is important to remark that these graphs already have shown potential to improve known computational methods. In a joint manuscript[56] with A. I. Weiss, we build infinite families of regular hypertopes (a generalisation of abstract polytopes) using Schreier coset graphs, solving an open question from a previous manuscript[57] where the authors were not able to find a single example using traditional computational tools (in particular `LowIndexNormalSubgroups` form MAGMA).

Maniplexes. Maniplexes are a graph theoretical generalisation of an abstract polytopes. A standard technique in mathematics is to use more general objects to solve problems then try to particularise the solution. By representing polytopes as graphs we are able to use graph-theoretical techniques such as *covers*, *voltage assignments* and *extensions* to build new maniplexes and hence determine which of those maniplexes are actually polytopes.

We shall emphasise that theses two previous approaches to build abstract polytopes sit in a great place for our research. The supervisor is an expert on methods of building datasets of graphs and both Schreier coset graphs and maniplexes are strong bridges between graph-theoretical techniques and problems on abstract polytopes.

Extensions. A polytope $\mathcal{P}$ is an extension of a polytope $\mathcal{K}$ if all the facets of $\mathcal{P}$ are isomorphic to $\mathcal{K}$. Symmetry conditions on $\mathcal{K}$ imply symmetry restrictions on $\mathcal{P}$. A natural way of constructing new polytopes is to determine when a given polytope admits an extension with prescribed symmetry conditions. This has proved to be a hard theoretical problem that we should attack as part of RO2 to then implement in the development of RO1. The specific techniques to attack this problem vary from graph theoretical techniques (using maniplexes and coset graphs) to purely group theoretical (such as free products with amalgamations). Observe that the use of extensions is a natural way to overcome the need of natural examples and datasets of higher rank polytopes.

Operations. Very informally, an operation is a mapping O that assigns a polytope $O(\mathcal{K})$ to each polytope $\mathcal{K}$. Usually the symmetries of $O(\mathcal{K})$ are related to the symmetries of $\mathcal{K}$. Very recently in a joint work with Hubard and Mochán[58], we have developed a theoretical technique to build polytopes with prescribed symmetry type. We shall use this technique to build new abstract polytopes from previously known ones by using known families of operations. Implementing these operations in a computational way should be one of our first approaches to attack both RO1 and RO2 and should allow us to build the first known dataset of non regular or chiral abstract polytopes.

Open science practices and FAIR principles

The nature of our research allows us to keep it fully open at every step. In fact, it is part of our research methodology that the users actively get involved in the process. Therefore, our research shall be able to fulfill most open science practice. We shall keep preliminary versions of our research manuscripts on ArXiv and submit the final versions to high quality open access journals. We shall use open-source software and keep the development of our own packages and datasets in a public git repository. Final version of our datasets will be publicly available on a website and in a FAIR-repository (such as Zenodo, MathDataHub).

As explained in Section 1.1, data management is still a young discipline in mathematics. Data production and storage has not been a key part of the traditional development of theoretical mathematics. Moreover, although most theoretical mathematicians embrace the notion of *open science*, the awareness of the FAIR principles for managing mathematical data is at a considerably lower level. A part of the problem might lie in the fact that specific nature of mathematics requires specific adaptations of the FAIR principles. This problem has been addressed in a recent

[56] A. Montero and A. I. Weiss. "Proper locally spherical hypertopes of hyperbolic type". en. In: *J Algebr Comb* (Oct. 2021).
[57] M. E. Fernandes, D. Leemans, and A. I. Weiss. "An Exploration of Locally Spherical Regular Hypertopes". In: *Discrete & Computational Geometry* (June 2020).
[58] I. Hubard, E. Mochán, and A. Montero. "Voltage operations on maniplexes". In preparation.

work of by Berčič et al.[59], where the notion of *Deep FAIR*. We shall follow their guidelines and at the same time use PolyData to promote the *Deep FAIR* principles.

We shall make our datasets *findable* by publishing datasets into an open FAIR-repository (Zenodo, MathDadaHub). We shall write appropriate metadata and documentation so that our datasets are not only accessible from the corresponding research papers (as it is usually the standard on mathematics) but from both a web-based interfaced and a downloadable source. This shall include corresponding software packages to manipulate and experiment with the datasets. Our data and metadata will be presented in web-based format as well as in platform independent formats (PDF, CVS). Full *interoperability* of software and mathematical objects is almost impossible but we shall at least make our datasets compatible with most popular computer algebra systems such as GAP, `SageMath` and MAGMA. We shall follow community standards in order to create datasets and software packages as *reusable* as possible.

We shall finish this section by pointing out that there the nature of our research, being purely abstract, *does not involve any gender dimension or other diversity aspects.*

1.3 Quality of supervision, training, and knowledge transfer

During the MCS fellowship in Ljubljana, I will be supervised by prof. Primož Potočnik. He is a leading expert in the area of algebraic graph theory. His work includes purely graph theoretical results, applications of group theory in algebraic graph theory, as well as computational aspects in group theory and discrete mathematics. He has proved a number of deep theoretical results as well as developed many new computational approaches that enabled him (and his coworkers Pablo Spiga, Gabriel Verret) to significantly increase the scope of existing datasets of highly symmetric graphs. His achievements include the census of all cubic vertex-transitive graphs of order up to 1280, the census of all tetravalent arc-transitive graphs of order up to 640, the census of all rotary maps on at most 1.500 edges etc. These datasets are one of the most used and cited resources in algebraic graph theory.

Prof. Potočnik has successfully supervised three PhD students (Gabriel Verret, Katja Berčič, Micael Toledo), currently supervises a postdoctoral fellow Alejandra Ramos and has informally advised several junior members of the department. He is the leader of a long-term research programme funded by the Slovenian Research Agency (ARRS) and has held numerous leadership positions (such as the Head of Department, Vice Dean of the faculty and the head of the PhD programme in mathematics). He has strong research ties with a number of leading research groups in discrete mathematics (such as the groups at University of Auckland, University of Ottawa, Comenius University in Bratislava, Univeristá degli Studi Milano etc) and regularly hosts top researchers in the area.

My joint research with prof. Potočnik will be supplemented by the training at the *mathematical knowledge management group* led by Katja Berčič. Dr. Berčič has recently returned from her postdoctoral training at the KWARC group at FAU in Erlangen, led by prof. Michael Kohlhase. She is now actively involved in a development of MathDataHub, a semantic portal that provides a web interface to datasets. The interface supports easy filtering, searching and customisable presentation of individual objects.

I will also regularly interact and discuss different aspect of my research with other members of a very strong discrete mathematics and theoretical computer science group at the University of Ljubljana, which includes high profile researchers, such as prof. Bojan Mohar (jointly appointed with Simon Fraser University, Canada), prof. Sandi Klavžar, prof. Riste Škrekovski, prof. Tomaž Pisanski, prof. Andrej Bauer etc. Having an opportunity to regularly meet and work with researchers of this level will contribute significantly to my professional growth.

Finally, a board of external advisors will be formed, consisting of top experts in the relevant areas of mathematics (including prof. Marston Conder, prof. Pablo Spiga, prof. Asia I. Weiss and prof. Gabe Cunningham and prof. Isabel Hubard,), who will regularly check on the progress of my research and advise on further directions.

Working under the supervision of prof. Potočnik a MSCA fellow, I hope to draw from his vast experience on theoretical and computational issues in algebraic graph theory. In particular, I hope acquire several new skills, including:

- ability of using advanced group theoretical methods relevant for the topic of the proposed research;
- proficiency in development of software packages (GAP, `SageMath` , MAGMA) for discrete mathematics;
- internet programming skills, such as construction of user-friendly internet platforms;
- understanding mathematical knowledge management (presenting and storing mathematical data under FAIR principles).

My training will consists of:

[59] K. Berčič, M. Kohlhase, and F. Rabe. “(Deep) FAIR mathematics”. en. In: *it - Information Technology* 62.1 (Feb. 2020).

- daily short research meetings with the supervisor (at least 4 times a week), where progress on the project and obstacles and possible solutions will be discussed;
- longer research sessions with the supervisor (once to twice per week);
- weekly meetings with the knowledge management group at the department (led by dr. Katja Berčič), where
- attending the meetings of the discrete mathematics group at the department (once a week) and research sessions with individual members of the group (based on the specific needs of the project)
- intensive research retreats (in duration of at least 5 days at least once per 2 months) where meetings with the advisory board will be organised.

On the other hand, my experience on the topic subject of abstract polytopes complements the more graph- and group-theoretical expertise of the supervisor and the discrete mathematical group at the host institution. The complementary nature of the expertise of the supervisor and myself will have synergetic effects needed to fulfil the objectives of PolyData.

2 Impact

2.1 Credibility of the measures to enhance the career perspectives and employability of the researcher and contribution to his/her skills development

The interdisciplinary nature of the proposed research will provide me with training in two mains sets of skills. On the one hand, with the guidance of the supervisor, I will consolidate my young career as a theoretical mathematician working with highly symmetric objects. In particular, I shall gain training on *permutation groups* and *symmetries of graphs*. The strong presence of prof. Potočnik will increase my own presence in the community which in turn will improve my chances to obtain a permanent academic job.

On the other hand, the computational skills needed to build the proposed datasets, such as the development of software packages, databases, and the mathematical knowledge management will make me a desirable researcher not only for pure math departments but also for computer-science-oriented institutions.

Moreover, FMF-UL host an undergraduate and graduate program in mathematics which is a great opportunity for me to increase my teaching experience.

Finally, the programming and data management training obtained as a result of the proposed research will not only improve my chances to get an academic position but also a non academic job as a software developer, data manager or any other data-oriented position.

2.2 Suitability and quality of the measures to maximise expected outcomes and impacts, as set out in the dissemination and exploitation plan, including communication activities

Our proposed research sits on the interplay of computer science and theoretical mathematics. However, as most basic research the end users will be other researchers working on symmetries of discrete objects. We should emphasise that our overall goal is to improve the way research on this area is performed.

Our plan of dissemination can be divided into two main categories: local audience and international audience.

For the local audience I will continuously participate on with talks on the seminar of Discrete Mathematics of the host institution (FMF-UL) as well as the seminar of Combinatorics and group theory of the Faculty of education of the University of Ljubljana (PeF-UL). Those two seminars will allow me to constantly disseminate my research among the local researchers. Those researchers can will test the quality and efficiency of the built datasets and will offer constant feedback.

For the international audience we should publish research articles in open access journals that show the potential of our research. Meaning that we should not only write and publish articles that explain how we build datasets of polytopes but we should serve as the firsts users of these datasets. We should direct our theoretical research towards the use of these datasets to show the potential they have to improve the way basic research is performed.

I will participate in international conferences to present and disseminate our research. I will present the first advances of our research in a talk in the International Slovenian Conference on Graph theory, which is an international forum that occurs every 4 years and has had more than 300 participants in the last editions.

In order to optimize the development of the computational part of our project, I shall organise at least one programming workshop per year were both researchers and students will get together and discuss problems regarding datasets of discrete objects. This will also serve to get users that will test our developed datasets.

Finally, I shall visit at least once a year a member of the external advisory committee in order to adapt the development of our research to the needs of the community.

On the other hand, our project will be a case of study of the KWARC group. They not only be beneficiated from the final research products but also from the process of developing these datasets as part of their research on mathematical knowledge management. We shall measure this impact by having constant meetings with Dr. Berčič, who participates in this group, but also by invinting active research on mathematical knowlege managemente to orient, supervise and participate on the organised workshops.

2.3 The magnitude and importance of the project's contribution to the expected scientific, societal and economic impacts

As mentioned before, the final users of our project are mostly on the scientific community.

Our research shall contribute to the overall development of research on symmetries of discrete objects. As mentioned in Section 2.2, PolyData shall benefit researchers and students of discrete mathematics by improving the way the conduct research. The first and probably most obvious way is that as a result of RO1 and RO2 we shall not only contribute with research papers to the community but to show an example of how datasets can be used to conduct research. Our data will be published as an open FAIR-repository with the appropriate documentation and software packages so that the users can easily include it on their own workflow. Furthermore, with the success of RO4 we expect to truly and substantially change the way research on discrete mathematics is performed.

The collaboration with the KWARC group will serve to promote the development of mathematical knowledge management. In particular, our project, as a whole, shall be a test case of the Deep FAIR principles.

3 Quality and Efficiency of the Implementation

3.1 Quality and effectiveness of the work plan, assessment of risks and appropriateness of the effort assigned to work packages

In the list below WP1 (Work package 1) is correspondence with RO1, WP2 with RO2, etc. For each item, T stands for *Task*, M for *Milestone* and D for *Derivable*. The number on parentheses after milestones and derivables indicates the expected month to achieve/deliver the item.

Since RO1 and RO2 feed each other, WP1 and WP2 will run on parallel throughout all the project development. WP3 should run smoothly at the beginning of the project and its progress will depend on the success of RO1 and RO2 towards the end, while WP4 will start once we have some progress to show in RO3.

WP1 (New datasets of abstract polytopes)

T 1.1 Use operations to build *truncations*, *medials* and other classical constructions from the existing datasets of regular and chiral polytopes.

M 1.1 First dataset containing polytopes with symmetry types other than regular or chiral. . . . . (4)

D 1.1 FAIR repository the first dataset of non-regular and non-chiral polytopes. . . . .(6)

D 1.2 Update on the website (D2.2) with these new datasets. . . . . (8)

T 1.2 Explore known libraries of groups looking for groups to build non-regular and non-chiral polytopes.

T 1.3 Use extensions to build higher rank new polytopes from those previously known.

T 1.4 Compute auxiliary Schreier coset graphs of constructed datasets.

M 1.2 First programming workshop organised. . . . .(12)

D 1.3 Update on the repository and the website. . . . .(14)

T 1.5 Development of software packages to implement the constructed datasets.

M 1.3 First version of software packages for the new datasets. . . . . (18)

D 1.4 Software packages for the new datasets and documentation to use them publicly available. . . . .(20)

T 1.6 Implement other theoretical constructions developed in WP2 to build new datasets.

M 1.4 Second programming workshop organised . . . . (22)

WP2 (Theoretical constructions of polytopes)

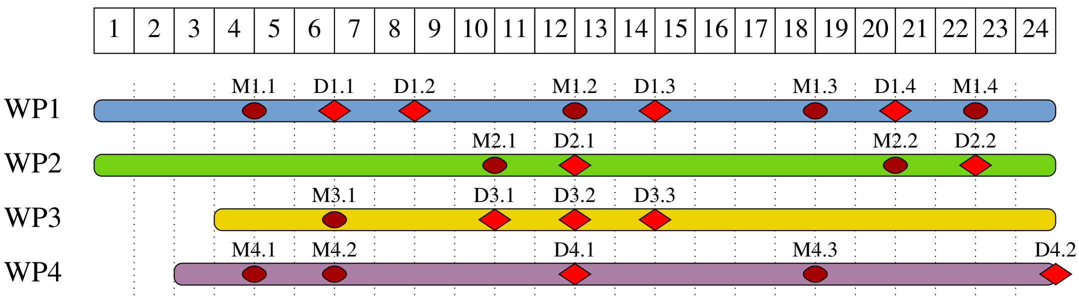
T 2.1 Use voltage operations to build polytopes with prescribed symmetry type.

T 2.2 Build extensions of regular and chiral polytopes on the existing datasets and explore the symmetry type possibilities.

T 2.3 Use Schreier coset graphs to build extensions of polytopes with prescribed symmetry type.
M 2.1 Give constructions of abstract polytopes with given symmetry type and 2, 3 and 4 orbits. . . . . (10)
D 2.1 Research manuscript on extensions of polytopes. . . . . (12)
T 2.4 Explore how classic techniques on graph theory can be implemented to build maniplexes and polytopes.
M 2.2 Construction of highly symmetric maniplexes and polytopes using graph theoretical techniques. . . . . . (20)
D 2.2 A manuscript on constructions of maniplexes with prescribed symmetry type . . . . (22)

WP3 (Publish and manage datasets of polytopes in a FAIR-ly way)
T 3.1 Collect an unify the existing datasets of abstract polytopes.
T 3.2 Compute the maniplex associated to each of the polytopes
T 3.3 Start building a database of polytopes with the already computed data.
T 3.4 Write documentation on how to use our repository.
M 3.1 Prepare data and metadata to start building a fair repository. . . . . (6)
D 3.1 First version of a repository including the existing computed datasets of polytopes. . . . . (10)
D 3.2 A website with a web-based version of the computed data. . . . . (12)
D 3.3 Write software packages to improve the user-data interaction. . . . . (14)

WP4 (Dissemination of PolyData to establish it as a standard)
T 4.1 Prepare a presentation of PolyData to introduce it to the community.
M 4.1 Introduce our project in an international forum. . . . . (4)
T 4.2 Evaluate the feedback obtained in M 4.1 and implement the appropriate changes.
Prepare an early version of D 2.1 to be tested by the local audience and the external committee.
M 4.2 First visit to a member of the external committee. . . . . (6)
T 4.3 Establish a web interface to receive feedback from the community
D 4.1 Publish the web interface in T 4.3 . . . . (12)
T 4.3 Work on the implementation of datasets according to the requests of the community.
M 4.3 Visit to a member of the external committee . . . . (18)
T 4.4 Write documentation and software packages to allow the users to contribute to PolyData .
D 4.2 Documentation and software package to allow the community to follow our standards and contribute to our repositories . . . . (24)



3.2 Quality and capacity of the host institutions and participating organisations, including hosting arrangements

The University of Ljubljana (UL) and Faculty of Mathematics and Physics (FMF-UL) provides to all researcher's office/lab space and personal computer with overall administrative and IT support. FMF-UL has its own meeting rooms and a specialised library. Other 37 libraries of the UL faculties/academies and departments, the National and University Library, and the Central Technological Library can also be used. UL researchers have access to about 20.000 subscription e-journals for free (Elsevier, Springer Nature, Wiley, etc.) and to more than 170.000 licenced e-books from one-point DiKUL (Digital Library of UL). Articles and monographs with one of the faculties of the University of Ljubljana as the affiliation, can be deposited and openly available through the Repository of the University of Ljubljana. Foreign researchers also get support from Research Offices and Human Resources Office at Rectorate and faculty level regarding their working/living arrangements, accommodation etc. UL owns several apartments, which are available to foreign researchers. UL offers excellent working conditions, innovative and multidisciplinary research environment and promotes high quality of exchange of interdisciplinary knowledge and ideas.

The Department of Mathematics at UL FMF hosts a very strong discrete mathematics and theoretical computer science group at the host institution, which includes high-level researchers, such as Bojan Mohar (affiliated also with Simon Fraser University, Canada), Sandi Klavžar, Tomaž Pisanski, Riste Škrekovski, Andrej Bauer, Matija Pretnar etc. Members of this group have lead several research projects and have extensive experience in supervising PhD students and postdoctoral researchers, including an MSC fellow (Daniel Ahman, under supervision of Matija Pretnar).