1. **Project description: Geometric combinatorial Hopf algebras.**

Introduction to Polytopes in Algebra

A combinatorial sequence that is created by a recursive process often carries the seed of a graded algebraic structure. An algebra reflects the process of building a new object from prior ones; and a coalgebra arises from deconstructing an object into its constituent components. We are building upon the foundations laid by many other researchers, especially Gian-Carlo Rota, who most clearly saw the strength of this approach. This proposal will transition between new polytopes, newly defined operadic structure, and the newly discovered algebras. At each stage we will highlight the broader impact of the project by pointing out the role student researchers will play.

1.1. **Review of important Hopf algebras based on trees.** The historical examples of Hopf algebras $\mathfrak{S}Sym$ and $\mathcal{Q}Sym$, the Malvenuto-Reutenauer Hopf algebra and the quasisymmetric functions, can be defined using graded bases of permutations and boolean subsets respectively. Loday and Ronco used the fact that certain binary trees can represent both sorts of combinatorial objects to discover an intriguing new Hopf algebra of planar binary trees, $\mathcal{Y}Sym$, lying between them. [21, 22]. They also described natural Hopf algebra maps which neatly factor the descent map from permutations to boolean subsets. Their first factor turns out to be the restriction (to vertices) of the Tonks projection from the permutohedron to the associahedron. Chapoton made sense

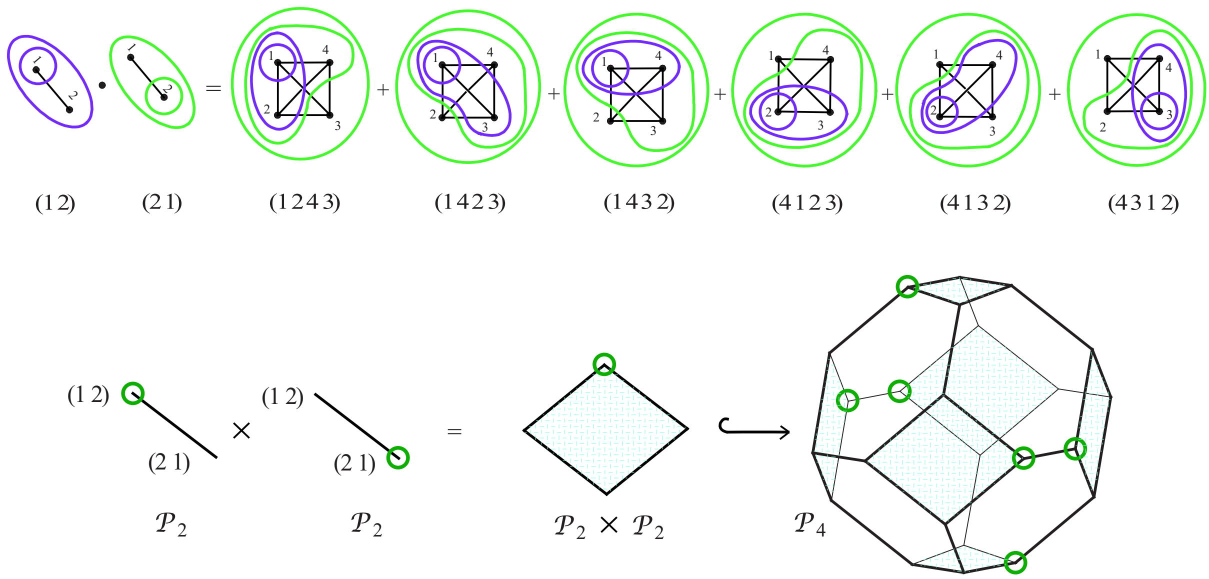

Figure 1. Multiplying in $\mathfrak{S}Sym$. The theme of [17] is that the product of two faces from a given recursive sequence of polytopes, here from terms $\mathcal{P}_i$ and $\mathcal{P}_j$ of the permutohedra, is described as a sum of faces of the term $\mathcal{P}_{i+j}$. The summed faces in the product are the images of maps which embed a cartesian product of the earlier terms of $\{\mathcal{P}_n\}$.

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of this latter fact when he found larger Hopf algebras based on the faces of the respective polytopes [8].

Much more of the structure of these algebras has been uncovered in the last decade. In 2005 and 2006 Aguiar and Sottile used alternate bases for the Loday-Ronco Hopf algebra and its dual to construct explicit isomorphisms [3],[2]. Several descriptions of the big picture of combinatorial Hopf algebras have put these structures in perspective, notably [1], and [19], and most recently the preprint of Loday and Ronco [20].

1.2. **New insights into $\mathfrak{S}Sym$, $\mathcal{Y}Sym$ and divided powers.** In our recent paper [17] we take the novel point of view of graph associahedra from which to study these algebras. First we show how the Hopf algebras $\mathfrak{S}Sym$ and $\mathcal{Y}Sym$ and the face algebras $\mathfrak{S}\tilde{Sym}$ and $\mathcal{Y}\tilde{Sym}$ containing them can be understood in a unified geometrical way, via cellular surjections and recursive facet inclusion. For an example of the product of basis elements of $\mathfrak{S}Sym$, see Figure 1. Then we capitalize on that unified viewpoint to build analogous algebraic structures on the vertices and faces of the cyclohedra and simplices, which we describe below in Section 3.1.

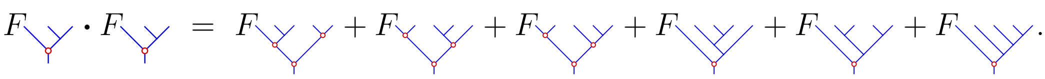
Now, in [15], we introduce a new characterization of $\mathfrak{S}Sym, \mathcal{Y}Sym$ and the divided power Hopf algebra. The latter is denoted $\mathcal{K}[x] := \text{span}\{x^{(n)} : n \geq 0\}$, with basis vectors $x^{(n)}$ satisfying $x^{(m)} \cdot x^{(n)} = \binom{m+n}{n} x^{(m+n)}$, $1 = x^{(0)}$, $\Delta(x^{(n)}) = \sum_{i+j=n} x^{(i)} \otimes x^{(j)}$.

Our new point of view sees all three of these as *graded Hopf operads*, which are graded monoids in the category of coalgebras, with the monoidal structure given by the composition product. In other words, they are simultaneously operads and coalgebras using the same grading, and with operad compositions required to be coalgebra morphisms. This implies their Hopf algebra structure, given by $A \cdot B = \gamma(\Delta^{(n)} A \otimes B)$ where $\Delta^{(n)}$ is the iterated coproduct.

1.3. **Cambrian lattices and their Hopf algebras.** In [27] Reading uses *insertional* and *translational* lattice congruences to build the Malvenuto-Reutenauer Hopf algebra as the limit of a sequence of smaller Hopf algebras: the first Hopf algebra in the sequence is the graded Hopf algebra with one-dimensional graded pieces and the second is the Hopf algebra of non-commutative symmetric functions. In the same paper Reading builds the Hopf algebra of planar binary trees as the limit of a similar sequence. Our work here is partly motivated by the question of whether the third leg of the triangle might also be amenable to such an approach. As an answer, in Sections 3.2 and 3.3 we build the Malvenuto-Reutenauer Hopf algebra as the limit of a sequence of smaller graded algebras where the first algebra in the sequence is the graded algebra of planar binary trees, and the second is based upon the cyclohedra.

2. Multiplihedra: trees

2.1. **The classic polytopes part 1: bileveled trees.** The vertices of the multiplihedra can be represented by trees whose nodes are divided into two levels. In [14] and [16] we have demonstrated a new graded algebra with basis these bileveled trees, graded by the numbers of internal nodes. Here is an example of the product:



The important role played by the new algebra, which we call $\mathcal{M}Sym$, is due to the fact that the Saneblidze-Umble cellular projection β from the permutohedra to the multiplihedra (restricted to vertices) is indeed an algebra homomorphism in this context. Thus we are led to ask:

Question 2.1. *Is there an extension of $\mathcal{M}Sym$ to the faces of the multiplihedra paralleling Chapoton's extension of $\mathfrak{S}Sym$ to the faces of the permutohedra? If so, does it also have a differential graded structure?*

We conjecture that the answer is yes. Students may chose to solve a precursor to this question by unraveling the geometric structure of the product in $\mathcal{M}Sym$ as observed from the cellular projection β.

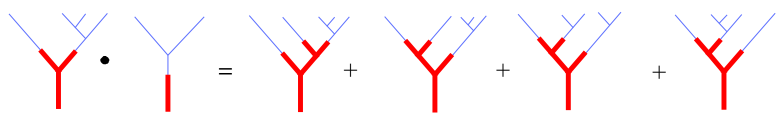
2.2. **A big commuting diagram of bileveled trees.** In [13] I introduced a new sequence of polytopes which are simultaneously quotients of the multiplihedra and categorified versions of the associahedra. The former is seen by forgetting tree structure in the upper portion of a bi-leveled tree; the latter is due to the fact that these new *composihedra* parameterize enrichment of categories. In fact, several authors had in the past assumed that the composihedra *were* the associahedra. Their mistake came in part due to the fact that the associahedra are indeed the result of forgetting tree structure of the lower level of the bi-leveled trees.

Since that paper, we have realized several additional polytope sequences exist whose terms' vertices correspond to forgetting ordering and or tree structure of the two levels at different times. When upper and lower tree structure is forgotten, what remains is a picture of a composition, that is, a vertex of a cube. Figure 2 is a pair of commuting diagrams, one showing examples of an ordered tree and all its simpler images, and the second showing the corresponding polytopes in 3d.

Each sort of tree promises to be a basis element of a new graded algebra; subalgebras of $\mathfrak{S}Sym$ which are either containing or contained within $\mathcal{M}Sym$. The main question that is begging for attention here is:

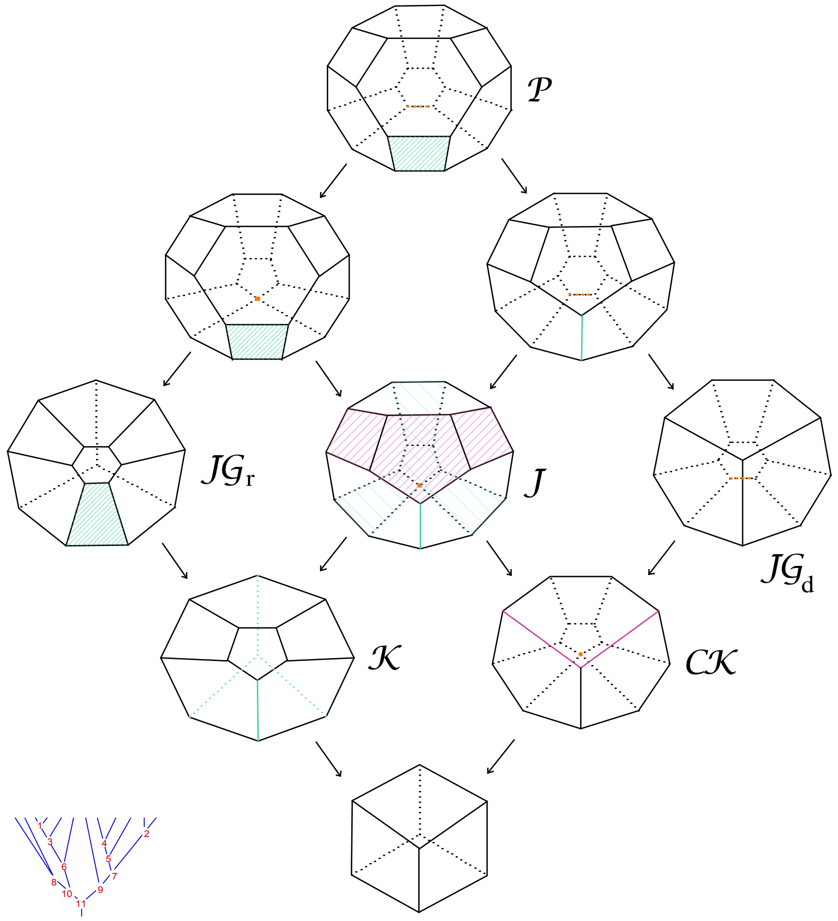
Question 2.2. *What relationships exist between the classic Hopf algebras $\mathcal{Y}Sym$ and $\mathcal{Q}Sym$ and our new algebras that use the same bases?*

2.3. **The classic polytopes part 2: painted trees.** In the process of writing the recent papers [14] and [16] we realized the existence of a new Hopf algebra based upon the vertices of the multiplihedra, but described via the pictures of painted trees. The coproduct is splitting of trees as in $\mathcal{Y}Sym$, from leaf to root. Here is an example of the product:



In [3] the authors use Möbius inversion on the Tamari lattice of binary trees to describe the primitive elements of $\mathcal{Y}Sym$.

Question 2.3. *We would like to find a nice description of the algebra of painted trees based on $\mathcal{Y}Sym$, including a characterization of primitive elements of the painted trees. Is there a sublattice of the multiplihedron whose Möbius inversion will provide a simple characterization of the space of primitives?*



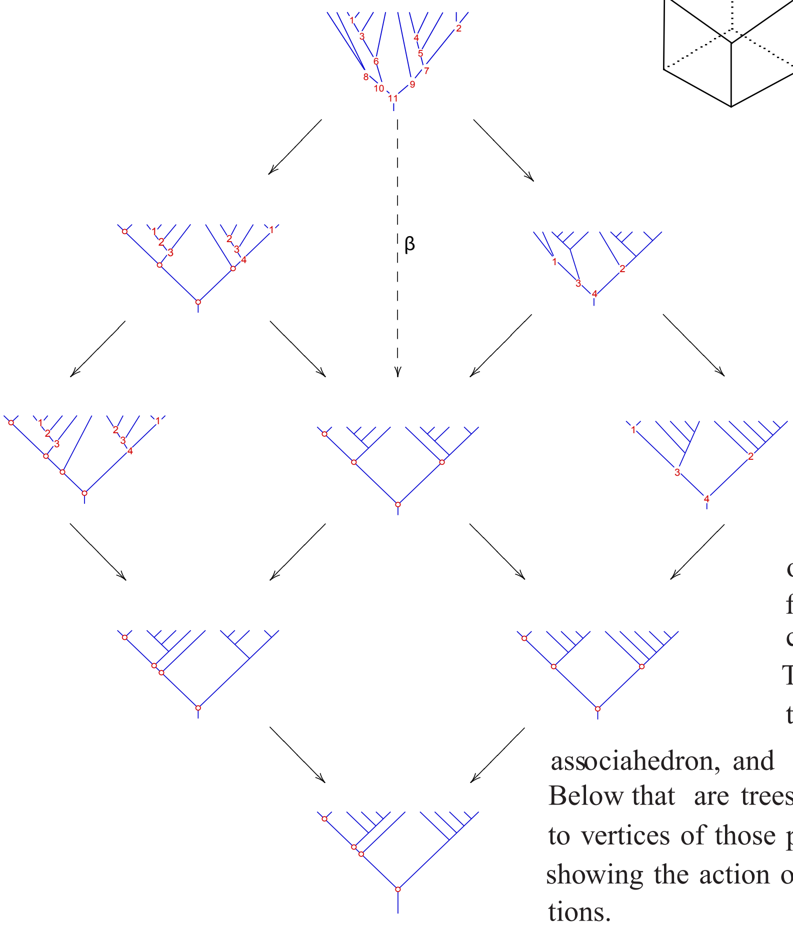


Figure 2.

On the top is a commuting diagram of polytopes in 3 dimensions, from the permutohedron to the cube. The multiplihedron is in the middle, $\mathcal{K}$ is the associahedron, and $\mathcal{CK}$ is the composihedron. Below that are trees corresponding to vertices of those polytopes (in ten dimensions) showing the action of the surjections.

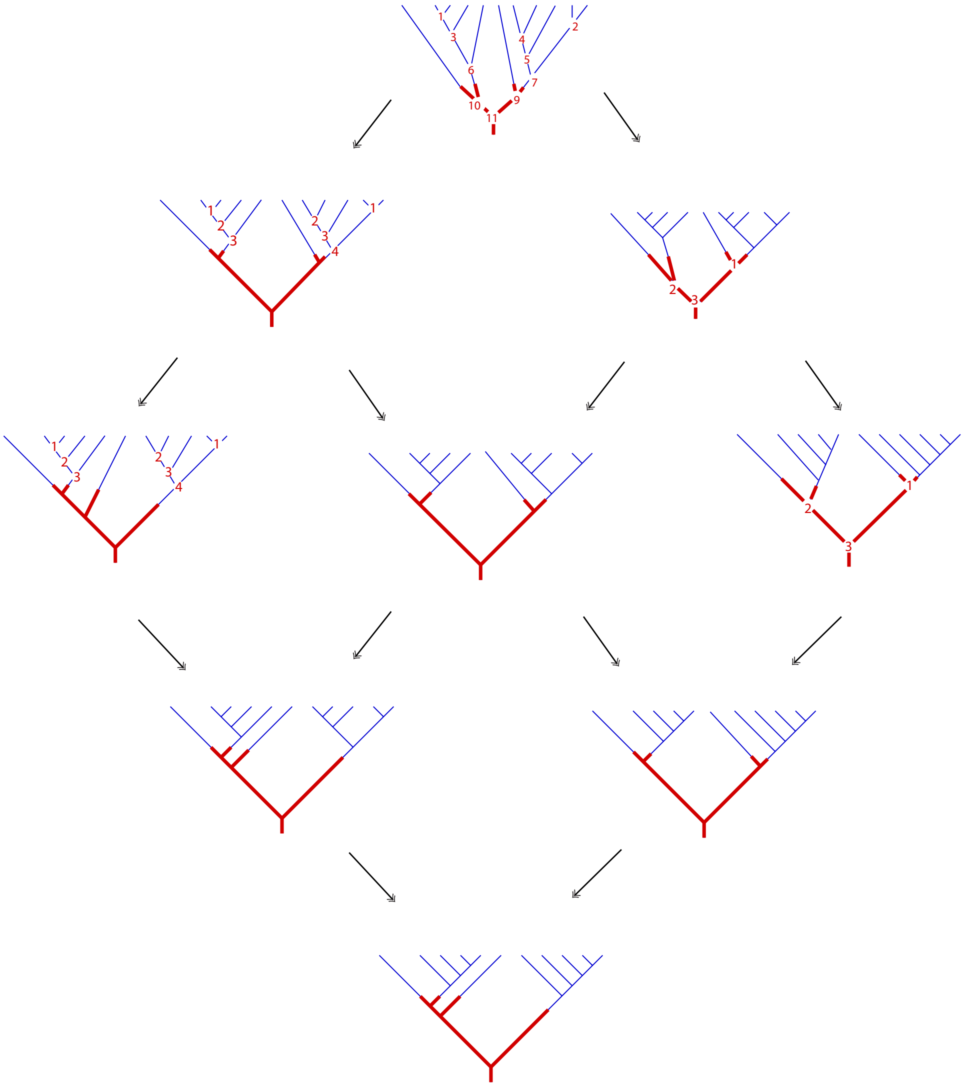


FIGURE 3. These trees correspond to the same vertices of polytopes (in ten dimensions) as the trees shown in Figure 2, but each of these allow us to describe Hopf algebras.

The preceding is a question for which we know the answer. In our forthcoming paper [15] we will show that there is a way to compose two coalgebras $\mathcal{C}$ and $\mathcal{D}$ in the style of an operad to get a new coalgebra $\mathcal{C} \circ \mathcal{D}$ whose new primitives have a simple explanation in terms of the old. Not only the painted trees but a whole family of tree-like examples turn out to fit into this picture of *compositional coalgebras.* More importantly, the tree-like cases we discuss next are examples of *graded hopf operads,* that is, graded coalgebras which are simultaneously operads under the same grading. In [15] we will demonstrate that the graded Hopf operads and their modules turn out to be Hopf algebras and modules. Then we define a precise way in which a module coalgebra can cover a Hopf algebra, and predict even more structure for these *covering module coalgebras.* Here are two of the main theorems:

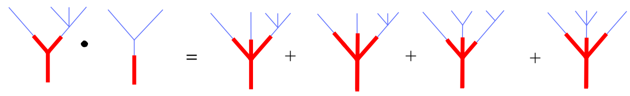
Theorem 2.4. *Let $\mathcal{D}$ be a graded Hopf operad and $\mathcal{C}$ a graded coalgebra. If there is a surjective coalgebra map $\tau : \mathcal{C} \to \mathcal{D}$ then both $\mathcal{E} = \mathcal{C} \circ \mathcal{D}$ and $\mathcal{E}' = \mathcal{D} \circ \mathcal{C}$ are covering module coalgebras over $\mathcal{D}$.*

Theorem 2.5. *A covering module coalgebra $\mathcal{E}$ over $\mathcal{D}$ has three additional structures: it is a Hopf module and a comodule algebra over $\mathcal{D}$; and it is a one-sided Hopf algebra with a one-sided unit.*

2.4. **The big commuting diamond of painted trees.** The bi-leveled trees of Figure 2 all have alternate representations, using painted tree versions with one less leaf. Figure 3 is the picture of the painted trees corresponding precisely to the ones in the same positions as in Figure 2.

Each of these new families of trees provides the basis for a graded Hopf algebra. Here is the new sort of product, using corollas rather than combs, and demonstrated on compositions.

$F_{13} \bullet F_2 =$

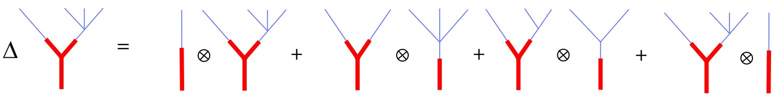


$$F_{113} \quad + F_{113} \quad + F_{122} \quad + F_{131}$$

The coproduct is the usual splitting of trees:

$\Delta\ F_{13} \quad =$

Δ



$$= F_1 \otimes F_{13} \quad + F_{11} \otimes F_3 \quad + F_{12} \otimes F_2 \quad + F_{13} \otimes F_1$$

This implies all new Hopf algebra structures on the familiar polytopes: permutohedra, associahedra and cubes. In [15] we show how the new coalgebras are formed by composing pairs of the old. Then we predict the new Hopf structure based on operad and operad action characteristics. Finally the cellular projections (different from the Tonks projection!) that are induced are shown to preserve algebraic structure. In the next stage of research we ask for further cause effect relationships:

Question 2.6. *How does the convex polytope geometry of our new algebras predict algebraic structure? Are there differential graded Hopf superalgebras based on the faces of the polytopes? What is the Hopf algebraic significance of the fact that the facet-inclusion operad of associahedra contains a suboperad of binary trees?*

3. Graph associahedra and cellular projections.

In [6] and [10] Carr and Devadoss show that for every graph G there is a unique convex polytope $\mathcal{K}_G$ whose facets correspond to connected induced subgraphs. I first suspected the existence of new algebras based on $\mathcal{K}_G$ after my discovery (published in [17]) that the Tonks projection from the permutohedron to the associahedron can be factored through a series of graph-associahedra. This fact is simple to demonstrate; it follows from Devadoss's discovery that the complete graph-associahedron is the permutohedron while the path graph-associahedron is the Stasheff polytope. Thus by deleting edges of the complete graph one at a time, we describe a family of quotient cellular projections. Figure 4 shows one of these. Our important result is that the cellular projections give rise to graded algebra maps.

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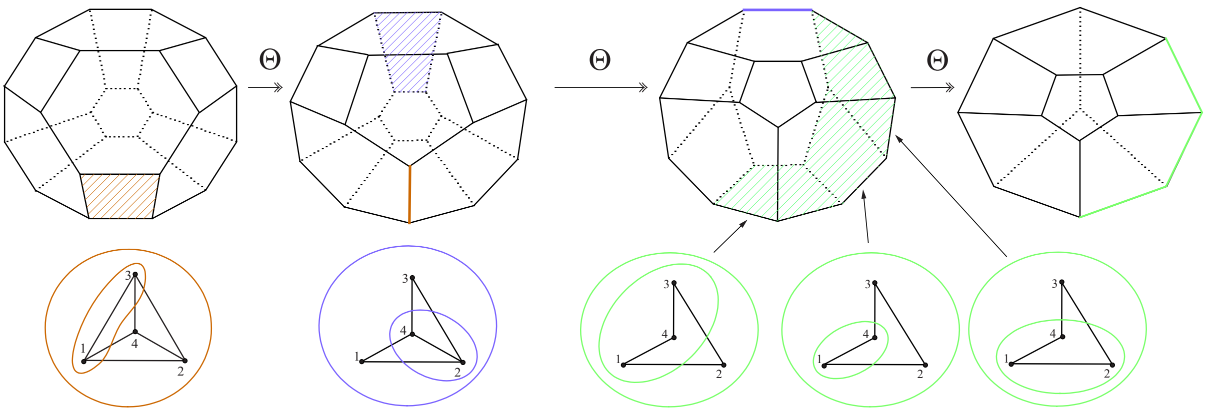


FIGURE 4. A factorization of the Tonks projection through 3 dimensional graph associahedra. The shaded facets correspond to the shown tubings, and are collapsed as indicated to respective edges. The first, third and fourth pictured polytopes are above views of $\mathcal{P}_4, \mathcal{W}_4$ and $\mathcal{K}_4$ respectively.

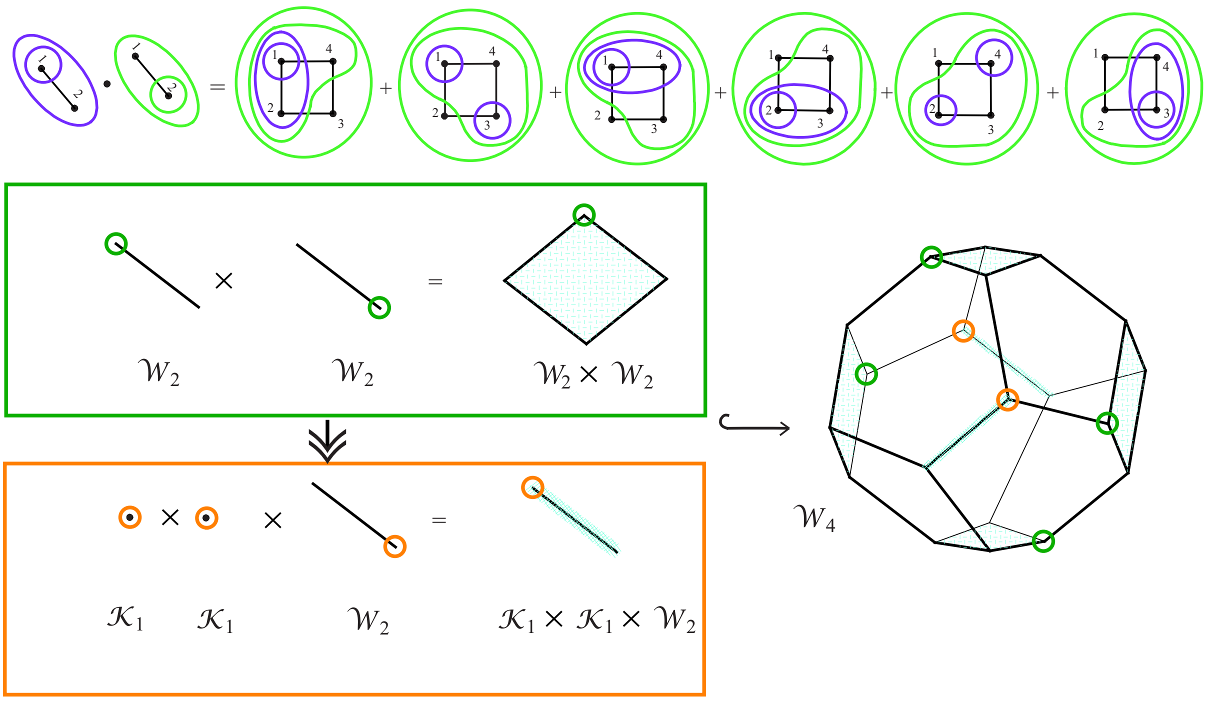


FIGURE 5. The theme of [17] is that the product of two faces, here from terms $\mathcal{W}_i$ and $\mathcal{W}_j$ of the cyclohedra, is described as a sum of faces of the term $\mathcal{W}_{i+j}$. The summed faces in the product are the images of maps which embed cartesian products of earlier terms of $\{\mathcal{W}_n\}$, composed with our new extensions of the Tonks projection.

3.1. **New algebras and modules: cyclohedron and simplex.** In our recent paper [17] we demonstrate associative graded algebra structures on the vertices of the cyclohedra and simplices, denoted $\mathcal{W}Sym$ and ΔSym. We also extend this structure to the full poset of faces. Figure 5 shows the product of a pair of vertices in the cyclohedron.

The number of faces of the n-simplex, including the null face and the n-dimensional face, is 2^n. By adjoining the null face here we thus have a graded algebra with n^{th} component of dimension 2^n. A fascinating convergence now appears.

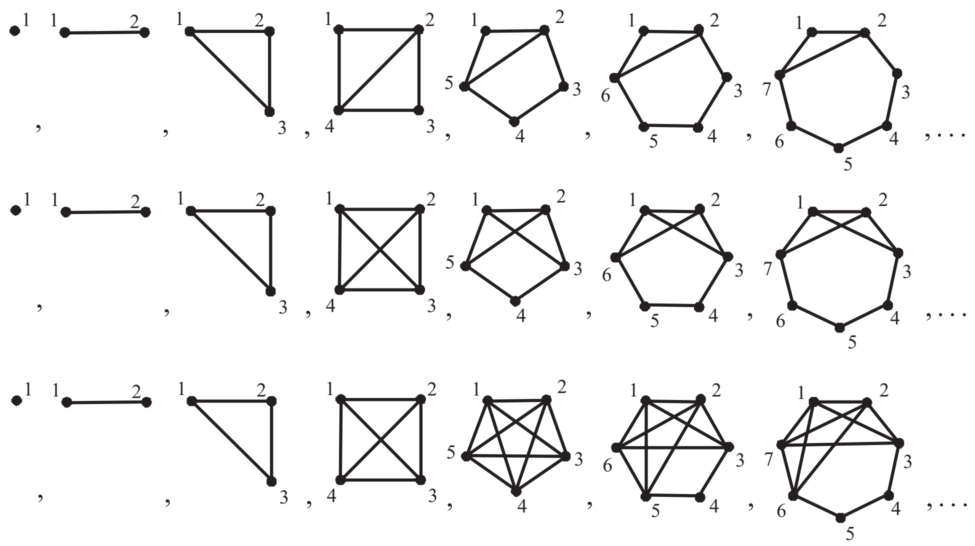
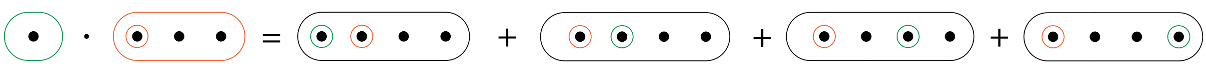


FIGURE 6. Hereditary graph sequences.

Conjecture 3.1. *The Hopf algebra of simplex faces $\Delta\tilde{Sym}$ is isomorphic to the algebraic opposite of the algebra of compositions with the painted tree product.*

The proof of this soon-to-be theorem will be in [15]. Here is an example; compare this with the example in section 2.4 by using the bijection between subsets $\{a, b, \dots c\} \subset [n]$ and compositions $(a, b-a, \dots, n+1-c)$ of $n+1$.

$$F_{\emptyset} \bullet F_{\{1\}} =$$



$$= \quad F_{\{1,2\}} + F_{\{1,2\}} + F_{\{1,3\}} + F_{\{1,4\}}$$

3.2. **More new algebras: filtering $\mathfrak{S}Sym$.** Next is a description of how to construct a graded algebra which lies between $\mathfrak{S}Sym$ and $\mathcal{Y}Sym$. First we need to define a sequence of graphs with numbered nodes, indexed by the number of nodes in each graph. The recursive property which they minimally must possess is as follows:

Definition 3.2 (**Hereditary graph sequence**)**.** *Given a graph G_n in our sequence, and any one of its nodes: the reconnected complement of G_n with that node deleted and with the inherited numbering of nodes must have as a subgraph the term G_{n-1} of our sequence. Figure 6 shows several examples.*

Conjecture 3.3. *The vertices of a polytope sequence $\mathcal{K}_{G_i}$ for $\{G_i\}$ a hereditary graph sequence form the basis of a subalgebra of $\mathfrak{S}Sym$.*

The product of two basis elements is performed in an analogous way to the product in $\mathfrak{S}Sym$ (and $\mathcal{W}Sym$). Figure 7 shows a partial example. The definition of hereditary graph sequence is designed to ensure that the product is well-defined. We have examples of this conjecture in the form of $\mathcal{Y}Sym$, $\mathcal{W}Sym$ and ΔSym. The proof of associativity rests upon a straightforward demonstration of the following fact:

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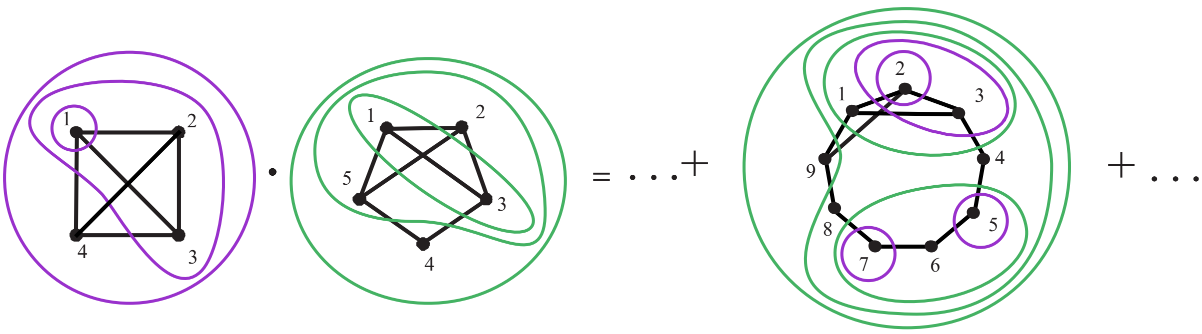

FIGURE 7. One term in a product of graphs from a hereditary sequence.

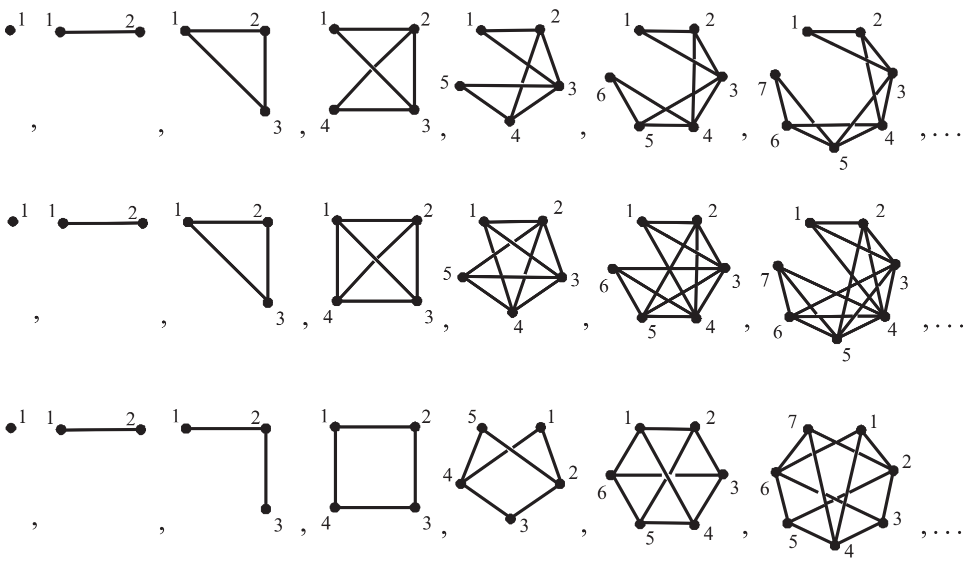

FIGURE 8. Restrictive graph sequences.

Conjecture 3.4. *The generalized Tonks projection from the permutohedra to a sequence $\mathcal{K}_{G_i}$ for a hereditary graph sequence is an algebra homomorphism.*

There is a lot to investigate here. From the examples in Figure 6 we conjecture that there is an infinite filtration of the algebra $\mathfrak{S}Sym$ based on incrementally increasing the connectedness of the early graphs in the hereditary sequence. The first algebra in the filtration is $\mathcal{Y}Sym$ and the second is $\mathcal{W}Sym$.

3.3. **New Coalgebras: another filter of $\mathfrak{S}Sym$.** We consider another class of sequences of graphs where G_n has numbered nodes $\nu_1, \ldots, \nu_n$.

Definition 3.5 (**Restrictive graph sequence**). *Given a graph G_n in our sequence: the induced subgraph of $G - \nu_n$ and the induced subgraph of $G - \nu_1$ both equal the term G_{n-1} of our sequence. Figure 3.3 shows examples.*

Conjecture 3.6. *The vertices of a polytope sequence $\mathcal{K}_{G_i}$ for $\{G_i\}$ a restrictive graph sequence form the basis of a subcoalgebra of $\mathfrak{S}Sym$.*

The coproduct of a basis element is performed in an analogous way to the coproduct in $\mathfrak{S}Sym$. Figure 9 shows an example. The definition of restrictive graph sequence is

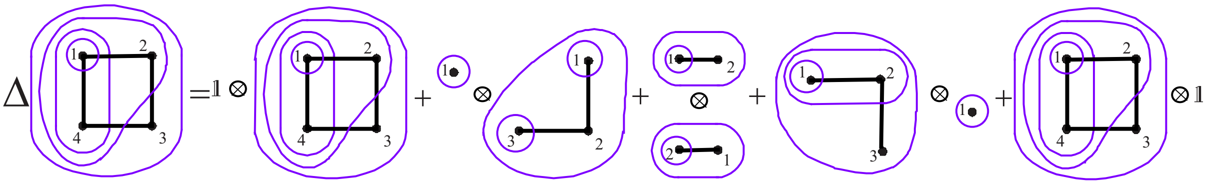

FIGURE 9. A coproduct in a restrictive sequence coalgebra.

designed to ensure that the coproduct is well-defined. The proof of coassociativity rests upon a straightforward demonstration of the following fact:

Conjecture 3.7. *The generalized Tonks projection from the permutohedra to a sequence $\mathcal{K}_{G_i}$ for a restrictive graph sequence is a coalgebra map.*

From the examples in Figure 3.3 we conjecture that there is an infinite filtration of the coalgebra $\mathfrak{S}Sym$ based on incrementally increasing the connectedness of the early graphs in the restrictive sequence. Again the first coalgebra in the filtration is $\mathcal{Y}Sym$.

3.4. **Face algebras.** As usual, we conjecture that the algebras and coalgebras based upon the graph associahedra for hereditary and restrictive graph sequences may be enlarged to respective structures on the faces of the polytopes.

3.5. **Investigative strategies.**

3.5.1. *Lattices.* One can represent the elements of the symmetric groups in multiple ways. Classically these pictures have allowed lattices such as the Tamari order on binary trees and the Boolean posets to be seen as projections of the weak order on symmetric groups. We have uncovered several new poset structures on the skeletons of the graph associahedra. Given a numbering of the nodes of a graph we define the *ordered graph lattice*. 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. Figure 10 shows an example.

Conjecture 3.8. *The 1-skeleton of each graph associahedron is a quotient lattice of the weak order on the symmetric group.*

Of course the projection map we have in mind is the generalized Tonks projection restricted to vertices. The answer to the following question will have important ramifications to finding Möbius inversion.

Question 3.9. *Do the generalized Tonks projections from $\mathfrak{S}_n$ to our new lattices form lattice congruences or interval retracts?*

3.5.2. *Möbius inversion.* By performing Möbius inversion on the elements of our basis, with respect to the various lattices, we can find a new basis for the algebra or coalgebra. As mentioned above, this new basis can prove to be perfect for describing primitives or finding structure constants. In [16] we show that the existence of an interval retract between our lattice and the weak order on $\mathfrak{S}_n$ implies a formula for the Möbius function.

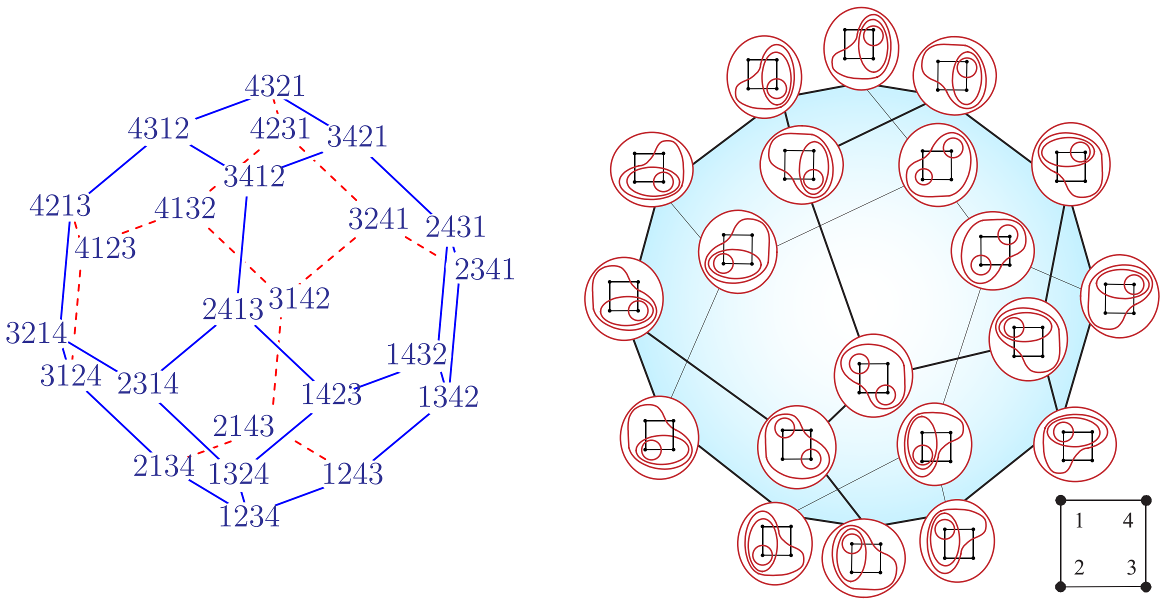

FIGURE 10. On the left is the 1-skeleton of the permutohedron demonstrating the weak order on $\mathfrak{S}_4$. On the right is the 1-skeleton of the cyclohedron, seen as a lattice of graph tubings. Möbius inversion on this lattice gives a new basis for the corresponding noncommutative graded algebra. Notice that the new poset structure is different than Reading's Cambrian lattice on the same set [28].

3.5.3. *Generating functions and group actions.* Generating functions have recently been discovered for many of the combinatorial sequences involved in our research. In [25] Postnikov, Reiner and Williams uncovered the generating functions for the vertices of many graph types, including cycles. I found the generating functions for the vertices of the multiplihedra and composihedra in [12] and [13]. These are useful both for finding dimension by counting basis elements and for existence theorems based on the fundamental theorem of Hopf modules.

Fellow researcher J.P. Cossey and students are currently looking at dihedral group actions on the catalan objects and their generalizations. We plan to consider algebraic interpretations of the orbits of those actions.

3.5.4. *Operads and Species.* Chapoton and Livernet [7] show 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 [30]. 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.

The Hopf algebra $\mathcal{Y}Sym$ has been fit into the construction of Moerdijk and Van der Laan, which builds Hopf algebras from operads [24],[31]. It seems very likely that this construction can be applied to operad bimodules in order to construct Hopf modules. We plan to investigate this possibility for several modules of the associahedra, including the cyclohedra (as described by Markl [23]), the multiplihedra and the composihedra.

Finally, our graded Hopf operads and modules use a specialization of the composition product of species. We plan to look for connections to the Hopf algebras of species, (including Postnikov's generalized permutohedra) studied by Marcelo Aguiar and collaborators.

4. Graph Multiplihedra: generalizing painted trees.

4.1. Graph multiplihedra and quotients. The idea of painted trees is not hard to apply in general to tubings on graphs. We refer to the result as *marked tubings*. We completed an initial study of the resulting polytopes, dubbed *graph multiplihedra* $\mathcal{J}_G$, published as [9]. That paper also describes the quotients of the graph multiplihedra which generalize the composihedra, and the corresponding quotients which arise from forgetting the tube structure within the painted region. Examples for the case of the edgeless graph on three nodes are seen in the central lower four maps of Figure 12. Since then, a pair of new revelations has revealed the complete analogy to the classic multiplihedron structure.

4.1.1. *Generalizing the Saneblidze-Umble map.* Recall that Saneblidze and Umble described a cellular surjection β from the permutohedra to the multiplihedra in [29], and that this map was used to transfer the algebra structure of $\mathfrak{S}Sym$ to that of $\mathcal{M}Sym$ in [14] and [16].

Since the permutohedra are precisely the graph multiplihedra of the complete graphs, there is automatically a cellular surjection from $\mathfrak{S}_n$ to any $\mathcal{J}_G$ for graph G on n nodes. The map is described by deleting edges. At each deletion we create the induced marked tubing, and at the end of the process we have a marked tubing of the graph G. Figure 11 demonstrates this process.

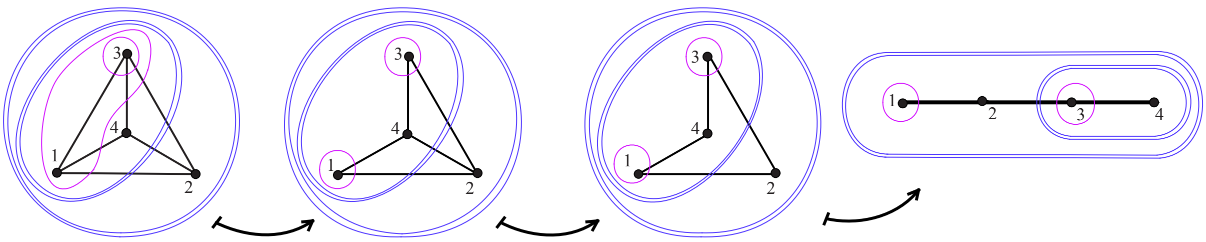

Figure 11. The surjection β factored. The corresponding cellular projections are of 4-dimensional polytopes.

Immediately this description of the Saneblidze-Umble projection suggests that there are a series of Hopf module algebras filtering the Hopf algebra of permutations, and which contain the Hopf module of painted trees. These have bases made up of the maximal marked tubings of the graphs in the restrictive and hereditary sequences described earlier.

4.1.2. *Special Factoring: edge deletion by tube marking.* The 3-dimensional case of the map β is shown factored in the top portion of Figure 2. There is an analogous picture for any graph. Thus for any of the generalized Saneblidze-Umble projections from $\mathcal{P}_n$ to $\mathcal{J}_G$ we can describe a factoring that is distinct from the one in Figure 11. In that figure we delete some edges and the projection equates two marked tubings which yield the same induced tubing after the deletion. With a certain set of edges in mind for deletion, we can factor the entire projection by first equating the tubings that originally differed only within thick tubes, and then equating the tubings that differed only in thin tubes. Or we could factor in the other order. For an example of the two options see the top four maps of Figure 12. Of course the plan is for students to study the algebraic structure of these new polytopes.

Conjecture 4.1. *Given a hereditary (respectively restrictive) sequence of graphs, the faces of corresponding polytopes at any one of the nine locations of the commuting diagram exemplified in Figure 12 form the basis of a graded algebra (respectively graded coalgebra.) In addition the new polytopes all have lattice structures on their 1-skeleta which generalize the Tamari lattice.*

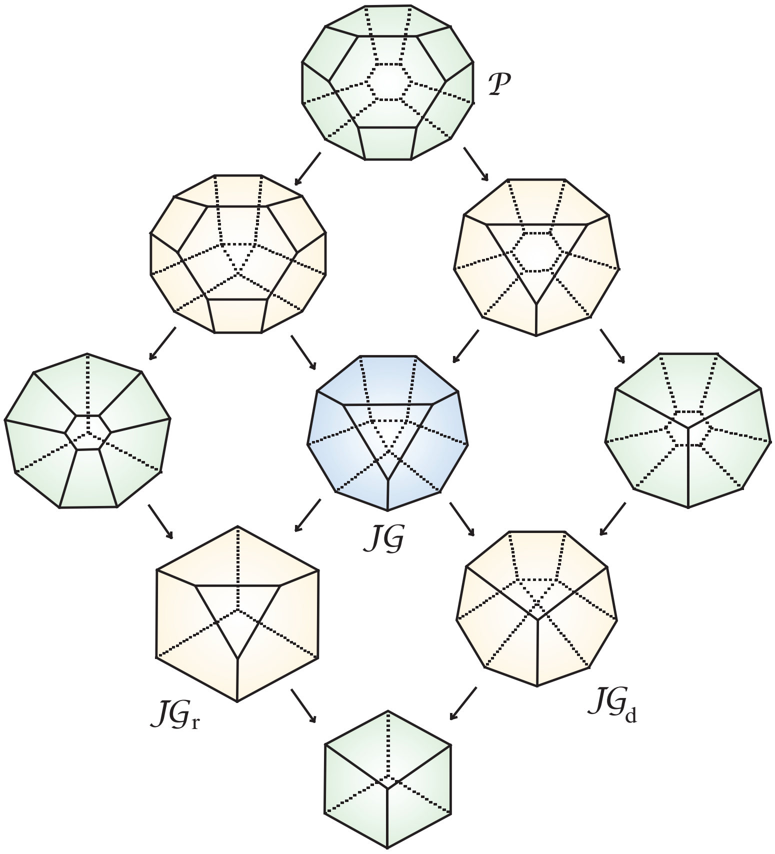

FIGURE 12. The commuting diamond of polytopes for G the edgeless graph on three nodes.

5. PSEUDOGRAPHS AND CW-COMPLEXES: NEW POLYTOPE SEQUENCES.

5.1. **Pseudograph associahedra.** The number of redundant edges in a pseudograph is the number of edges which would need to be removed to make it a simple graph. We dicovered a generalization of associahedra to pseudographs, simply by defining a tube to be any connected subgraph containing at least one of the edges between each of its pairs of nodes. In the recently submitted [5], a collaboration with Mike Carr and Satyan Devadoss, we have found that these polytopes are simple and have dimension $= n - 1 + |\{redundant\ edges\}|$, where n is the number of nodes. Figure 13 shows some examples in 3d.

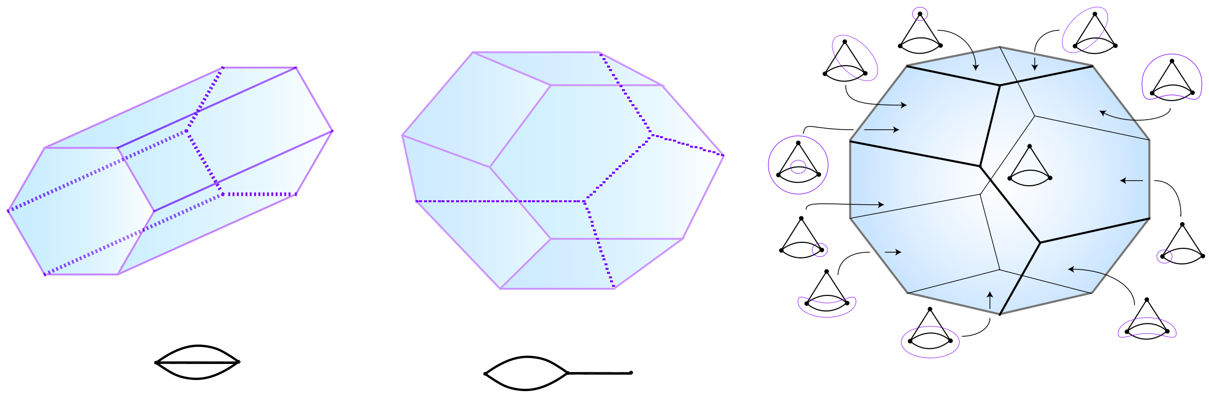

FIGURE 13. Several pseudograph associahedra. The third is shown with labeled facets, and the reader may reconstruct the others in similar fashion.

5.1.1. *Discrete geometry.* We, especially collaborator Mike Carr, have discovered a method of truncation which yields the pseudograph associahedron. The main purpose of this tool will be its use in gaining understanding of the recursive nature of the polytopes. I have proven that $\mathcal{K}_G$ for G the graph with two nodes and n edges is equivalent to $\mathcal{P}_n \times [0,1]$.

We answer the first of the following pair of questions in [5]:

Question 5.1. *How can we characterize facets of a pseudograph associahedron in terms of cartesian products of smaller pseudograph associahedra? What sort of generalized operad structure does this exemplify?*

We believe that the answer to this is crucial to a full understanding of the algebraic nature of these polytopes. From observations of how the products in $\mathfrak{S}Sym, \mathcal{W}Sym, \mathcal{Y}Sym$ and ΔSym depend on the recursive stucture of the polytopes, the answer to this question should clarify which sequences of pseudograph support algebras and coalgebras. Another route to better understanding lies in finding how they fit into the picture of generalized permutohedra developed by Postnikov and Zelevinsky. Graph-associahedra are examples of Postnikov's *nestohedra*, and the collection of tubings on a graph exemplify a *nested set* [26]. In fact, more specifically they are *graphical nested sets* as defined by Zelevinsky [32].

Conjecture 5.2. *The face posets of pseudograph associahedra are (generalized) graphical nested sets, and the pseudograph associahedra themselves are nested polytopes.*

This conjecture is plausible in light of Proposition 6.4 of [32]: Every two-dimensional face of the nested polytope is a d-gon for $d \in \{3, 4, 5, 6\}$. However, the the set of tubes of a pseudograph do not form in general a building set, so the definition of nested set will have to be generalized to encompass *multi-buildings*. If two elements of the multi-building intersect then there is another element of the building which contains their union.

5.1.2. *Hopf algebras.* There are several sequences of pseudograph associahedra that we can immediately use to construct graded Hopf algebras. They are found simply by adding redundant edges to the path graphs and complete graphs, as shown in Figure 14. Recall that the path graph associahedron is the classic associahedron, the basis for $\mathcal{Y}Sym$. We have a proof that the pseudograph associahedron for the graph with two nodes and n multiedges is a prism on the n^{th} permutohedron. Therefore we are compelled to ask:

Question 5.3. *What sort of combination of $\mathcal{Y}Sym$ and $\mathfrak{S}Sym$ is described by the Hopf algebras based on the multi-path graphs?*

An example of the multiplication of basis elements in a multipath Hopf algebra is in Figure 15.

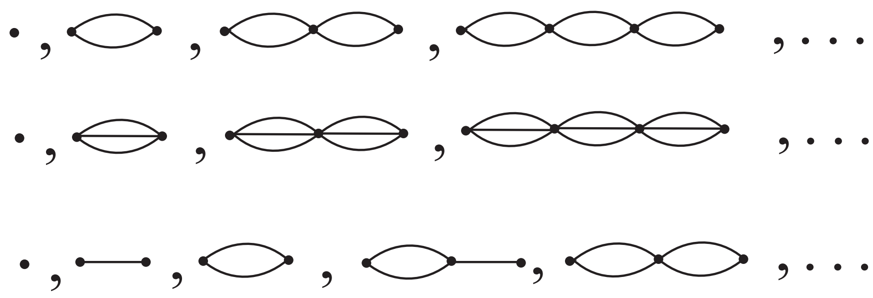

FIGURE 14. Some sequences of pseudographs which support new Hopf algebras (the first two) and a coalgebra.

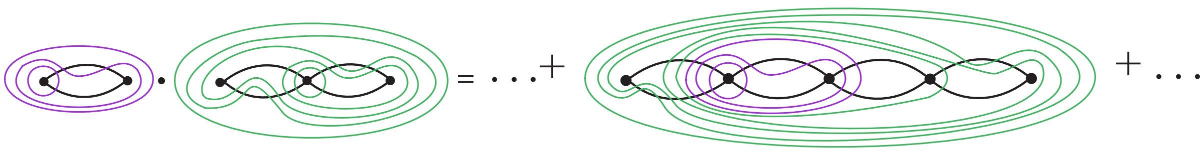

FIGURE 15. One term in the multiplication.

5.1.3. *Graded algebras and coalgebras.* Again we can immediately describe new graded algebras and coalgebras by adding redundant edges to the graph sequences that support graph associahedra algebras and coalgebras. In addition, there are new coalgebras that may be described using new sequences of pseudographs such as the third sequence pictured in Figure 14.

5.2. **Pseudographs with loops.** When the pseudograph is allowed to have loops (which are counted as redundant edges) then the associahedron is no longer a convex polytope. Rather we have proven that the geometry is that of a polytopal cone. The dimension is as expected: the associahedron for a pseudograph with n nodes and m redundant edges including loops is $n + m - 1$. We have some preliminary results. For instance, the pseudograph-associahedron of a single node graph with n loops is equivalent as a CW-complex to the quotient of the pseudograph-associahedron of a two-node graph with n multiedges under identification of the two facets which correspond to its two trivial tubes.

5.3. **Cell-complex associahedra.** For each sphere S^k of any dimension contained in a CW-complex X, we count the number of higher dimensional cells attached by their boundary along that sphere and define the number of *redundant cells* to be one less than the total.

Definition 5.4. A tube T of X is a set of cells which span a connected subcomplex, such that for every set of dimension k-cells in T which form a copy of the k-sphere S^k, T includes at least one of the $(k+1)$-cells whose boundary is that copy of S^k.

Two compatible tubes are either nested or far apart. That is, T is compatible with T' if $T \subset T'$ or if the two are disjoint and not connected by any 1-cell. A tubing of X is a set of compatible tubes. Tubings are partially ordered by inclusion. For any CW-complex X, the corresponding CW-complex associahedron $\mathcal{K}_X$ is the polytopal cone whose face poset is isomorphic to the poset of tubings on X.

Conjecture 5.5. *In the experiments we have performed, for X a CW-complex with n 0-cells and m redundant cells, and all attaching maps homotopically nontrivial, the associahedron $\mathcal{K}_X$ is a convex polytope with dimension $n+m-1$. If there are p homotopically trivial attaching maps, then $\mathcal{K}_X$ will be a polytopal cone with dimension $n+m+p-1$.*

Example 5.6. Consider the *k-globular* cell complex G homeomorphic to S^k. It has two 0-cells (a copy of S^0), two 1-cells attached to that 0-sphere, two 2-cells attached to the resulting 1-sphere, and so on up to two k-cells. The polytope K_G is the $(k+1)$-dimensional cube. Note that the cell complex G' formed from G by the attachment of one more $(k+1)$-cell to make a $k+1$-dimensional disk also has $\mathcal{K}_{G'}$ the $(k+1)$-cube.

Example 5.7. Figure 16 shows a facet of a four dimensional CW-complex associahedron.

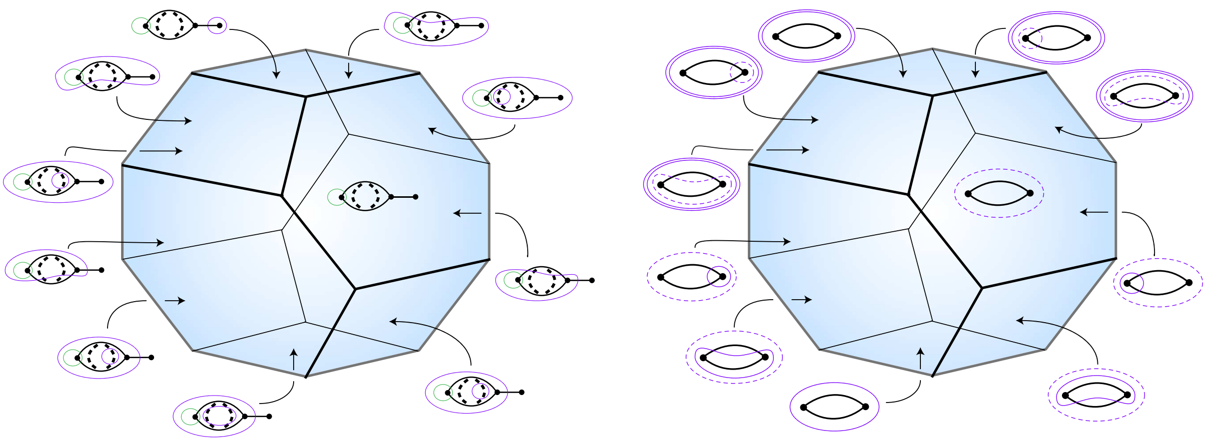

FIGURE 16. On the left is a single facet in the associahedron for the shown CW-complex. The CW-complex is constructed from three nodes, three edges, and then two disks (shown as dashed curves) attached to the copy of S^1. The facet corresponds to the singleton tube of the leftmost node. On the right, the same polytope appears as a pseudograph multiplihedron.

The first example of an algebraic structure will come from CW-complexes made by gluing together a string of globular cell complexes of homogenous dimension to form globular paths.

Question 5.8. *Does the sequence of k-globular paths (whose n^{th} term has n 0-cells) give rise to a sequence of CW-complex associahedra whose vertices form the graded basis of a Hopf algebra combining the structures of $\mathcal{Q}Sym$ and $\mathcal{Y}Sym$?*

5.4. **Pseudograph and CW-complex multiplihedra.** The *pseudograph-multiplihedron* can be described simply by the poset of marked tubings on a pseudograph. A marked tubing is a set of compatible marked tubes of the pseudograph, with compatibility defined just as in [9]. An example is in Figure 16. We conclude with a conjecture and several questions germane to the existence of algebraic structures based on these objects.

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Conjecture 5.9. *In the experiments we have performed, for G a pseudograph with n nodes (loop free), the multiplihedron $\mathcal{J}_G$ is a convex polytope with dimension $n + |\{$ redundant edges $\}|$.*

Question 5.10. *Are the loop-free pseudograph multiplihedra convex polytopes, and if so, can we describe their facets recursively as cartesian products? When we allow loops, are the pseudograph multiplihedra polytopal cones?*

Question 5.11. *Are CW-complex multiplihedra realized as convex polytopes and polytopal cones? What is their facet structure?*

Question 5.12. *Are the range and domain quotients of pseudograph and CW-complex multiplihedra convex polytopes? Do the 1-skeletons of the pseudograph and CW-complex associahedra and multiplihedra form generalized Tamari lattices?*

6. Application

6.1. **Combinatorial chemistry.** 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 [18], [4]. 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 17 shows the five of these with 2 or fewer hexagons, including the one with zero hexagons.

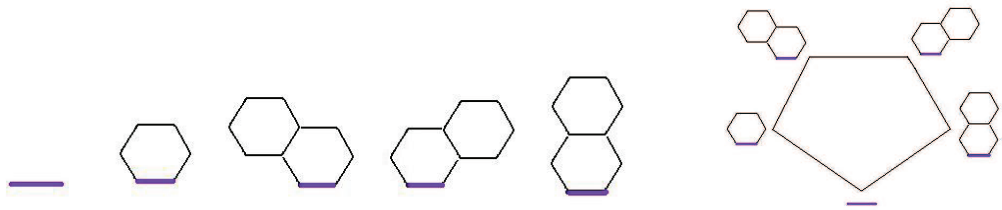

FIGURE 17. $\leq$ 2-cell rooted polyhexes; arranged around a composihedron.

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 17 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. See Figure 18 for examples.

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 [11]. 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.

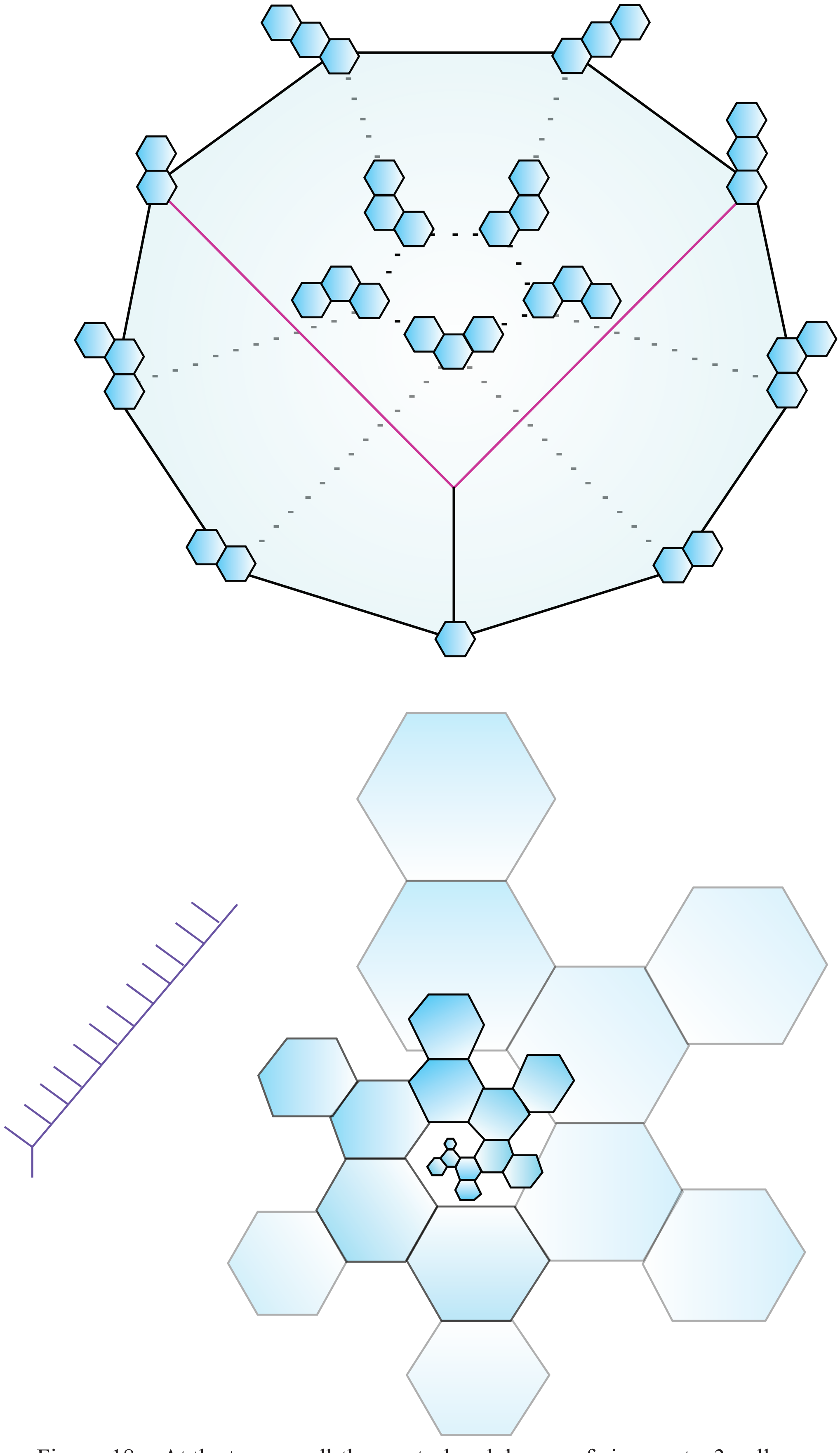

Figure 18. At the top are all the rooted polyhexes of size up to 3 cells, arranged on the composihedron CK(4). Just below them is a binary hex-tree and its associated polyhex.