Nested Polytopes with Non-Crystallographic Symmetry Induced by Projection

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Abstract

Inspired by the structures of viruses and fullerenes in biology and chemistry, we have recently developed a method to construct nested polyhedra and, more generally, nested polytopes in multi-dimensional geometry with non-crystallographic symmetry. In this paper we review these results, presenting them from a geometrical point of view. Examples and applications in science and design are discussed.

Introduction

Polyhedra and symmetry are fascinating topics that have attracted the attention of scientists and artists since ancient times. There are innumerable examples of polyhedral shapes in nature; Radiolaria are single-cell micro-organisms that live in the ocean, with shapes resembling the Platonic solids, that were first described by E. Haeckel after his voyage on H.M.S. Challenger in the late nineteenth century [1]. Most viruses are made up of a protein shell, called capsid, that contains the genomic material and in many cases possesses icosahedral symmetry. Caspar-Klug theory and generalisations thereof [2] exploit this symmetry in order to predict the positions of the capsid proteins by representing the capsid as an icosahedral surface. In chemistry, icosahedral symmetry occurs in fullerenes, molecules of carbon atoms arranged to form icosahedral cages [3]. In fact, the name itself comes from Buckminster Fuller, who designed the geodesic dome in 1948, with an icosahedral shape.

Mathematics provides a beautiful and powerful language to describe symmetry in nature. In 1872, F. Klein, in his Erlangen Program, proposed the idea to study the symmetries of a geometrical shape through abstract objects called *groups*. Since then, group theory has become a very important branch of mathematics, and provides a bridge between algebraic methods and geometric visualisations. In particular, crystal patterns in the plane and in space were studied by A. Bravais and E. Fedorov in the nineteenth century, who identified the 17 *wallpaper groups* and the 230 *space groups* [4]. Crystal patterns, or, in more mathematical terms, *lattices*, consist of regular arrangements in two or three dimensions that are periodic, i.e. they are invariant under translations. The crystallographic restriction dictates that the symmetry groups of lattices in the plane

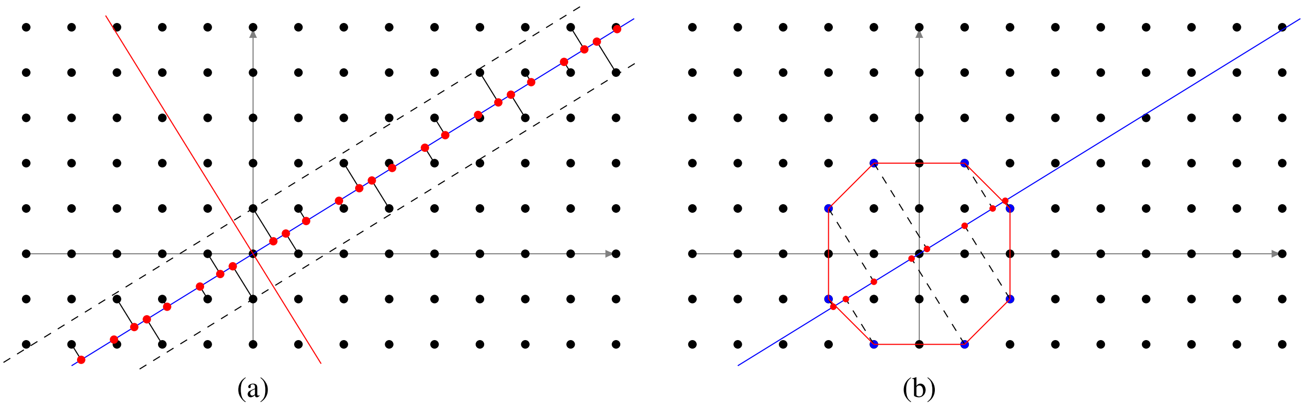


Figure 1 : *(a) Illustration of the cut-and-project method for a one-dimensional quasicrystal (Fibonacci lattice): lattice points lying within the stripe defined by the dashed lines are projected orthogonally onto the blue line (the "physical space"). The result is an infinite point set which is quasiperiodic, i.e. with long-range order but no translational periodicity, that does not fill the line densely. (b) Illustration of our method to construct nested point sets, showing the connection with the cut-and-project method. Lattice points forming the vertices of a polygon (or in group theoretical terms, belonging to the orbit of the symmetry group of the lattice) are projected into the physical space, resulting in a finite nested point set, in this case one-dimensional.*

or in 3D space can only have two-, three-, four- or six-fold rotational symmetry. As a consequence, five- and n-fold symmetries, with n greater than six, are called *non-crystallographic*. These include the symmetry of viruses, the geodesic dome and fullerenes.

In 1984, Shechtman announced the discovery of *quasicrystals*, solids with long-range order that exhibit non-crystallographic symmetry in their atomic organisation [5]. Since then, the theory of quasicrystals has become an active field of research among physicists and mathematicians, who have developed a method to study the properties of quasicrystals based on higher dimensional geometry [6, 7]. The main idea is to select points from a "generalised" lattice in a suitable higher dimension, and then "project them down" into the plane or 3D space. This is the so-called *cut-and-project* method [8]. In Figure 1 (a) we provide a visual example of this method in the case of a one-dimensional quasicrystal.

The idea of geometry in higher dimensions dates back to the second half of the nineteenth century. In 1884, E.A. Abbott explores the concepts of multi-dimensionality in his novella *Flatland*; in particular, he describes a two-dimensional world populated by polygons, in which one day a Sphere from space arrives, showing the three-dimensional world to a Square. The Sphere explains the concept of "solids" to the Square using analogies: a cube in space is the analogue of the square in the plane, and consists of 6 faces and 8 vertices; thus, a four-dimensional hypercube (also called *tesseract*) will be made up of 8 "3D faces" (called *cells*) and 16 vertices. In other words, it is possible to generalise the concept of polyhedron to any dimension: specifically, a generalised polyhedron (or *polytope*) in dimension k is the convex hull of a finite set of points in the k-dimensional space. H.S.M. Coxeter [9] gave a systematic study of regular polytopes, and introduced the concept of *reflection groups*, i.e. groups generated by reflections through hyperplanes, to study their symmetry properties.

In our recent paper [10], we proposed a method to construct *nested* polytopes with non-crystallographic symmetry. In particular, these are obtained from the projection of lattice points in a higher dimensional space forming the vertices of a single polytope. The connection with the cut-and-project method is explained in Figure 1 (b). The idea was motivated by the fact that a significant number of viruses and fullerenes display nested shell arrangements of material and atoms with icosahedral symmetry. This is evident, for example, in the structure of Pariacoto virus (PaV) [11], and in the atomic organisation of carbon onions [12].

In this paper we review the method we developed from a geometrical point of view. The mathematics is explained through visual examples, and so are the applications in the natural sciences. This approach has led to a close collaboration between mathematicians, biologists and designers, and opens up new opportunities for dialogue between science and art.

Nested polytopes induced by projection

When the Sphere in *Flatland* presents itself to the Square, the latter sees a circle, a two-dimensional object. In fact, from a geometrical point of view, when we cut a sphere with a plane we obtain circles of various sizes, the limit points being the poles. The circles thus constructed are *sections* of the sphere. If a source of light is placed behind the sphere, we can visualise its shadows on the plane while the position of the sphere varies. These are *projections* of the sphere into the plane. These methods, by the principle of analogy, can be generalised to any dimension; Coxeter gave a detailed explanation of this in his study of regular polytopes [9]. This is the way in which we, as three-dimensional beings, can "grasp" ideas of higher dimensional geometry.

The idea of nesting arrangements originates from this easy example. In particular, Figure 2 shows the projection of the twelve vertices of an icosahedron onto a plane perpendicular to a three-fold axis. The result is a compound of two nested hexagons, i.e. two hexagons situated at different radial levels. Let us then consider this simple process "backwards"; we start from the inner hexagon and then "lift" its vertices in space, by putting them in correspondence to six vertices of the icosahedron. At this point we *extend* the symmetry of the hexagon into 3D by considering the icosahedron as a whole, i.e. by adding the remaining six vertices to the "lifted" ones. The projection of these 12 vertices will then consist of the hexagon we started with *plus* the outer one. From a group theoretical point of view, the symmetry of the hexagon (in the plane) is *extended* into space via the icosahedron, whose symmetry group contains the symmetry of the hexagon as a subgroup.

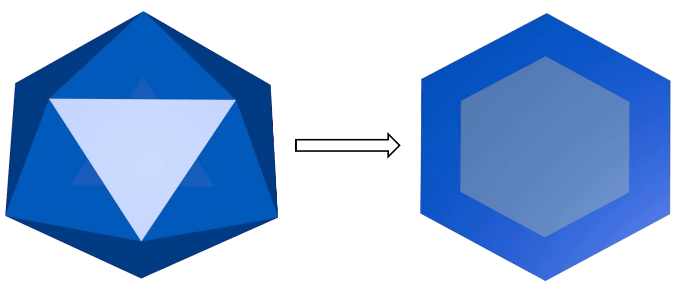


Figure 2: *An example of the construction method in 3D: projection of an icosahedron onto a plane perpendicular to a three-fold axis, resulting in two nested hexagons.*

By analogy, we can generalise this simple example to any number of dimensions in a purely mathematical way. Let us consider a polytope $\mathcal{P}$ in dimension k with non-crystallographic symmetry which is *isogonal* or *vertex-transitive* [13], i.e. every vertex can be carried to any other by a symmetry operation. The symmetry group of $\mathcal{P}$, which we denote by G, does not leave any (generalised) k-dimensional pattern invariant. From an abstact point of view, it is possible to find a pattern in a higher dimension d that is left invariant by G [8]. More precisely, the vertices of $\mathcal{P}$ can be "lifted" to some points that are part of a d-dimensional lattice. The number d is called the (minimal) *crystallographic dimension* of G. The convex hull of these points forms a d-dimensional polytope with symmetry G; however, just as the six vertices of the hexagon are lifted to the icosahedral vertices, it is possible to "extend" the symmetry described by G by considering more

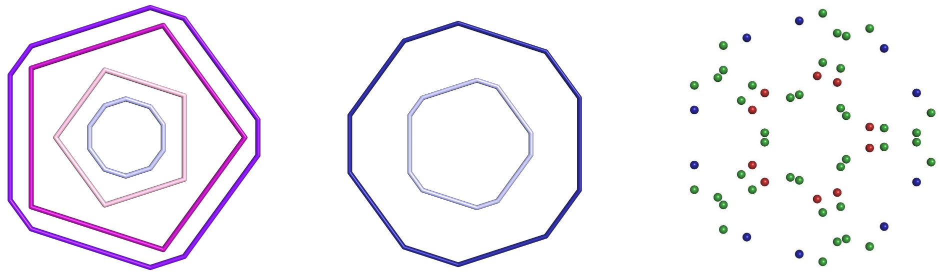


Figure 3 : *Planar nested structures with five-fold symmetry, induced by projection of points of the four-dimensional honeycomb lattice. The polygons are obtained by computing the convex hull of the points situated at each radial level.*

points of the lattice. Here group theory plays a crucial role: the points added are such that the symmetry group of the resulting polytope contains G as a subgroup. The projection of the vertices thus obtained in dimension k consists of polytopes with symmetry G situated at different radial levels.

In Figure 3 we show examples of planar nested structures with five-fold symmetry thus obtained. These are projections of vertices of four-dimensional polytopes (usually called *polychora*), whose vertices are points of the four-dimensional A_4 lattice, also called *honeycomb* lattice.

Icosahedral symmetry and applications to virus architecture

Icosahedral symmetry plays a fundamental role in virology. Since the theory of Caspar and Klug in 1962, scientists have realised the importance of geometry as a predictive tool for virus architecture. In their seminal paper [14], they describe the construction of a family of polyhedra with icosahedral symmetry, called *icosideltahedra*, that predict the position and relative orientation of the capsid proteins, inspired by the work on the geodesic dome by Buckminster Fuller. More recently, Twarock [2] proposed a generalisation of Caspar-Klug theory, called *Viral Tiling theory*, where, inspired by quasicrystals, the surface of a capsid is tesselated using tiles similar to the ones used in the Penrose tiling.

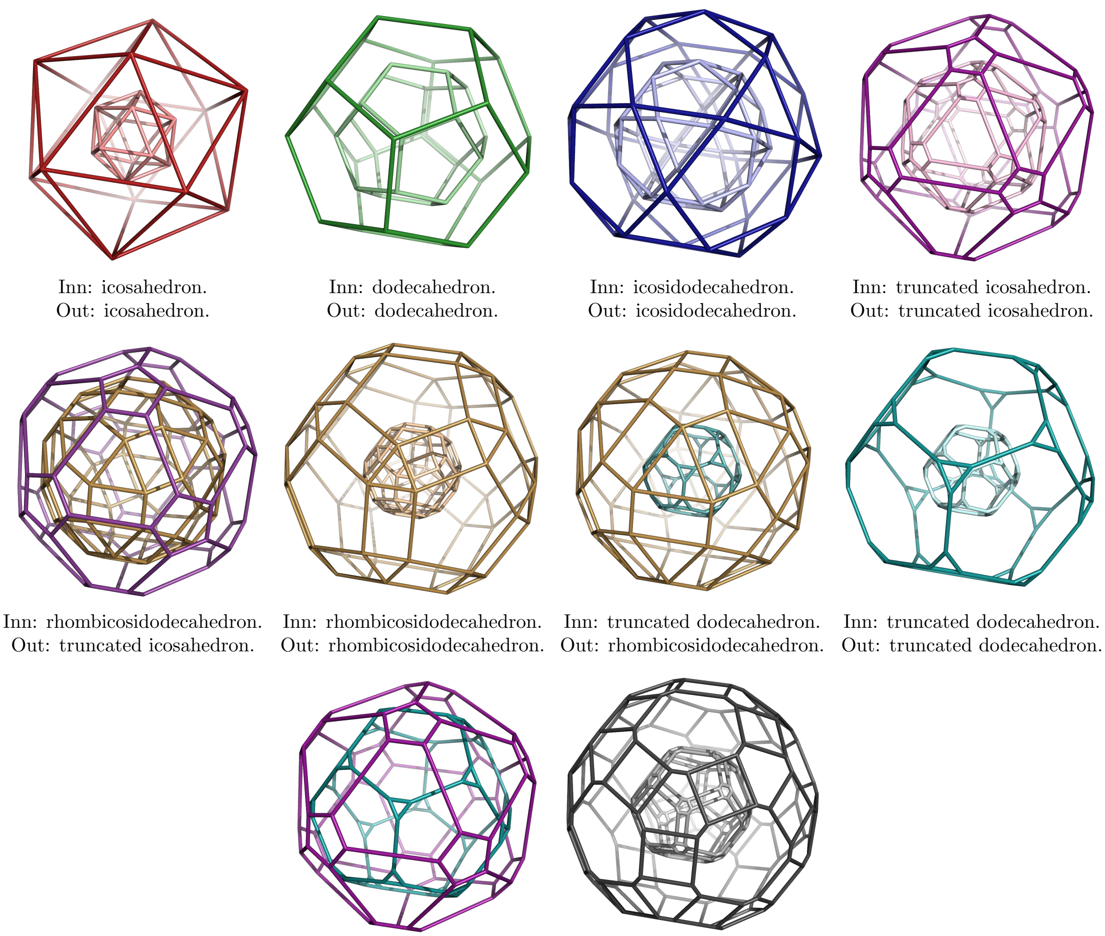
These methods describe the capsid as a two-dimensional object rather than a three-dimensional one. The construction of nested polytopes that we developed originates in the idea to extend Caspar-Klug theory and study in more depth the capsid architecture, in particular obtaining information about its thickness and radial distribution of material to formulate simultaneous constraints on capsid geometry and genome organisation.

From a group theoretical point of view, icosahedral symmetry (including reflections) is described by the Coxeter group H_3. Since this group contains five-fold symmetry, it is non-crystallographic in the 3D space; the minimal crystallographic dimension, where the symmetry-retaining projection is possible, is six. In fact, let $\tau := \frac{1}{2}\left(1+\sqrt{5}\right)$ denote the golden ratio. The points $(\pm\tau, \pm 1, 0)$ and all the cyclic permutations of their coordinates form the 12 vertices of an icosahedron centered at the origin. On an abstract level, these points can be “lifted” in the six-dimensional space to form a basis of the simple cubic lattice in six dimensions [8].

At first, we concentrated on double shell structures, and studied in detail pairings of nested polyhedra with icosahedral symmetry, which are induced by projection from points of the hypercubic lattices in six dimensions that are related by one of its symmetries. Again, group theory plays an important part in this task. In particular, we extended the symmetry in the six-dimensional space so that the symmetry group of the resulting polytope contains the group H_3 as a *normal* subgroup [4]. The assumption of normality allows further characterisation of the geometrical properties of the projected structures. In particular, the polyhedra constituting the layers in the resulting compound must each have the same number of vertices (for a rigorous mathematical proof of this, see [10]). In this case there are (at most) two nested polyhedra in projection, since the order (i.e. "size") of the extension is twice the order of H_3. These properties are used to classify the possible pairings thus constructed. Specifically, in Table 1 we list all the isogonal polyhedra with full icosahedral symmetry [13]. Since each polyhedron in the resulting compound must have the same number of vertices, there are in total 10 possible configurations (up to reordering), which we present in Figure 4.

Polyhedron	Number of vertices
Icosahedron	12
Dodecahedron	20
Icosidodecahedron	30
Truncated icosahedron	60
Truncated dodecahedron	60
Rhombicosidodecahedron	60
Truncated icosidodecahedron	120

Table 1 : *Isogonal polyhedra with icosahedral symmetry.*



Inn: icosahedron. Out: icosahedron.
Inn: dodecahedron. Out: dodecahedron.
Inn: icosidodecahedron. Out: icosidodecahedron.
Inn: truncated icosahedron. Out: truncated icosahedron.
Inn: rhombicosidodecahedron. Out: truncated icosahedron.
Inn: rhombicosidodecahedron. Out: rhombicosidodecahedron.
Inn: truncated dodecahedron. Out: rhombicosidodecahedron.
Inn: truncated dodecahedron. Out: truncated dodecahedron.
Inn: truncated dodecahedron. Out: truncated icosahedron.
Inn: trunc. icosidodecahedron. Out: trunc. icosidodecahedron.

Figure 4 : *Classification of all possible pairings of nested polyhedra with icosahedral symmetry as projection of vertices of polytopes in 6D, whose symmetry group contains H_3 as a normal subgroup. "Inn" and "Out" stand for inner and outer shell, respectively.*

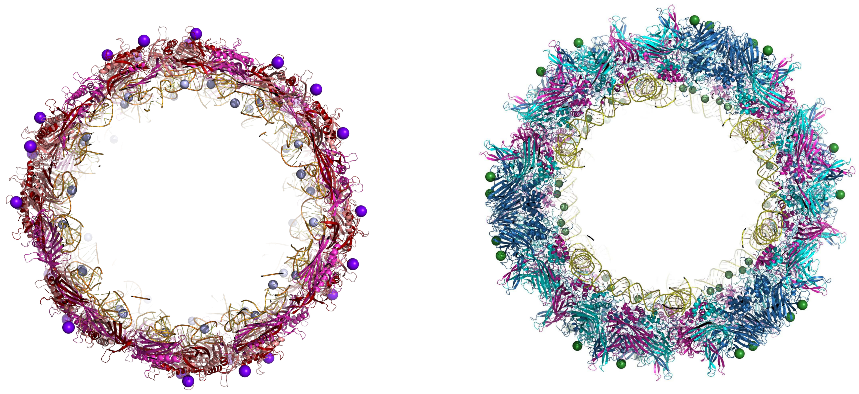


Figure 5: *Section of two viral capsids with icosahedral symmetry: Bacteriophage MS2 (left) and Pariacoto Virus (right). The points in purple (left) and green (right) are obtained with the projection method, and they encode constraints on the structures and positions of the inner and outer surfaces of the capsid.*

These structures provide blueprints for simple viral capsids, specifically for those with a low T-number in the Caspar-Klug classification. In particular, we used the vertices of two nested rhombicosidodecahedra and the compound of a rhombicosidodecahedron and a truncated icosahedron to model the architecture of the capsids of Bacteriophage MS2 and Pariacoto Virus, respectively (see Figure 5). The vertices of the outer shell describe the location of the capsid proteins, whereas the inner shell gives information on the genomic material (RNA) inside the capsid.

Inspired by this, we designed a 3D model based on the structure of the Pariacoto virus capsid (see Figure 6). This artwork opens up new possibilities of collaboration between mathematicians, biologists and designers with potential in public outreach. In fact, the model can be used as a visual aid to explaining the structure of a virus, and how mathematics plays a fundamental role in understanding its architecture in depth.

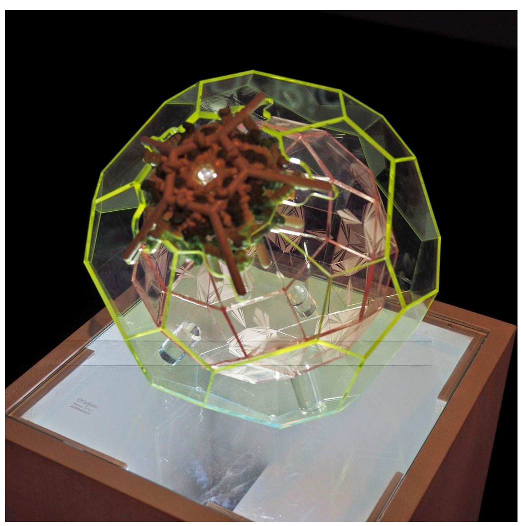


Figure 6: *Pariacoto structure* $\#1$*; mixed media, 2014. The model represents the structure of the capsid of Pariacoto Virus: the outer shell recreates the location of capsid proteins, with a close-up view on a cluster of proteins modeled via 3D printing, based on PDB-id 1f8v. The inner shell represents the architecture of the RNA cage inside the capsid.*

Four-dimensional icosahedral polytopes

Four-dimensional polytopes (polychora) were first analysed by A. Boole Stott and H.S.M. Coxeter in the first half of the twentieth century [9, 15]. By analogy to the two- and three-dimensional case, polychora are bounded by 3D "faces", called cells, which are themselves polyhedra. Generalised icosahedral symmetry in four-dimensional space is described by the Coxeter group H_4. In particular, the 4D analogues of the icosahedron and the dodecahedron are the so-called *600-cell* and *120-cell*, respectively. The four dimensional isogonal polytopes with symmetry group H_4 have been classified in [16].

In complete analogy with icosahedral symmetry in 3D space, the group H_4 is non-crystallographic in four dimensions. Its minimal crystallographic dimension is eight [8]. With the same techniques as in the 3D case, it is possible to construct nested polychora with H_4 symmetry via projection from the eight-dimensional E_8 lattice. However, in order to "visualise" these objects it is necessary to draw three-dimensional sections and/or projections of them. Although it is *a priori* possible to take sections in any direction, it is convenient to "cut" the polychora perpendicularly to a symmetry axis, as in this case the resulting polyhedron retains symmetrical properties. In Figure 7 we provide a 3D example of this for the case of an icosahedron. In Figure 8 we present two examples of sections of nested polychora, taken through "3D solids" (or in more mathematical terms, *hyperplanes*) perpendicular to some symmetry axis of the polychora.

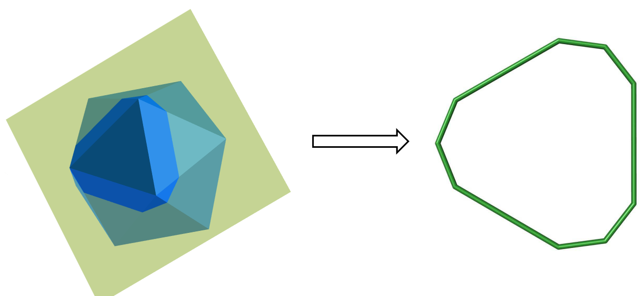


Figure 7 : *Section of an icosahedron, taken perpendicular to a three-fold axis: the result is a polygon with three-fold symmetry.*

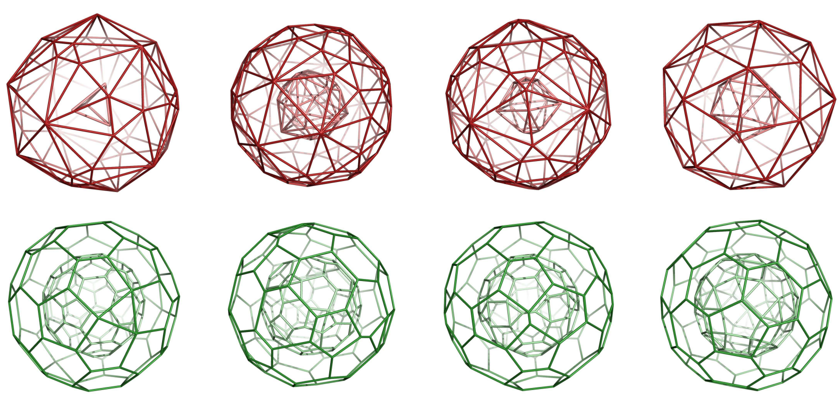


Figure 8 : *Section of nested polychora with H_4 symmetry: two nested 600-cells (top row) and two nested 120-cells (bottom row). The sections taken possess, from left to right: tetrahedral symmetry, symmetry of a triangular prism, symmetry of a pentagonal prism and icosahedral symmetry.*

These results show the possibility of using multi-dimensional geometry to visualise and design complex structures with high symmetry. These are examples of "computational art": scientific computing meets design to create shapes with prescribed features, which are characterised mathematically. In particular, the nested polyhedra and the sections of polychora displayed in this paper were computed numerically and visualised with the aid of Python programming language and the software PyMol. We think that this work could inspire new collaborations between geometers and designers, and emphasise the role of group theory in contexts outside the mathematical framework.

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