

Project description: Geometric combinatorial Hopf algebras and modules

1. INTRODUCTION

In 2008 several researchers made exciting advances in the application of algebra and combinatorics to particle physics. The crucial mathematical ingredients included Hopf Algebras and subalgebras, in regard to the specific physical principle of renormalization in quantum electrodynamics and chromodynamics.

Renormalization refers to the addition of counterterms to a sequence of divergent integrals for probability amplitudes in particle physics. Yielded is a calculable result which has been demonstrated to match experimental values to extremely high precision. The process of renormalization has previously appeared suspect to mathematicians, as it is often based on ill-defined path integral procedures. Hopf-algebraic techniques introduced by Connes and Kreimer in 2000 have promised to afford a deeper understanding and a firmer footing [12]. Simultaneously with Brouder and Frabetti, they found Hopf algebra structures on sets of rooted trees and on sets of Feynman diagrams [8]. The two isomorphic Hopf algebras encode renormalization by providing a formula for the counterterms via the antipode. The latter is found as a recursive sum of products whose operands are relative residues, or reconnected complements Γ/γ of diagrams Γ with loop subdiagrams γ . An example is in the second part of Figure 1. There is solid evidence now that the techniques developed in this area will also be applicable to unified field theories and even quantum gravity [30].

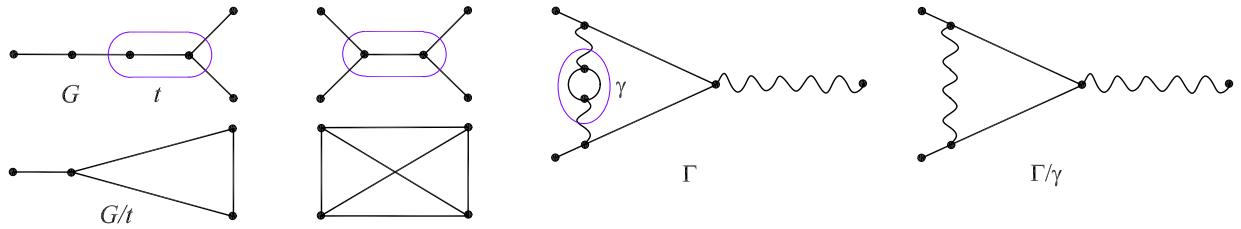


FIGURE 1. Connected subgraphs are circled, and the respective reconnected complements are shown below the graphs and to the right of the Feynman diagram. [9], [30]

One physicist currently considering the Hopf algebra approach is van Suijlekom, who this year showed how to find a Hopf subalgebra of the Feynman diagrams which corresponds to using the powerful Batalin-Vilkovisky formalism for renormalization, as opposed to the one-at-a-time consideration of Feynman graphs [47], [48]. Of the mathematicians, the work of Chapoton and Livernet stands out; their paper [10] shows that the commutative Connes-Kreimer Hopf algebra of rooted trees is in fact the incidence algebra based upon the operad of rooted trees, as defined by Schmitt in [42]. Furthermore Chapoton points out that this incidence algebra is always a surjective image of the Hopf algebra of representative functions of a certain group built directly from the operad.

It seems to be imperative that the structure of these combinatorial Hopf algebras, subalgebras, quotients and embeddings/projections be further investigated. Not only is there physical importance, but also the implication of deep mathematical ideas connecting some of the biggest growth areas in algebra today. These connections have been scrutinized in earnest throughout the last decade. In 1998 Loday and Ronco found an intriguing triangle of Hopf algebras [32]. Their newly defined Hopf algebra of planar binary trees lies between the Malvenuto-Reutenauer Hopf algebra on permutations and the Solomon descent algebra [33]. They also described a factoring of the surjection. Thanks to work of Foissy, Hivert-Novelli-Thibon, Holtkamp, Van der Laan, and Moerdijk, the Loday-Ronco Hopf algebra has been shown to be isomorphic to the non-commutative Connes-Kreimer algebra [16], [28], [29], [46], [35]. Much more of the structure is known, especially since in 2005 and 2006 Aguiar and Sottile used alternate bases for the Loday-Ronco Hopf algebra and its dual to construct explicit isomorphisms [4], [3]. Several descriptions of the big picture of combinatorial Hopf algebras

have put these structures in perspective, notably [1], and [27], and most recently the preprint of Loday and Ronco this month [31].

Along with the study of combinatorial Hopf algebras, an area of algebra currently experiencing extraordinary growth is the study of cluster algebras and their combinatorics. The connections between the two areas are extensive, as illustrated by the work of Reading on Cambrian lattices and their congruences in the last three years [39], [37]. Reading generalized the classic Tonks projection from permutations to binary trees to a family of maps defined for any oriented Coxeter diagram. (The original projection corresponds to type A_n .) The generalized lattices constituting the domain and codomain of Reading's maps correspond precisely to the generalized associahedra of Fomin and Zelevinsky, which in turn encode the structure of cluster algebra generators [11], [20]. Reading also discovered sequences of Hopf subalgebras of the permutations and binary trees based upon the fact that there is a lattice structure on both classes of objects which can be gradually collapsed by use of lattice congruences [38].

The theme of our current project is to develop a diverse new family of combinatorially defined posets united by the common characteristics of forming several of the following structures: lattices, convex polytopes, nested complexes, and bases of graded Hopf algebras or Hopf modules. The immediate aim of this research is to use the new Hopf modules and Hopf subalgebras, and the new projections and commuting diagrams relating those structures, to shed fresh light on well-known objects such as the Loday-Ronco algebra, the descent algebra, the permutation algebras, Reading's Cambrian lattices and related algebras, and the Connes-Kreimer algebra. An overarching goal is the unification via common generalization of existing approaches. For instance, a problem posed by Zelevinsky is to find a common generalization of his and Fomin's generalized associahedra and Postnikov's generalized permutohedra [49], [36]. The former specialize to the usual associahedron and cyclohedron via Dynkin diagrams, where the latter specialize to those same polytopes via Devadoss's *graph-associahedra* on the path and cycle graphs. Both areas are based upon certain fundamental concepts, such as nested sets of elements, and pairwise compatibility of those sets.

Carr and Devadoss first developed the theory of graph-associahedra in 2006 in order to generalize the role played by the associahedron and cyclohedron in tiling compactification spaces [9]. These polytopes have faces corresponding to *graph tubings*, which are sets of connected subgraphs each pair of which are either nested or not adjacent (their union is not connected.) Our first order of business will be to take a factorization of the Tonks projection through the graph-associahedra, as illustrated in Figure 2, and use it to define algebra and coalgebra structures on the graph tubings. In close concert with this effort we will also develop module and comodule structures based upon the graph multiplihedra, utilizing a parallel factorization of the projection from permutohedron to multiplihedron found by Saneblidze and Umble.

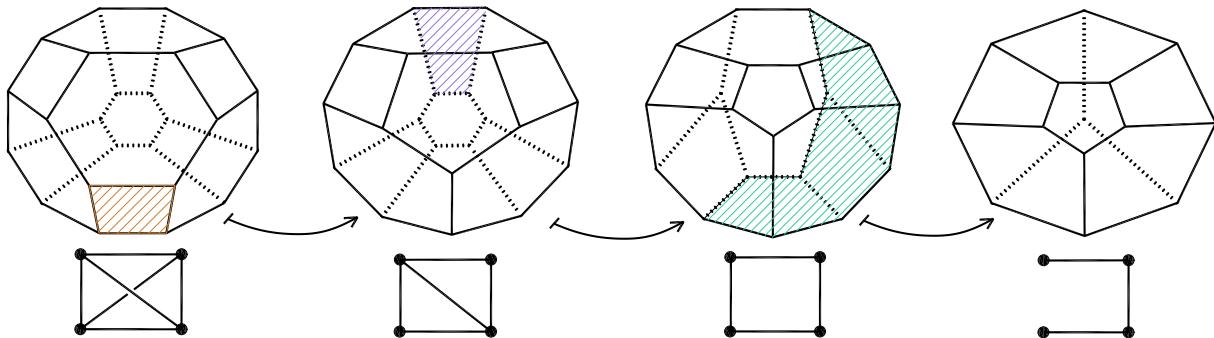


FIGURE 2. The cellular projection from the permutohedron to the associahedron, factored through two graph-associahedra. The third polytope is the cyclohedron [7]. The colored facets in the first 3 pictures are collapsed by the projection.

Secondly we plan to extend our scope to new combinatorial objects. These include generalizations of several well known examples of combinatorially defined polytopes: the graph-associahedra to multigraph-associahedra, the graph-multiplihedra to multiplihedra of Postnikov's nested sets, and the standard multiplihedron to generalized multiplihedron in the sense of Fomin and Zelevinsky. Of course then we will study the Hopf algebras, subalgebras, and modules implied by the structure of these new examples.

Thirdly there are a couple of long term goals that go beyond the Hopf algebra and module research. One is to seek out a deeper understanding of the common themes that run beneath the structures. A solid goal here would be to find a common generalization of all the polytopes involved which reflects the three features of compatibility, inheritance and restriction. In Fomin's generalized associahedra the vertices correspond to clusters, and the facets are cluster variables. For any collection of pairwise compatible cluster variables there is a cluster containing all of them [18], [19]. In Devadoss's graph-associahedra the vertices are maximal tubings and the facets are tubes, or connected subgraphs. For any collection of pairwise compatible tubes there is a tubing containing all of them. Thus the feature of pairwise compatibility links the two fields of study. The second two features are prominent in Postnikov's nestohedra and in the study of species. The feature of restriction is seen in the graph-associahedra as the appearance of the subgraph induced by a set of vertices. The feature of inheritance is found in the reconnected complement, where subgraphs are deleted but then replaced by cliques. Figure 1 displays some tubes and their reconnected complements.

A fourth long term goal is the application of some of the combinatorics studied in this project to questions in enumerative organic chemistry. It turns out that a quotient polytope of the multiplihedron has the same number of vertices as the number of all the rooted tree-like polyhexes with up to n cells. The initial question we would like to answer is how the polyhexes might be arranged according to the vertices of that polytope, and what the edges and facet groupings of the diagrams and their corresponding hydrocarbons might mean.

Much of the early work of the project has already been completed including the publication of results on the multiplihedra, its quotient polytopes, and the graph multiplihedra. Many of the initial experiments are done or underway, but the bulk of proving and deepening of conjectures and concepts is still to come. The funding we seek will largely free up time, our most scarce resource, both for the principal investigator and for several talented students—all of whom are prevented from devoting more effort to this important endeavor simply due to financial pressures.

Our secondary objective is to engage undergraduate math majors and masters degree candidates in this area of research. It is elementary enough to allow students to quickly be able to participate in the actual research, designing and conducting experiments, looking for patterns in the collected data, and helping to formulate and prove conjectures. The principal investigator has directed three masters theses and three senior research projects, one in this precise area and the others in closely related topics. Two of those theses became part of collaboratively published papers. A third paper with the third masters student and a fourth with a senior are in progress. Currently a fourth masters student and several undergraduates are engaged in the research.

The proposed project has as a partial goal the strengthening of ties between Tennessee State University and its counterparts in the region and wider academic community. The principal investigator has given invited and contributed talks about topics related to this project at TSU and at the neighboring Vanderbilt and Middle Tennessee State Universities, both in seminars and AMS functions. Visits have been exchanged, or invited talks given by the PI, with Frank Sottile at Texas A&M, Satyan Devadoss at Williams College and Jim Stasheff currently at Pennsylvania State University. Collaborative work with Devadoss has been accepted for publication, and new work has begun with Sottile, Devadoss, Aaron Lauve and Nathan Reading. A visit to North Carolina for the AMS sectional there is planned. This will include attendance at the session given by Reading, where Lauve will likely give a talk about our work, and an invited talk by the PI at the

session organized by Stasheff. One of the foremost goals at the moment is to help students, who already must present their work to the department, to participate in the seminar and conference arenas.

2. ALGEBRAS

The two most important existing mathematical structures in regard to the first stage of our project are the Malvenuto-Reutanauer graded Hopf algebra of permutations, MR , and the Loday-Ronco graded Hopf algebra of binary trees, LR . The n^{th} component of MR has basis the symmetric group S_n , with number of elements counted by $n!$. The n^{th} component of LR has basis the collection of binary trees with n interior nodes, and thus $n + 1$ leaves. These are counted by the Catalan numbers.

The connection discovered by Loday and Ronco between the two algebras is due to the fact that a permutation on n elements can be pictured as a binary tree with n interior nodes, drawn with attention given to the lengths of edges in order to ensure that the interior nodes are at n different vertical heights from the base of the tree. This is called a tree with levels. The interior nodes are numbered left to right. We number the leaves $0, 1, \dots, n - 1$ and the nodes $1, 2, \dots, n - 1$. The i^{th} node is “between” leaf $i - 1$ and leaf i where “between” might be described to mean that a rain drop falling between those leaves would be caught at that node. The vertical levels of the nodes are numbered top to bottom. Then for a permutation $\sigma \in S_n$ the corresponding tree has node i at level $\sigma(i)$. The connection between permutations and binary trees then is achieved by forgetting the levels, and just retaining the tree. This surjection was first noticed by Tonks, who found the corresponding cellular projection from permutohedron to associahedron [45]. Figure 3 shows an example.

The new revelation of Loday and Ronco is that the Tonks surjection is actually a Hopf algebraic projection, so that by choosing an inverse the algebra of binary trees is seen to be embedded in the algebra of permutations. Much more has been discovered about the structure of these Hopf algebras in the last decade. The binary tree algebra in particular has been shown to be self dual [4], [2]. It has also been characterized as a free dendriform algebra, and as the Hopf algebra determined by a particular Hopf operad [46]. Many of the properties of LR are inherited from MR . One purpose of our research is to parse this inheritance by investigating a large family of interesting combinatorial algebras which lie between the algebra of permutations and the binary trees.

Our new approach is made possible by the recent discovery of Devadoss that the graph-associahedron developed by himself and others is, in the case of the complete graph on n vertices, precisely the n^{th} permutohedron [13]. The vertices of the graph-associahedron of the complete graph on n nodes are originally defined to correspond to maximal tubings of that graph. Here is a way to describe a bijection from the maximal tubings to the permutations. First a numbering of the n nodes must be chosen. Then given an n -tubing, since the tubes are all nested we can number them starting with the innermost tube. Then the permutation $\sigma \in S_n$ pictured by our tubing is such that node i is within tube $\sigma(i)$ but not within any tube nested inside of tube $\sigma(i)$. Figure 3 shows an example.

The binary trees with $n + 1$ leaves (and n internal nodes) correspond to the vertices of $(n - 1)$ -dimensional associahedron, or Stasheff polytope. In the world of graph-associahedra, these vertices correspond to the maximal tubings of the path graph on n nodes. This correspondence can be described by creating a tube of the path graph for each internal node of the tree. Each trivalent node has a left and right branch, which each support a subtree. The tube contains the same numbered nodes of the path graph (left to right) as the nodes of the subtree determined by the internal node. Figure 3 shows an example.

Now the Tonks projection from permutations to binary trees can be described in terms of the tubings. Given a permutation pictured as a maximal tubing of a complete graph with n numbered nodes, we can define the *induced tubing* of the path graph on n nodes. To achieve the path graph, we delete all the edges of the complete graph except for those connecting the nodes in consecutive order from 1 to n . As a single edge

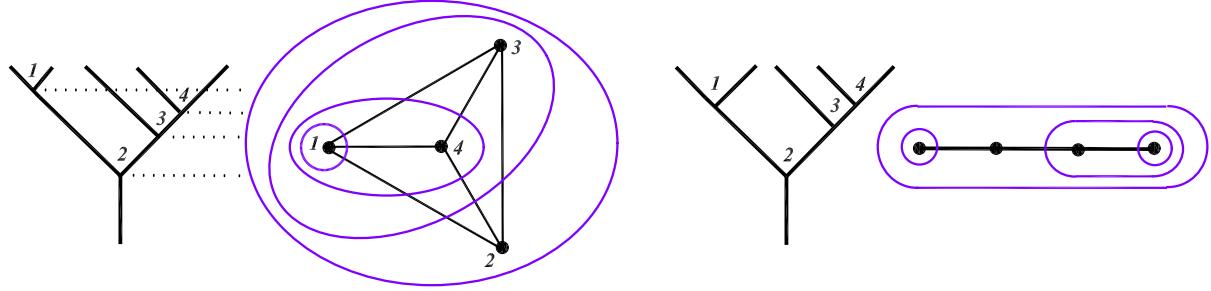


FIGURE 3. The permutation $\sigma = (1432) \in S_4$ pictured as an ordered tree and as a tubing of the complete graph; the unordered tree, and its corresponding tubing.

is deleted, the tubing is preserved up to connection. That is, if the nodes of a tube are no longer connected, it becomes two tubes made up of the two connected subgraphs spanned by its original set of nodes. If there are redundant tubes created in this process only one of them is kept. The result of deleting the extra edges gives exactly the induced tubing on the path which corresponds to the binary tree that is the image of the Tonks map on the permutation. In fact, there is a factorization of the Tonks cellular projection through various graph-associahedra. An example is shown in Figure 4.

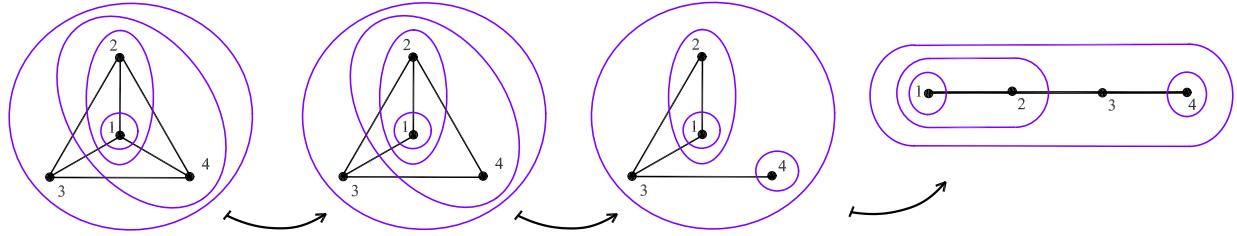


FIGURE 4. The Tonks projection, factored by graphs.

The products and coproducts of MR and LR can also be described in terms of the maximal tubings on complete and path graphs respectively. The product of two permutations from S_n and S_m (seen as basis elements) is a sum of $\binom{n+m}{n}$ basis elements from S_{m+n} . These summands, pictured as tubings of the complete graph on $n+m$ numbered nodes, are each determined by first choosing n of the numbered nodes and then drawing the first permutation upon the subgraph induced by those nodes with numbering determined by their original order. The second permutation is drawn upon the subgraph determined by the remaining m nodes, but each of its tubes are expanded to include the first subgraph as well. An example is in Figure 5.

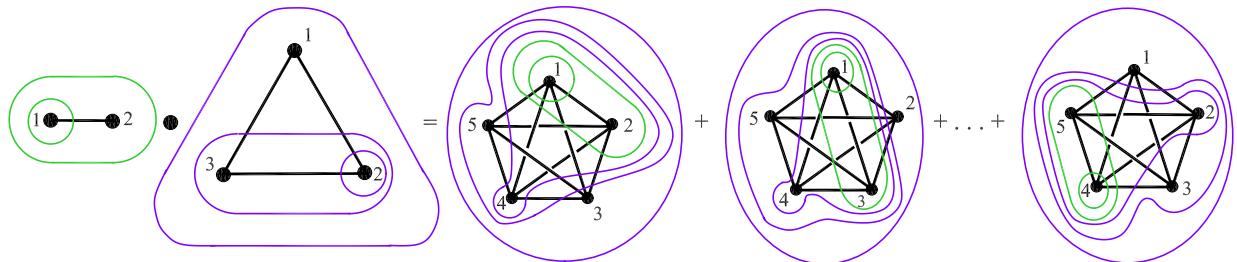


FIGURE 5. The product in MR . See [3] for all 10 terms, described there as compositions with inverse shuffles.

The coproduct of the MR can be described in terms of the graph tubings also. Given a maximal tubing of the complete graph on n vertices, the coproduct is a sum of $n+1$ terms, each a tensor product of basis

elements. These elements are all found as induced tubings on subgraphs. The two elements of a tensor product are found by choosing a node p and inducing the tubings on the subgraph induced by nodes $1 \dots p$ and on the subgraph induced by nodes $p + 1 \dots n$. An example is in Figure 6.

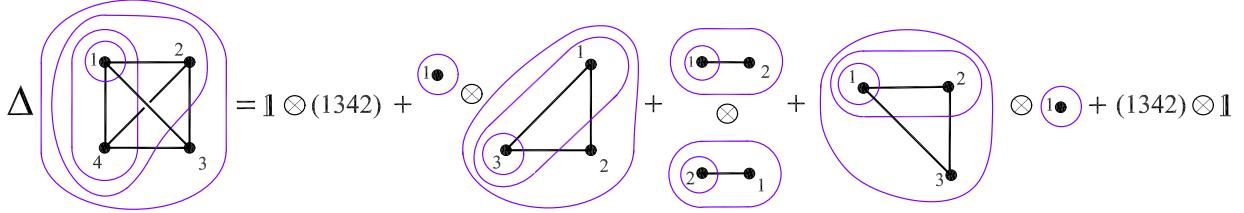


FIGURE 6. The coproduct in MR .

The product and coproduct of LR is described by Aguiar and Sottile in terms of splitting and grafting binary trees [4]. We can vertically split a tree into smaller trees at each leaf from top to bottom—like a lightning strike that hits a leaf and splits the tree along the shortest path to the root. We graft trees by attaching roots to leaves, without creating a new interior nodes at the graft. The product of two trees with $n + 1$ and $m + 1$ leaves (in that order) is a sum of $\binom{n+m}{n}$ terms, each an $(n + m + 1)$ -leaved tree. Each is achieved by vertically splitting the first tree into $m + 1$ smaller trees and then grafting them to the second tree, left to right.

This product of trees can be described in terms of the path graph tubings as well. To create a term of the product we need a tubing on a path graph of $n + m$ nodes. We choose n of these nodes, and then put the n -tubing on them by first breaking it up into components that match the subgraph induced by our choice of n nodes. Then the second m -tubing can be placed on the remaining m nodes, expanding each tube that is adjacent to an existing one in order to include it. Even more simply we can describe this process as:

- (1) Lifting our n and m -tubings to preimages of the Tonks projection in the complete graphs on n and m nodes.
- (2) Performing the product of these complete graph tubings in the MR algebra,
- (3) and projecting the resulting terms back to tubings of the path graph on $n + m$ nodes.

The coproduct of a tree in LR is again described by Aguiar and Sottile [4]. It is a sum of $n + 1$ terms, each a tensor product of basis elements. The two elements in a tensor product are found by choosing a leaf along which to vertically split the tree into two smaller trees. In terms of a coproduct of an n -tubing of the path graph, the elements are all found as induced tubings on subgraphs. The two elements of a tensor product are found by choosing a node p and inducing the tubings on the subgraph induced by nodes $1 \dots p$ and on the subgraph induced by nodes $p + 1 \dots n$.

From the viewpoint of tubings on graphs, there is a clear path to generalization of the products and coproducts in MR and LR . Not only can we extend the structure to certain sequences of graphs, but we can do so in such a way that we produce extremely interesting subalgebras and sub-coalgebras of MR . In fact, there is the potential for a series of finely tuned filters of MR , possessing important relationships with LR . The first goal of the proposed project is to seriously investigate these filters, with an eye to classification and application to the well known structures.

Here is a brief description of how to construct a graded coalgebra which lies between the MR and LR coalgebras. First we need to define a sequence of connected graphs with numbered nodes, indexed by the number of nodes in each graph. The collective property that they minimally must possess is as follows: given a graph in our sequence, and a consecutively numbered subset of its nodes, the subgraph induced by those nodes must also occur as a term in our sequence. We call this a *restrictive graph sequence*. An example, in

Figure 7, is formed by connecting any two numbered nodes whose difference is odd. There are many more similar examples.

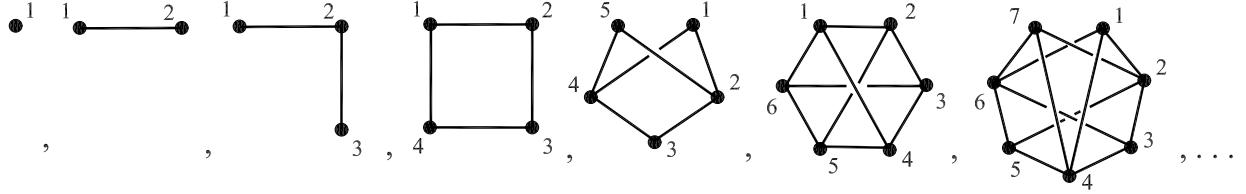


FIGURE 7. Example of restrictive graph sequence.

From such a restrictive graph sequence, we can form a fundamental basis for a graded coalgebra. The n^{th} component of the basis is comprised of the maximal tubings on the n -node graph, the n^{th} graph in our sequence. The coproduct of an n -tubing T_n on the graph g_n in our sequence is given by:

$$\Delta T_n = \sum_{p=0}^n (\text{induced tubing on } g_p) \otimes (\text{induced tubing on } g_{n-p})$$

where the induced tubings are determined by taking the subgraphs of g_n with nodes $1 \dots p$ and $p+1 \dots n$ respectively. Figure 8 shows an example in the coalgebra based on the sequence shown in Figure 7.

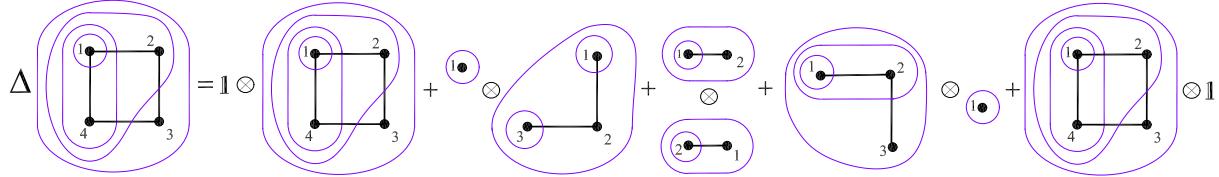


FIGURE 8. A coproduct in a restrictive sequence coalgebra.

Next is a description of how to construct a graded algebra which lies between the *MR* and *LR* algebras. First we need to define a sequence of connected graphs with numbered nodes, indexed by the number of nodes in each graph. The collective property that they minimally must possess is as follows: given a graph g_n in our sequence, and one of its nodes, the reconnected complement of the graph g_n with that node deleted must occur as the term g_{n-1} in our sequence. We call this a *hereditary graph sequence*. One example is the cycle graphs on n vertices. A related example is shown in Figure 9.

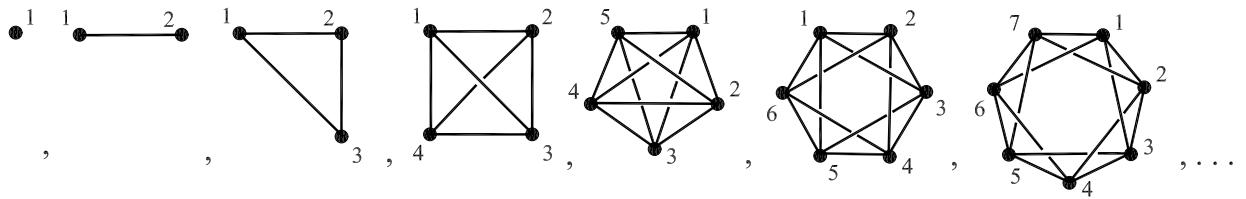


FIGURE 9. Example of hereditary graph sequence.

From such a hereditary graph sequence, we can form a fundamental basis for a graded algebra. The n^{th} component of the basis is comprised of the maximal tubings on the n -node graph, the n^{th} graph in our sequence. The product of tubings T_n and T_m on the graphs g_n and g_m in our sequence is given by $\binom{n+m}{n}$ terms, each a tubing of the graph g_{n+m} . Each is achieved by:

- (1) Lifting our n and m -tubings to preimages of the Tonks projection in the complete graphs on n and m nodes.
- (2) Performing the product of these complete graph tubings in MR ,
- (3) and projecting the resulting terms back to tubings of the graph g_{n+m} .

An example is shown in Figure 10.

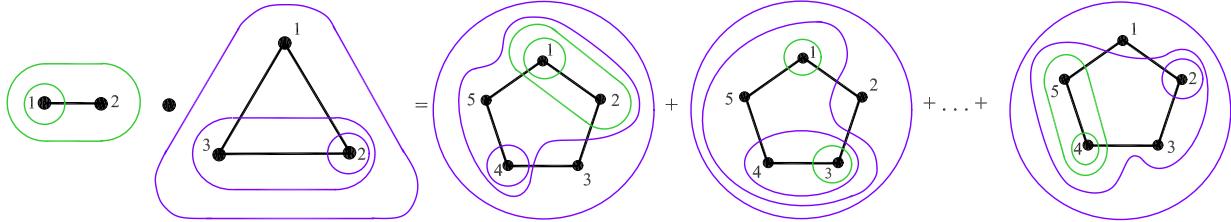


FIGURE 10. A product of cycle graph tubings (10 terms total).

Our intense interest in these subalgebras and sub-coalgebras is due to the fact that they occur naturally as the intermediate domains of a factorization of the Tonks projection. Recall that the Tonks projection can be described by deleting edges of the complete graph with numbered nodes, creating at each deletion the induced tubing, until the path graph is achieved. The new subalgebras and sub-coalgebras we have described all occur as intermediaries of this process. A factor of the Tonks projection is described simply by deleting only certain of the edges of a graph sequence, to achieve a new sequence, as exemplified in Figure 4. The result is a cellular projection of polytopes, here restricted to vertices. The full cellular projection, as shown in Figure 2 is of even greater importance in describing lattice congruences and differential algebra projections.

Much is still to be learned about the nested embedding of these graph-theoretic sub-coalgebras and subalgebras of the permutations. There is a tantalizing parallel here to the research of Fomin and Reading [17]. In his analysis of the MR and LR Hopf algebras Reading focuses on the fact that the components of their grading form classic lattices: the weak order on the permutations and the Tamari lattice respectively. He then defines lattice congruences of two varieties: the *translational* families of congruences on the permutations guarantee that their equivalence classes form subalgebras of the MR algebra, and *insertional* families of congruences guarantee sub-coalgebras [38]. Our next step, already proceeding via communications with Reading, is to see whether various families of polytopes we describe arise from lattice congruences. The goal here, beyond simply drawing useful analogies, is to look for graph sequences that are both hereditary and restrictive in order to construct Hopf subalgebras. This project seems difficult, but the tool of pattern avoidance in permutations has already allowed Reading to successfully describe families of congruences that are both translational and insertional.

A fact which makes our project plausibly successful along these lines is that, given a graph G , the collection of maximal tubings form the vertex set of a convex polytope—the graph-associahedron K_G . The edges of this polytope then have the potential to be the covering relations of a lattice. Following from the examples of the permutations and binary trees seen as graph tubings, we can describe the conjectural covering relations as follows: a maximal tubing covers another if the collection of all the tubes of both splits into identical pairs except for one pair of tubes which are unique to their respective tubings. Ordering the numbered nodes in the two tubes which make up this pair, the greater tubing is the one whose unique tube has a lexicographically greater list of nodes. This ordering generalizes both the weak order on permutations and the Tamari ordering of binary trees.

The fact that the tubings form polytopes also opens up the question of considering higher dimensional faces as basis elements in the algebras. This creates at least two intriguing possibilities. One is that the

restrictive sequences could yield the foundational basis for an actual Hopf algebra. The reason that they generally do not when considering only the maximal tubings (vertices of the graph-associahedra) is that the product via lifting is not well defined. However, since the faces of a polytope form a lattice, the collection of possible results of a lifting could be replaced with a join of those maximal tubings in the face lattice, making the product well defined. The other intriguing possibility is that the faces of a single graph-associahedron could be organized into a graded differential Hopf algebra, perhaps embedded in the original Hopf algebra based upon the entire restrictive sequence. That this possibility is actually the case for the permutohedron has been verified by communication with F. Sottile. We have also experimentally verified the Leibnitz rule for trees.

Reading's sufficient conditions for a lattice congruence to yield a Hopf subalgebra apply more generally to a large class of lattices arising in the study of cluster algebras. As stated above, an overriding goal of ours is to unite the differing viewpoints, seen most starkly as differing generalizations of the associahedron, via a common generalization. First, however, there is the sub goal of extending new findings about the Hopf algebras on graph sequences and on the vertices of single graph-associahedron to the next larger family of mathematical objects of which these are members. Graph-associahedra are examples of Postnikov's *nestohedra*, and the collection of tubings on a graph exemplify a *nested set* [36]. In fact, more specifically they are *graphical nested sets* as defined by Zelevinsky [49]. The first theoretical aspect of this work will be to transfer the definitions of restrictive and hereditary sequences, and the associated products and coproducts, to the general graphical nested sets.

Experimentally, we look forward to investigating a whole new class of polytopes which might lie within the class of nested sets, but may need a broader description than graphical. We believe that it makes perfect sense in the definition of graph-associahedron to replace "graph" with "multigraph" (loop free) and replace "tube" with "connected sub-multigraph". The conjecture is that the new posets of multi-tubings are still realized by the face structure of polytopes. During his recent visit, Devadoss opined that, for an n -node multigraph G , the associahedron K_G should have dimension $n - 1 + |\{\text{redundant edges}\}|$, where the number of redundant edges means the number of edges that minimally must be removed to result in a simple graph. Our first task would involve more experimentation, and then the proving of all the relevant theorems about multigraphs. Both of these are planned student projects. Theorems will include the dimension and the product structure of faces of the polytopes, as well as useful realizations.

Here are some examples. The simplest case is the multigraph with two nodes and two edges. K_G in this case is a quadrilateral, with dimension $2 - 1 + 1 = 2$. The multigraph G with two nodes and three edges has K_G a hexagonal prism. The multigraph G with three nodes and three edges shown in the second part of Figure 11 has dimension 3 for K_G . The classical 3 dimensional associahedron, the path graph-associahedron, is shown for comparison.

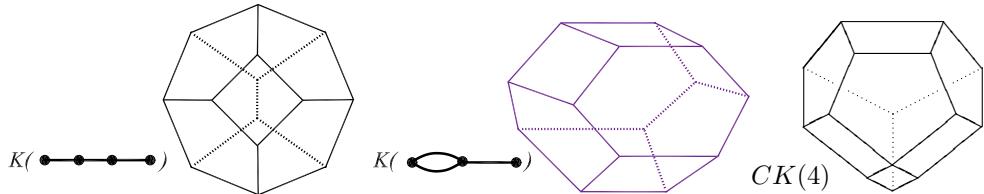


FIGURE 11. The associahedron [44], a multigraph associahedron, and the composihedron [23].

3. MODULES

The complexes now known as the multiplihedra, usually denoted $\mathcal{J}(n)$, were first discussed by Stasheff in [43]. Pictures in the form of *painted binary trees* can be drawn to represent the multiplication of several

objects in a monoid, before or after their passage to the image of that monoid under a homomorphism. A painted binary tree is painted beginning at the root edge (the leaf edges are unpainted) and in such a way that painted regions must be connected, painting must never end precisely at a trivalent node, and painting must proceed up both branches of a trivalent node. For instance, given a, b, c, d elements of a monoid, and f a monoid morphism, the tree in Figure 12 represents the operation resulting in the product $f(ab)(f(c)f(d))$.

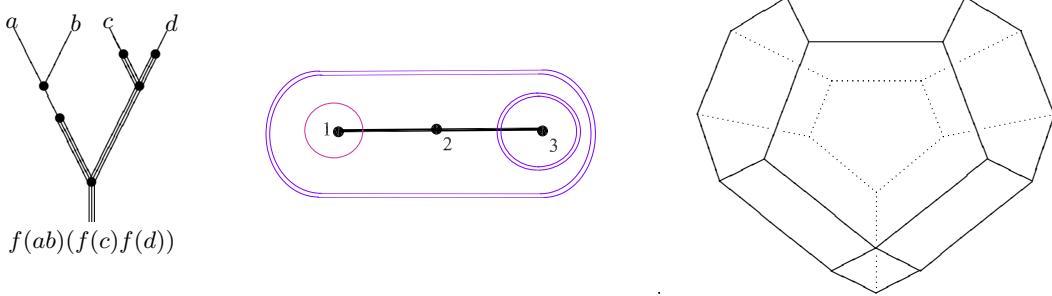


FIGURE 12. A painted tree, the corresponding marked tubing and the 3d multiplihedron where both represent a vertex.

Of course in the category of associative monoids and monoid homomorphisms there is no need to distinguish the product $f(ab)(f(c)f(d))$ from $f(abcd)$. These diagrams were first introduced by Boardman and Vogt in [6] to help describe multiplication in (and morphisms of) topological monoids that are not strictly associative (and whose morphisms do not strictly respect that multiplication.) The n^{th} multiplihedron is a CW-complex whose vertices correspond to the unambiguous ways of multiplying and applying an A_∞ -map to n ordered elements of an A_∞ -space. Thus the vertices correspond to the binary painted trees with n leaves. The edges of the multiplihedra correspond to either an association $(ab)c \rightarrow a(bc)$ or to a preservation $f(a)f(b) \rightarrow f(ab)$. The associations can either be in the range: $(f(a)f(b))f(c) \rightarrow f(a)(f(b)f(c))$; or the image of a domain association: $f((ab)c) \rightarrow f(a(bc))$. The 2-dimensional multiplihedron is a hexagon, and Figure 12 shows the 3 dimensional $\mathcal{J}(4)$.

The overall structure of the associahedra is that of a topological operad, with the composition given by inclusion. The multiplihedra together form a bimodule (left and right module) over this operad, with the action again given by inclusion. That is, there exist inclusions:

$$\mathcal{K}(k) \times (\mathcal{J}(j_1) \times \cdots \times \mathcal{J}(j_k)) \hookrightarrow \mathcal{J}(n)$$

where n is the sum of the j_i . This is the left module structure. The right module structure is from existence of inclusions:

$$\mathcal{J}(k) \times (\mathcal{K}(j_1) \times \cdots \times \mathcal{K}(j_k)) \hookrightarrow \mathcal{J}(n)$$

where n is the sum of the j_i . This structure mirrors the fact that the spaces of painted trees form a bimodule over the operad of spaces of trees, where the compositions and actions are given by the grafting of trees, root to leaf.

Two significant advances in understanding the multiplihedra were made in 2008. I published results earlier this year about the geometric and combinatorial structure of the multiplihedron, including the fact that its vertices are counted by the Catalan transform of the Catalan numbers [22]. Also in that paper is a description of how to calculate the vertices in Euclidean space whose convex hull realizes the n^{th} multiplihedron. This in fact answered the open question of whether or not the multiplihedra could indeed be realized as convex polytopes. The first part of Figure 14 shows the actual geometric realization of the multiplihedron with some of the points labeled.

The other relevant advance, unpublished as yet, was made by Lauve and Sottile. They discovered that the vertices of the multiplihedron, often pictured as painted trees, comprise the fundamental basis of a graded Hopf module over the LR Hopf algebra. They constructed the action and the coaction: the module action of the binary trees on the vertices of the multiplihedron in the fundamental basis, and the comodule coaction of the binary trees on the vertices in a new basis called the monomial basis. The two bases are related to each other by Moebius inversion. Since their discovery, working together we have uncovered several additional related Hopf algebraic structures on the multiplihedra and permutohedra.

These latter advances open the question of the existence and classification of other module structures over the other subalgebras and sub-coalgebras of the MR Hopf algebra. We are in excellent position to attack that problem, since in 2008 we published descriptions of the first generalization of the multiplihedron along the line of development parallel to the graph-associahedron [14]. Just as the faces of the classical multiplihedra can be labeled with painted trees, the vertices of the graph-multiplihedra correspond to maximal tubings of the graph using two colors of tube. We draw the two colors as thick and thin. These are referred to as marked tubings. Marked tubes u and v are *compatible* if

- (1) u and v do not intersect,
- (2) u and v are not adjacent (their union is not connected), and
- (3) if $u \subset v$ where v is not thick, then u must be thin.

A *marked tubing* of G is a collection of pairwise compatible marked tubes of G . An example on a path graph is shown in Figure 12.

The collection of marked tubings on a graph G can be given the structure of a poset. For a graph G with n nodes, the *graph-multiplihedron* \mathcal{J}_G is a convex polytope of dimension n whose face poset is isomorphic to the poset of marked tubings of G . The classic dimension n multiplihedron is the graph-multiplihedron on the path graph with n nodes. In our paper we show that the graph-multiplihedron for the complete graph on n vertices is the permutohedron of dimension n [14]. This is done by producing a poset isomorphism, which when restricted to the vertices of the permutohedron gives a set bijection between permutations on n elements and maximal marked tubings of the complete graph on $n - 1$ nodes. This description seems to indicate that the permutations form a non-trivial graded Hopf module over themselves; that is, over the MR Hopf algebra.

Saneblidze and Umble were the first to describe a surjection π from the permutations to the painted binary trees; more precisely from the permutohedron to the classic multiplihedron [40]. Their projection can be described in terms of the marked tubings just as above we described the Tonks projection in terms of ordinary tubings. Beginning with a maximal marked tubing of the complete graph on n ordered nodes, we delete the edges of the graph except for those between node i and $i + 1$. At each deletion we create the induced marked tubing, and at the end of the process we have a marked tubing of the path graph. Figure 13 demonstrates this process.

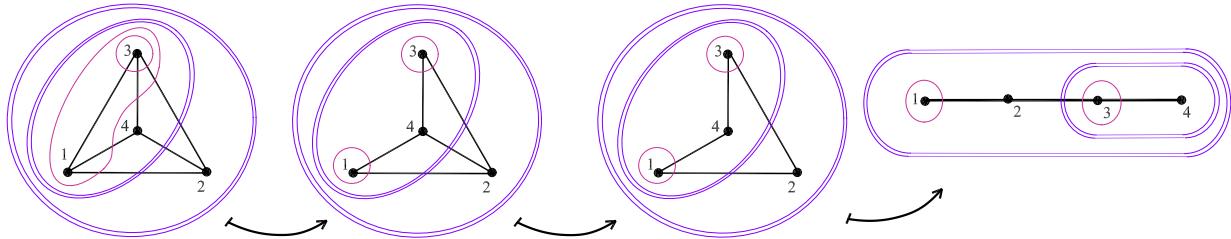


FIGURE 13. The surjection π factored.

Immediately this description of the Saneblidze-Umble projection suggests that there are a series of submodules and subcomodules of the Hopf module of permutations which filter the latter, and which contain

the Hopf module of painted trees discovered by Sottile and collaborators. These have bases made up of the maximal marked tubings of the graphs in the restrictive and hereditary sequences described earlier. The Saneblidze-Umble projection will factor through a selection of these submodules simply by a choice of specific order in which to delete edges of the complete graph, one at a time.

The *LR* Hopf algebra of trees has been fit into the construction of Moerdijk and Van der Laan, which builds Hopf algebras from operads [35], [46]. It seems very likely that this construction can be applied to operad bimodules in order to construct Hopf modules. We plan to explore this route both for its own interest and in order to get a clearer picture of the Hopf module of painted trees—since the multiplihedra do indeed form an operad bimodule over the associahedra. Once verified on this known example, our newly developed method for constructing Hopf modules will be applied to other operad module structures. These include the characterization of the cyclohedra as a module over the associahedra, as described by Markl [34].

The discovery of another module over the associahedra was published by the PI in 2008 [23]. This is the sequence of polytopes known collectively as the *composihedra*. The 3d composihedron is pictured in Figure 11. These characterize A_∞ -maps from a topological monoid to an A_∞ -space. Therefore each of these polytopes is a quotient of the corresponding multiplihedron. In our paper of this year we show how these polytopes are used to parameterize compositions in the formulation of the theories of enriched bicategories and pseudomonoids in a monoidal bicategory. We also present a simple algorithm for determining the vertices in Euclidean space whose convex hull is the n^{th} polytope in the sequence of composihedra, that is, the n^{th} composihedron $\mathcal{CK}(n)$. The vertices are counted by the binomial transform of the Catalan numbers. Early work with Sottile and Lauve demonstrates the possibility of Hopf algebraic structures based on the composihedra, both algebras and modules.

The associahedra reappear as the quotient of the multiplihedron for the case of maps from an A_∞ -space to a monoid. This implies that the *LR* algebra has an interesting module structure over itself. Both quotients generalize to the graph associahedra, and the polytopes thus created are denoted JG_r and JG_d (becoming the associahedra and composihedra respectively for G a path graph) [14]. We plan then to describe Hopf module structures on JG_r and JG_d in general which specialize via the path graphs to the originals. This may lead to further results relating module and algebra constructions, since certain identities exist. For instance $JG_r = JG_d$ in the case of the complete graph G . Also K_G for G a star graph is conjecturally congruent to JG_r for G the cycle graph.

Having satisfied ourselves with the fine structure of the Hopf modules just described, we will turn to even further generalizations. Again, there are two directions in which the research will proceed. One is in the path of Postnikov, where we will seek to define generalized multiplihedra for his generalizations of the associahedra. We of course already have this done for the case of graph-associahedra, and the case of the nestohedra for graphical nested sets and even more general nested sets should follow quickly. In our paper with Devadoss we find a Minkowski sum description of the graph-multiplihedron for the edgeless graph on n nodes, denoted ∇_n . If C_n is the n -cube $[0, 1]^n$ in \mathbb{R}^n , then the hyperplane $\sum x_i = 1$ cuts C_n into two polytopes, the simplex Δ_n and its complement $C_n - \Delta_n$. The polytope ∇_n is combinatorially equivalent to $\Delta_n \oplus (C_n - \Delta_n)$.

For the nestohedra, Postnikov gives a realization formulated as a Minkowski sum of simplices. A question deserving of further thought is whether there is a consistent definition of *marked nested sets* which would specialize to our marked tubings. It would be especially interesting to elucidate whether the Minkowski sum for ∇_n discussed here has a nice generalization in that context.

It is fairly easy though to describe a multiplihedron for the family of generalized permutohedra that Postnikov calls nestohedra. These polytopes are defined as Minkowski sums of standard simplices of various dimension that correspond to subsets of $[n]$. For instance the ordinary associahedra are the Minkowski sums of the simplices corresponding to all the subsets of $[n]$ that are consecutive strings. For each of these subsets

the corresponding simplex is just the convex hull of the endpoints of the unit vectors on the coordinate axes listed in the string of integers.

For any of these nestohedra that include all the single element subsets of $[n]$ the resulting polytope will be in the positive quadrant of R^n , perpendicular to the vector $(1, \dots, 1)$. Conjecturally the multiplihedra can be constructed geometrically by creating another copy of the nestohedra one half the size, parallel to the original but closer to the origin, and then connecting corresponding vertices by shortest paths from the large nestohedra to the little one, always adding edges that are parallel to the coordinate axes, and putting in both paths whenever there are two possible routes. The intuition of this construction is a generalization of the geometric realizations for the classical multiplihedra in [22] and the graph-multiplihedra in [14].

For even more examples we will return to the multigraph generalization of the graph-associahedron. Now the *multigraph-multiplihedron* can be described simply by the poset of marked tubings on a multigraph. In the experiments we have performed, for G a multigraph with n nodes (loop free), the multiplihedron J_G has dimension $n + |\{\text{redundant edges}\}|$.

Finally we plan to continue investigations already in progress into the proper definition of a multiplihedron corresponding to Fomin and Zelevinsky's generalized associahedra. This will have both the potential of affording us with new Hopf module structures over the Hopf algebras described by Reading, and may also have important consequences for the study of cluster algebras. So far it is still unclear what the generalized multiplihedron for a generalized associahedron of Fomin and Zelevinsky should be. There are a couple of good hints, however. Figure 14 displays a candidate for the generalized multiplihedron for the cyclohedron, or type B associahedron.

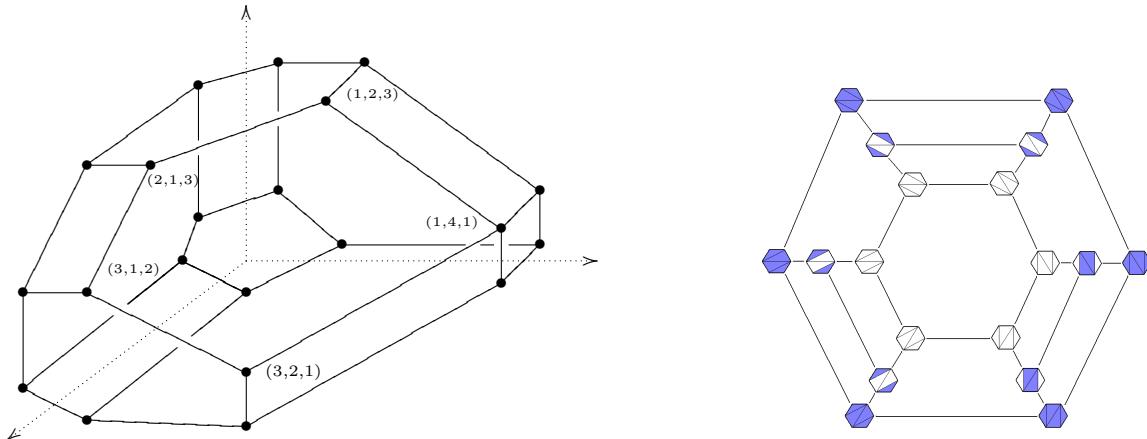


FIGURE 14. The 3d type A multiplihedron realized as a convex hull; and the 3d type B multiplihedron, as a Schlegel diagram.

Note that it is definitely different from the graph multiplihedron based upon a cycle graph. Here we followed the example of creating the classical multiplihedron by shading triangulations, starting with a chosen base edge of the n -gon. Since the vertices of the cyclohedron are centrally symmetric triangulations, we required the shading to also be centrally symmetric.

The generalized associahedra are connected to cluster algebras via the creation of adjacency matrices for the vertices and then mutation matrices for the edges. The adjacency matrix of a shaded triangulation should have a factor of $q \in (0, 1)$ multiplying each entry corresponding to shaded triangle(s). This intuition comes from the fact that the same process is used to create the convex hull of the graph-multiplihedron.

Another tool that will be brought to bear in the effort to find common constructions of Hopf modules is that the 1-skeleton of the multiplihedron does possess a lattice structure. It contains within it the Tamari lattice, since the multiplihedron contains two copies of the associahedron. Other covering relations are

described as extending the painted portion of a tree past a single additional interior node. This lattice is easy to generalize to the graph multiplihedra, and so we will look for interesting lattice congruences which can generate Hopf submodules from marked tubings on subgraphs of the complete graph.

This discussion brings us back to the possibility of finding a unified approach to both the Hopf algebras based on graph sequences, those related to cluster algebras, and more generally based on lattice congruences. There are several category theoretical possible approaches to this problem, which might have the potential of describing the various Hopf algebras all at once. One is the concept of *species*, or *structure types*, which are a way of seeing sequences of combinatorially defined sets as functors from finite sets to sets. Schmitt defines Hopf algebra structures on certain types of species which he refers to as *species with restriction* and *hereditary species* [41]. Using this Schmitt defines a different Hopf algebra structure on the permutations. It would be very interesting to know whether the *MR* and *LR* Hopf algebras fit into the species construction. We have already mentioned the operadic constructions of Hopf algebras. A third possibility is to look for a categorical PROP which encodes all Hopf algebras. The existence of such an object is an open question.

Early results of the PI and others paint a tantalizing picture. A book in progress by Aguiar and Mahajan is entitled *Monoidal functors, species and Hopf algebras*. In this work they demonstrate that various pairs of products on species form 2-fold monoidal categories. The PI and collaborators have published several papers about the latter structures, their classification, and operads within them [25], [21], [24]. Included are examples of n -fold monoidal structures based upon Young diagrams and braids. It would be very interesting to investigate in this context the Hopf algebra structures on Young diagrams from a species point of view.

4. AN APPLICATION

We plan to study the polyhexes, which consist of arrangements of a number of hexagons which share at least one side with another in the group. These arrangements look very familiar to an organic chemist, since they are the pictures of *polycyclic benzenoid hydrocarbons*. This name refers to the way that carbon often occurs in a molecule as a hexagonal ring of six atoms. One of these rings alone is the molecule benzene, C_6H_6 . There has been much recent research into the enumeration of hydrocarbons. The state of knowledge here is that it is still unknown how to calculate the number of possible hydrocarbons of a given size. Many partial results have been discovered [26], [5]. Enumeration of hydrocarbons is closely related to purely mathematical constructions like the polyhexes. Especially so when we restrict our attention to special polyhexes, such as the tree-like ones with a chosen “root” edge. Figure 15 shows the five of these with 2 or fewer hexagons, including the one with zero hexagons.

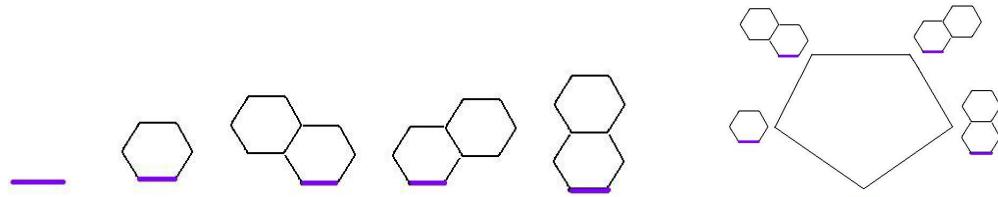


FIGURE 15. ≤ 2 -cell rooted polyhexes; arranged around a composihedron.

If collections of molecules could be arranged around facets of a polytope then there might be revealed interesting insights into the properties of those molecules and their relationships. This knowledge should also accelerate the computer processes of building and searching libraries of molecules. The sequence of total numbers of tree-like rooted polyhexes starts out 1,2,5,15,51,188... and then eventually grows as quickly as 5^n . It turns out that the n^{th} composihedron has the same number of vertices as the number of all the rooted tree-like polyhexes with up to n cells. The sequence of composihedra has numbers of facets which start

out 0,2,5,10,19,36... and that grow only as quickly as 2^n . This is important to the possible applications of molecular library searching, since it means that a facet-based search has the potential to proceed much more quickly. If the facets have meaning in terms of the chemical properties of the molecules, then the search process could be sped by screening for entire groups of molecules that share a facet. Even better, perhaps only certain facets need be represented in the library. This would help in the building stage, which can be the most time consuming.

Another advantage is that the polytope can be thought of as a solid in space, made of all its interior points rather than just the vertices. This can lead to the solution of problems by use of continuous optimization techniques. By this we mean that a property such as the conductivity of the molecule we are building might be represented by a continuous function on the polytope. Then we could find a point (not necessarily a vertex) somewhere in the solid polytope where that function value is at a maximum. Finally we could find the nearest vertex to that point and predict its associated molecular structure to realize maximum possible conductivity.

In the second part of Figure 15 we show the rooted polyhexes arranged around a pentagon. This is only one possible arrangement. The question is how to choose the “right” arrangement so that it extends meaningfully to an arrangement around the 3-dimensional composihedron of all 15 of the tree-like polyhexes with 3 or fewer hexagons. In fact, we want to find a recipe for putting the polyhexes with n or fewer hexagons at the vertices of the n -dimensional composihedron. The tools for attacking the problem of finding a meaningful recipe include a list of known one-to-one complete correspondences (bijections) between the polyhexes and other combinatorial objects. These include strings of words made with a given alphabet, trees with a whole number assigned to each leaf, trees with extra long branches, and branching polyhexes. Others with unknown arrangements (in addition to the rooted tree-like polyhexes) include Dyck paths and the symmetric polyhexes with $2n + 1$ hexagons [15]. By linking together the various bijections we hope to find useful new ones. Another tool is to understand the polytope edges as moves made between objects. Specific bijections are often also found using generating function techniques. Communications with Emeric Deutsch have greatly facilitated the possibility of this application of the combinatorics in our research.

Among the open questions to be researched or assigned to students are: What are the geometrical properties of the realizations of various polytopes—centers, volumes, symmetries, edge lengths and facet areas? Also of interest are the combinatorial properties—number of vertices, numbers of faces, numbers of triangulations, and space tiling properties. When the numbers of vertices of a particular sequence of polytopes are known, then there is the opportunity to find other (molecular) interpretations of those numbers which the polytopes also help to organize.

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