Polyhedral Knots and Links

Slavik Jablan, Ljiljana Radović, and Radmila Sazdanović
The Mathematical Institute
Knez Mihailova 37
P.O.Box 367
11001 Belgrade
Serbia
E-mail: sjablan@gmail.com
E-mail: ljradovic@gmail.com
E-mail: radmilas@gmail.com

Abstract

This paper contains a survey of different methods for generating knots and links based on geometric polyhedra, suitable for applications in chemistry, biology, architecture, sculpture (or jewelry). We describe several ways of obtaining 4-valent polyhedral graphs and their corresponding knots and links from geometrical polyhedra: mid-edge construction, cross-curve and double-line covering, and edge doubling constructions. These methods are implemented in *LinKnot* and can be applied to the data bases of polyhedra. In a similar way, an edge doubling construction transforms fullerene graphs into alternating knot and link diagrams.

Introduction

The initial interest in knot theory was motivated by Kelvin's theory of atomic structure (1867). By the turn of the century, scientific confirmation of Mendeleev's periodic table showed that Kelvin's theory was incorrect, so chemists were no longer interested in classifying knots, but mathematicians, in particular topologists, continued to study them.

However, around 1960 the focus of chemists turned towards attempts to synthesize molecular knots and links. The first pair of linked rings in a form of the Hopf link, a *catenane*, was synthesized by H.Frisch and E.Wasserman in 1961. In 1989 C.Dietrich-Bushecker and J.-P.Sauvage produced the first molecular knot, a trefoil made out of 124 atoms. They introduced *stereochemical topology*: synthesis, characterization, and analysis of topologically interesting molecular structures [1,2].

Synthesis of the first molecular Moebius ladder with three rungs by D.Walba, R.Richards and R.C.Haltiwanger in 1982, and the addition of twists to it managed by Q.Y.Zheng in 1990, enabled the generation of numerous knots and links. In fact, breaking rungs in the Moebius multi-strand twisted ladders turns it into a molecular closed braid representation of a knot or link.

Indonesian weaving and Tamari balls inspired the original tensegrity researchers, B.Fuller and K. Snelson to use knots and links in architecture. Their approach became more popular during the last decades, with the use of light-weight materials, tensegrity and computer design tools (CAD/CAM).

From the point of view of organic chemistry, molecular biology, or architecture the most interesting cases are complex knotted and linked structures with a high degree of symmetry. However, tabulation of knots and links, as well as computing of knot invariants is restricted to knots and links with relatively small number of crossings.

In some sources the end of the 19th century is called the "dark age of the knot theory", because the only ways to distinguish knots was by a few "non-exact methods". However, the first knot tables were created during that period by P.G.Tait, T.P. Kirkman and C.N.Little. The next big step in knot tabulation happened almost a century later, when M.Thistlethwaite and his collaborators compiled new knot and link tables using computers. At the moment, even supercomputer cannot improve on these computations. The existing knot tables contain alternating knots up to 24 crossings, and non-alternating knots up to 16 crossings. Very recently, M.Thistlethwaite tabulated non-alternating knots up to 19 crossings, alternating links up to 18 crossings, and non-alternating up to 12 crossings [3]. These tables are insufficient for

applications because knots and links relevant to biology, chemistry or architecture have a higher number of crossings. Moreover, most tabulated knots and links have a low degree of symmetry, unlike the knotted natural structures, because nature, art, and architecture prefer symmetry and complexity. Hence, many chemists have tried to determine whether knots and links are new forms of molecular structures [4-6]. Geometrical characteristics and the polyhedral shapes of biological molecules have attracted much attention, and remarkable discoveries were made in the control and syntheses of polyhedral links or catenanes, such as the DNA tetrahedron, DNA cube, DNA truncated octahedron [4], DNA octahedron, and more recently DNA bipyramids and DNA prisms. Topologically linked protein catenane − a 72-hedral link discovered in the context of virology, has been found in the mature empty capsid of a double-stranded DNA bacteriophage. This and similar discoveries extended the domain of forms that are possible in the biochemical world. Many questions about newly discovered structures can be formulated in the language of knot theory and answered by using mathematical-topological and geometrical methods. The concept of "polyhedral links" is a novel mathematical model, proposed by Qiu's group for the first time in 2005 and later leading to a series of papers in this field [5-6].

We propose using some well-known construction methods in knot theory, such as the mid-edge construction, for modeling knots and links that arise in chemistry and biology. For example, the mid-edge construction consists of replacing mid-edge points of a graph by 4-valent vertices and joining the adjacent loose ends. Furthemore, we can transform graphs into alternating knot and link diagrams by introducing over-crossings and under-crossings, i.e., specifying the top and bottom strand in each vertex.

All considerations in this paper are restricted to alternating knots and links. A detailed description of the Conway notation for knots and links, as well as the background material can be found [7-9]. S*ource link* is link corresponding to a Conway symbol containing only tangles ±1 and ±2, and a link given by a Conway symbol containing only tangles ±1, ±2 and ±3 is called a *generating link*. Informally, a family of knots (or links) is obtained by adding twists to chains of digons in source or generating links. Note that adding an even number of twists preserves the number of components [9-11].

Additional material, including easy to use interactive *webMathematica* functions for experimenting and creating knots and links using all constructions described in this paper, can be found online at http://math.ict.edu.rs:8080/ webMathematica/poly/cont.htm .

Polyhedral Knots and Links and their Construction

The first class of graphs we consider is the 4-valent basic polyhedra corresponding to alternating polyhedral knots and links. *Basic polyhedron* is a 4-regular, 4-edge-connected, at least 2-vertex connected plane graph without digons. The derivation of basic polyhedra was completed up to 12 crossings by T.P.Kirkman, with one omission: the basic polyhedron 12E. Kirkman derived basic polyhedra by eliminating digons in knot and link diagrams, using only diagrams which satisfy the following necessary condition: each contains at most three digons belonging to the same face. Eliminating digons is achieved by inscribing triangles into faces, with the vertices belonging to the face edges (e.g., coinciding with their midpoints). The complete list of the basic polyhedra with n=12 crossings was obtained by A.Caudron in 1982 by composing hyperbolic tangles. The program *LinKnot* contains the data base of basic polyhedra up to 20 crossings. The database of basic polyhedra is produced from the list of simple 4-regular 4-edge-connected, but not 3-connected plane graphs generated by Brendan McKay using the program "plantri" written by Gunnar Brinkmann and Brendan McKay (http://cs.anu.edu.au/~bdm/plantri/). This data base contains in total 83 177 basic polyhedra up to 20 crossings. The list of basic polyhedra includes 2-vertex connected basic polyhedra which are not actual geometrical polyhedra. The first example of that kind is the basic polyhedron 12E. The term "*polyhedral links*" stands for knots and links derived from different geometric polyhedra by mid-edge construction (Fig. 1a) or cross-curve and double-line covering (Fig. 1b), as well as the alternating source links derived from 3-valent geometrical polyhedra by edge doubling (Fig. 1c).
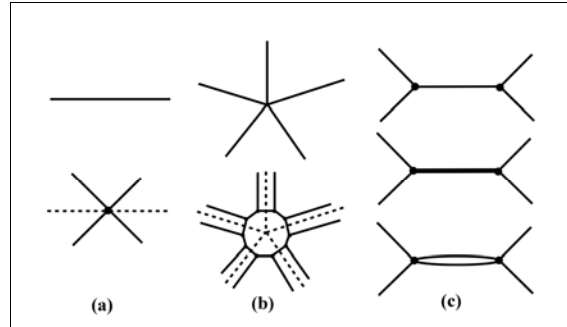
Figure 1: (a) Mid-edge construction; (b) cross-curve and double-line covering construction; (c) edge doubling construction. Broken lines denote edges of the original graph deleted during the construction.

Mid-edge Construction

The middle graph $M(G)$ of a polyhedral graph G, is obtained by connecting the mid-edge points of G (Fig. 1a) belonging to the adjacent edges of G. Clearly, the resulting $M(G)$ is always a 4-valent graph, i.e., a basic polyhedron. Every at least 3-vertex connected basic polyhedron is the middle graph of some geometrical polyhedron. After turning $M(G)$ into an alternating link diagram D_L, by introducing over-crossings and under-crossings in an alternating manner, the graph G is the graph of the link diagram D_L, i.e., $G(D_L)=G$, so the constructions of a graph of a link diagram $G=G(D_L)$ and a middle graph $D_L=M(G)$ are mutually dual. If the original graph G does not contain digons, the same holds for its middle graph.
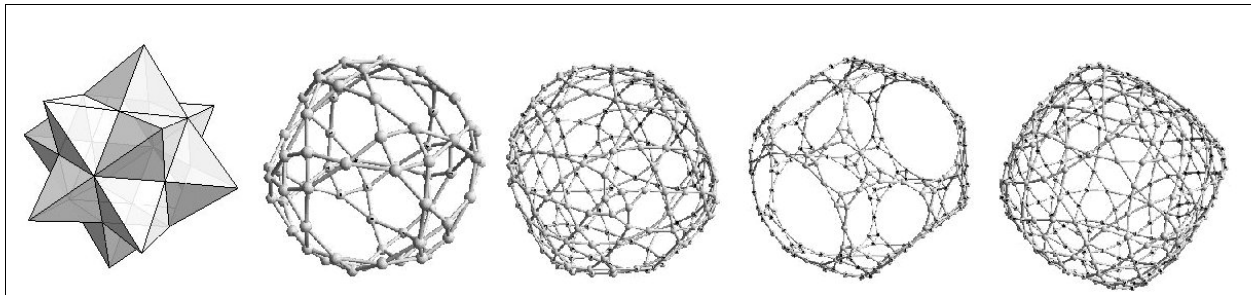

Figure 2: Escher's solid from the *Mathematica* data base of polyhedra [12] and basic polyhedra obtained from it and its transforms (truncated, stelated and geodesated Escher solid) by mid-edge construction.

Cross curve and Double-line Covering

In the paper [6] a new methodology for understanding the construction of polyhedral links has been developed based on the Platonic and Archimedean solids by using the method of the "cross-curve and double-line covering" introduced by the authors (Fig. 1b). In order to obtain 4-valent graphs they introduce the cross-curve and edge doubling construction: first replace *n*-valent vertices of a polyhedral graph by *n*-cross-curves, and then join the adjacent loose ends to obtain a double-line covering.

Edge Doubling

The next construction, called *edge doubling* (Fig. 1c), can be used for obtaining 4-regular graphs from 3-regular graphs: in every vertex of a 3-regular graph one edge is replaced by a double edge (digon) [8-11]. In particular, the edge doubling construction can be applied to graphs of truncated polyhedra, which are always 3-valent, yielding various polyhedral source links.
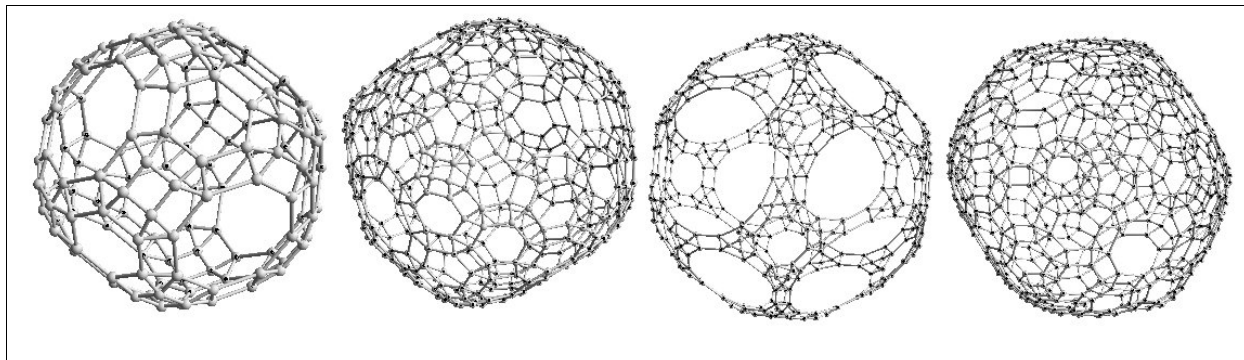
Figure 3: Basic polyhedra obtained from Escher's solid and its transforms by cross-curve and double-line covering.

Mathematica **Data Base of Polyhedra and Transformed Polyhedra**

The database of polyhedra in *Wolfram Mathematica* contains more than 100 interesting polyhedra, that can be used as an input for the construction methods described in this paper (Figs. 2-3). Moreover, by choosing between four different options: 0 for original input polyhedron, 1 for truncated, 2 for stellated, and 3 for geodesated, you can work with various transforms of the original polyhedra. Using as an input any of the mentioned families of polyhedra, polyhedra from the *Mathematica* database, their transforms, or basic polyhedra from the *LinKnot* database, you can obtain mid-edge graphs after *s* iterations.

Knots and Links and Fullerenes

Among the chemical elements, carbon, C, is the basis of all life. A whole branch of chemistry, organic chemistry, is devoted to the study of C-C bonds and different molecules originating from them. So far, carbon is the only known 4-valent element able to form long homoatomic stable chains or different 4-valent nets. Another candidate is silicon, whose homoatomic chemistry is rapidly developing.
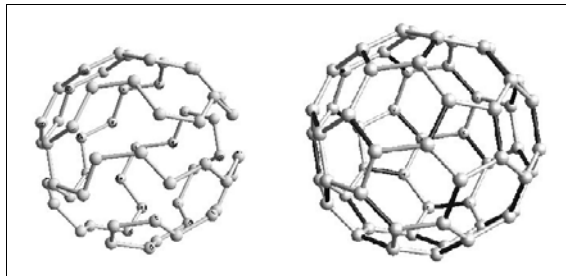

Figure 4: Hamiltonian cycle on fullerene C_{60} and edge doubling applied to C_{60}.

Fullerene is a 3-planar graph with pentagonal and hexagonal faces. In addition to the well-known diamond and graphite, a new form of carbon, the fullerene C_{60}, was first synthesized by H.W.Kroto, R.F.Curl and R.E.Smalley in 1985. Along with its remarkable 3-dimensional structure, a spherical closed pentagonal/hexagonal homoatomic shell, it contains exceptionally rare rotational symmetry of order 5 (which according to Barlow's *crystallographic restriction theorem* is forbidden in crystallographic space or plane symmetry groups) and the highest possible, icosahedral, point-group symmetry. Since the discovery of C_{60}, different fullerenes (e.g., C_{70}, C_{76}, C_{78}, C_{82}, C_{84}, *etc*.) have been synthesized, opening a new field for research of potentially different possible fullerene structures from the point of view of geometry, graph theory, or topology. The most complete discussion of fullerenes is given by P.D.Fowler and D.E.Manolopoulos [13].

Every fullerene has exactly 12 pentagonal faces. For every even $n>23$ there exists at least one fullerene C_n. Chemical fullerenes are obtained from fullerene graphs by substituting vertices with carbon atoms.

In the paper "Geometry of Fullerenes", republished in [9] the first author proposed considering fullerenes as alternating knots and links. First, we can consider all 4-valent graphs on a sphere. In chemistry, vertices of type 1111 (×) are only theoretically acceptable. In knot theory, 4-valent graphs on a sphere with all vertices of the type 1111 are exactly the basic polyhedra. A *general fullerene* is a graph whose vertices are of the type 211 (=<). Every general fullerene can be derived from a 3-valent graph by edge doubling (Fig. 4b). In knot theory, general fullerenes are source links derived from basic polyhedra by vertex tangle substitutions. In this paper we derive general fullerenes by edge doubling applied to 3-valent polytope graphs derived by the program *plantri* written by Brendan McKay. Different link diagrams can be obtained from the same general fullerene graph by edge doubling.

A special class of fullerenes consists of 5/6 fullerenes: those which have only pentagonal and hexagonal faces. If n_5 denotes the number of pentagons, and n_6 the number of hexagons, n_5 must be 12 by the Euler theorem, and the relation $3v=2e$. Hence, C_{20}, the regular dodecahedron {5,3}, is the first 5/6 fullerene with $n_6=0$. It has two non-isomorphic edge-colorings, resulting in two chemically different isomers of the same geometric dodecahedral form.

By using the program *fullgen* written by Gunnar Brinkmann, 5/6 fullerenes can be derived. The first fullerene satisfying Isolated Pentagon Rule (IPR) is C_{60}. A complete list of fullerenes is computed for $19<n<121$ vertices, where for $n>59$ only fullerenes satisfying IPR are computed. For every fullerene from this list it is possible to obtain a graph obtained by edge doubling.

Applications in Art and Architecture

In the history of art and architecture knots and links, in particular basic polyhedra, played an important role. Typical examples are the plan of Michelangelo's plaza based on the shadow of a torus knot (13,5) or Celtic "basic polyhedron" shown in Fig. 5. In contemporary architecture, even some very simple knots such as trefoil served as the basis for the construction of buildings, e.g., Mercedes-Benz Museum in Stuttgart [14]. With the advance of digital techniques and availability of ultra-light materials ground plans representing shadows of knots and links now become 3D structures made from flexible elastic rods. Instead of rigid bodies, the buildings of the future can be transformable entities erasing from flat 4-valent nets to their 3D embeddings, similar to NODUS-structures proposed by D. Kozlov [15]. Usual geodesic domes based mostly on rigid 3-valent graphs can be replaced by 4-valent flexible geodesic domes.
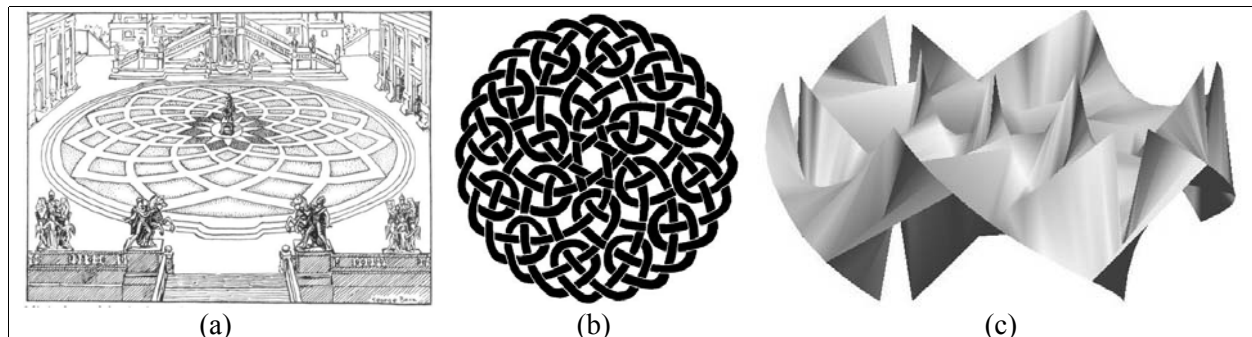

(a)   (b)   (c)

Figure 5: (a) Michelangelo's plaza; (b) Celtic "basic polyhedron"; (c) Seifert surface created in *LinKnot*.

For every knot or link we obtain the corresponding Seifert surface: a surface whose boundary is a given knot or link. Seifert surfaces are very succesfully used in sculpture beginning from 1930-ties, e.g., in the works by Naum Gabo. In the contemporary art typical examples are sculptures by Bathsheba Grossman [16] created by the program *Seifert View* by J.J. van Wijk [17], or sculptures by A. Bulatov (http://bulatov.org/). In the program *LinKnot* we are able to create Seifert surfaces based on polyhedral

knots and links (Fig. 5c), preserving the symmetry and beauty of polyhedra, but having the additional flexibility and variability.

Conclusion

Because of their regularity and symmetry, polyhedra occupied the attention of mathematicians, natural scientists, and architects for centuries. In this paper we proposed several constructions of knots and links originating from regular, uniform (Archimedean), and other polyhedra. Knots and links obtained in this way preserve important symmetry properties of the original polyhedra and represent the basis for the construction of polyhedral knotted structures from the nano to the macro level. For a long time chemists strove to synthesize polyhedral molecules. Despite the recent achievements, there is still a gap between the great variety of polyhedral shapes observed in nature (such as viral protein capsids) and the relatively limited molecular polyhedra constructed by small organic molecules. Recently, DNA was shown to be an excellent material for polyhedral knotted constructions, such as the DNA tetrahedron, cube, octahedron, dodecahedron, icosahedron, *etc*. We hope that this paper offers some theoretical background for development of general construction methods for polyhedral knots and links in stereochemical topology or architecture.

References

[1]   J.P. Sauvage and C. Dietrich-Buckecker, *Molecular Catenanes, Rotaxanes and Knots*, New York: Wiley, 1999.

[2] E. Flapan, *When Topology Meets Chemistry: A Look at Molecular Chemistry*, Cambridge University Press, Cambridge, 2000.

[3]   J.Hoste and M.Thistlethwaite, Knotscape, http://www.math.utk.edu/~morwen/knotscape.html (M.Thistlethwaite, Private communication, 10. Feb. 2010).

[4] Y. Zhang, N.C. Seeman, Construction of a DNA-truncated octahedron, J. Am. Chem. Soc. (1994), **116**, 1661-1669.

[5] W.-Y. Qiu and X.-D. Zhai, Molecular design of Goldberg polyhedral links, J. Mol. Struc. (Theochem) (2005) **756**, 163-166.

[6] W.-Y. Qiu, X.-D. Zhai and Y.-Y. Qiu, Architecture of Platonic and Archimedean polyhedral links, Science in China, Ser. B: Chemistry **51**, 1 (2008) 13-18.

[7] J. Conway, An enumeration of knots and links and some of their related properties, in *Computational Problems in Abstract Algebra*, ed. J. Leech, Proc. Conf. Oxford 1967, (Pergamon Press, New York, 1970), pp. 329-358.

[8] A. Caudron, *Classification des noeuds et des enlancements*, Public. Math. d'Orsay 82. Univ. Paris Sud, Dept. Math., Orsay, 1982.

[9] S.V. Jablan and R. Sazdanović, *LinKnot − Knot Theory by Computer*, World Scientific, New Jersey, London, Singapore, 2007; http://math.ict.edu.rs/, http://www.mi.sanu.ac.rs/vismath/linknot/index.html

[10] S. Jablan, Lj. Radović, R. Sazdanović, Pyramidal Knots and Links and their Invariants, MATCH Commun. Math. Comput. Chem., **65**, 3 (2011) 541-580.

[11] S. Jablan, Lj. Radović, R. Sazdanović, Knots and Links Derived from Prismatic Graphs, MATCH Commun. Math. Comput. Chem., (to appear).

[12] *Mathematica* Polyhedron Data, http://reference.wolfram.com/mathematica/ref/PolyhedronData.html

[13] P.D. Fowler, D.E. Manolopoulos, *An Atlas of Fullerenes*, Oxford University Press, Oxford, 1995.

[14] T. Vallisser, Other geometries in architecture: bubbles, knots and minimal surfaces, http://www.google.com/#q=knots,+architecture&hl=en&biw=1440&bih=713&prmd=ivns&ei=tf23TeP_M432sgaY5qTrAw&start=10&sa=N&bav=on.2,or.r_gc.r_pw.&fp=69c80c2345c6abc6

[15] D. Kozlov, N. Raasn, Topological method of construction of point surfaces as physical models, http://www.marhi.ru/AMIT/2008/spec08/papers/Kozlov/Kozlov02_paper_EAEA2007.pdf

[16] B. Grossman, Bathsheba Sculpture, http://www.bathsheba.com/

[17] J.J. van Wijk, Seifert View, http://www.win.tue.nl/~vanwijk/seifertview/