Exhaustive generation of atomic combinatorial differential operators

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Abstract

Labelle and Lamathe introduced in 2009 a generalization of the standard combinatorial differential species operator D, by giving a combinatorial interpretation to $\Omega(X, D)F(X)$, where $\Omega(X, T)$ and $F(X)$ are two-sort and one-sort species respectively. One can show that such operators can be decomposed as sums of products of simpler operators called atomic combinatorial differential operators. In their paper, Labelle and Lamathe presented a list of the first atomic differential operators. In this paper, we describe an algorithm that allows to generate (and enumerate) all of them, subject to available computer resources. We also give a detailed analysis of how to compute the molecular components of $\Omega(X, D)F(X)$.

Keywords: enumerative combinatorics, species theory, molecular species, differential operator, algorithm

1. Introduction

Since its introduction by Joyal in 1981 [9], the theory of species of structures has a noticeable influence in a variety of fields including combinatorics, algebraic data types [16], and also for the generation of combinatorial structures, either random [5, 3] or exhaustive [12]. Many aspects have been developed and the theory remains an active research domain for which the reader can find a comprehensive account in the monography of Bergeron et al. [2].

One of its fundamental concepts is the notion of derivative of a species. Indeed, for any species F, the combinatorial interpretation of DF is well known: A DF-structure on a set U is simply a F-structure on the set $U \cup \{*\}$ where $*$ is an element not in U. In other words, a DF-structure is a F-structure with a

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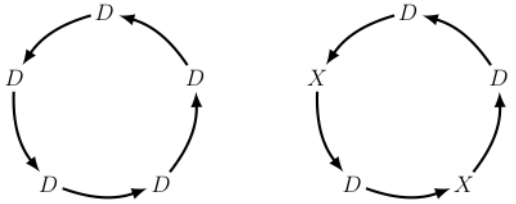
(a) (b)

Figure 1: (a) A DL_6-structure on the set $U = \{1, 2, 3, 4, 5\}$ where L_6 denotes the species of six elements lists. The placeholder element is represented as a white square ($\square$); (b) The differential operator D^n as a $L_n(D)$-structure.



(a) (b)

Figure 2: (a) The general differential operator $\mathcal{C}(D)$ as a $\mathcal{C}(D)$-structure; (b) A circular arrangement of operators D and singletons species X.

placeholder for one element as Figure 1a illustrates. Moreover, we have a good grip on the notion of D^nF, obtained from n successive applications of D on a species F. We often describe the differential operator D^n as a $L_n(D)$-structure, that is a n-list of operators D (see Figure 1b).

Joyal further developped this idea of graphical arrangements of the differential operator D by introducing in [10] a more general differential operator. It gives, for any species G, a combinatorial interpretation to a combinatorial operator denoted by $G(D)$. For example, Figure 2a illustrates the differential operator $\mathcal{C}(D)$ where $\mathcal{C}$ is the species of oriented cycles. But what combinatorial interpretation can one give to a circular arrangement of D's and X's as in Figure 2b?

Labelle and Lamathe answered this question in [11] (see also [13]) by introducing a generalization of the differential operator $G(D)$. For any two-sort species $\Omega(X, T)$, they defined a differential operator $\Omega(X, D)$, called generalized combinatorial differential operator. In the same manner as ordinary species, such operators can be decomposed as a sum of products of operators $X^m D^k/K$ called atomic combinatorial differential operators, where K is some suitable subgroup of $S_{m,k}$. They provide a partial list of all such operators for $m+k \leq 7$ (see also [4] for molecular species). The main purpose of this paper is to develop an algorithm which extends this list to include all atomic operators for $m + k \leq n$, $n \in \mathbb{N}$.

2. Preliminaries

A *species of structures* F is a functor $F : \mathbb{B} \longrightarrow \mathbb{B}$ from the category $\mathbb{B}$ of finite sets with bijections to itself. A number of combinatorial operations are defined

on species, namely addition, multiplication, cartesian product, composition and derivation. Those concepts can be extended to sets with k different sorts of elements. To denote one-sort and two-sort species, we use the notation $F(X)$ and $\Omega(X,T)$ for $k=1$ and $k=2$.

Molecular and atomic species play a very important role in the study of species. A species M is said to be *molecular* if and only if $M = F+G \Rightarrow F=0$ or $G=0$. In the same manner, a molecular species A is said to be *atomic* if and only if $A = FG \Rightarrow F=1$ or $G=1$.

One can show that any molecular species $M = M(X)$ is isomorphic to a species X^n/H, where H is a subgroup of S_n. This species is defined by setting for every finite set U

$$\frac{X^n}{H}[U] = \left\{\lambda H \mid \lambda : [n] \xrightarrow{\sim} U \text{ is a bijection}\right\}, \tag{1}$$

where $\lambda H = \{\lambda \circ h \mid h \in H\}$. One can then show that two molecular species X^n/H and X^m/K are isomorphic if and only if $n=m$ and H is conjugate to K in S_n. Similarly, any molecular two-sort species $M = M(X,T)$ is isomorphic to a species $X^m T^k/H$ where H is a subgroup of $S_{m,k}$. Here, $S_{m,k}$ denotes the Young subgroup of S_{m+k} permuting independently $\{1,2,\ldots,m\}$ and $\{m+1, m+2, \ldots, m+k\}$. Note that $S_{m,k} \simeq S_m \times S_k$ (see [15, 2] for more details).

For our purpose, we need a few important and useful results about products of two-sort molecular species.

Definition 2.1. *Let H and K be subgroups of S_{a_1,b_1} and S_{a_2,b_2} respectively. The subgroup $H * K$ of $S_{a_1+a_2,b_1+b_2}$ is defined by*

$$H * K = \{\omega = h * k \mid h \in H \text{ and } k \in K\},$$

where $h * k$ is the permutation obtained by the following shift operation on the four blocks of h and k:

$$\begin{array}{lll}
\textit{Block of size } a_1 \longrightarrow & \omega_1 \ldots \omega_{a_1} & = \quad h_1 \ldots h_{a_1} \\
\textit{Block of size } a_2 \longrightarrow & \omega_{a_1+1} \ldots \omega_{a_1+a_2} & = \quad a_1 + k_1 \ldots a_1 + k_{a_2} \\
\textit{Block of size } b_1 \longrightarrow & \omega_{a_1+a_2+1} \ldots \omega_{a_1+a_2+b_1} & = \quad a_2 + h_{1+a_1} \ldots a_2 + h_{b_1+a_1} \\
\textit{Block of size } b_2 \longrightarrow & \omega_{a_1+a_2+b_1+1} \ldots \omega_{a_1+a_2+b_1+b_2} & = \quad a_1 + b_1 + k_{1+a_2} \ldots a_1 + b_1 + k_{b_2+a_2}
\end{array}$$

Figure 3 illustrates this shift $(*)$ operation.

Example 2.2. If $h = 2\ 3\ 1\ 5\ 4 \in S_{3,2}$ and $k = 1\ 2\ 6\ 4\ 5\ 3 \in S_{2,4}$, then

$$h * k = 2\ 3\ 1\ 4\ 5\ 7\ 6\ 11\ 9\ 10\ 8 \in S_{5,6}$$

as Figure 4 illustrates.

Proposition 2.3. [2] *Let $X^{a_1}T^{b_1}/H$ and $X^{a_2}T^{b_2}/K$ be a pair of two-sort molecular species, where H and K are subgroups of S_{a_1,b_1} and S_{a_2,b_2} respectively. Then,*

$$\frac{X^{a_1}T^{b_1}}{H} \cdot \frac{X^{a_2}T^{b_2}}{K} = \frac{X^{a_1+a_2}T^{b_1+b_2}}{H * K}.$$

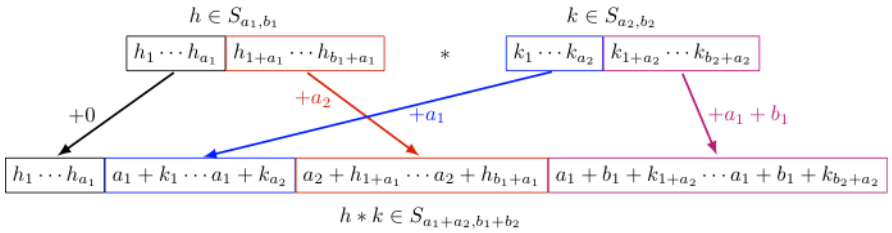


Figure 3: The definition of the shift performed on h and k to obtain $h * k$ in Definition 2.1.

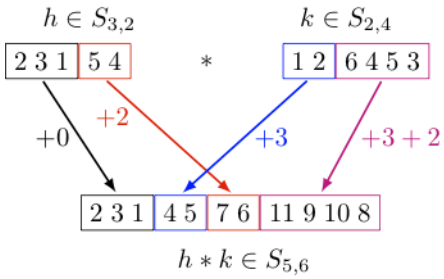


Figure 4: The result of $h*k$ with $h = 2\ 3\ 1\ 5\ 4 \in S_{3,2}$ and $k = 1\ 2\ 6\ 4\ 5\ 3 \in S_{2,4}$.

The cartesian product $H \times K$ can be identified to the group $H * K$ through the isomorphism $(h, k) \mapsto h * k$. From there, we deduce the following corollary, which is fundamental for the construction of the group $H * K$.

Corollary 2.4. *If H and K are generated by the sets $\{h_1, h_2, \ldots, h_p\}$ and $\{k_1, k_2, \ldots, k_q\}$ respectively, then $H * K$ is generated by the set*

$$\{h_1 * \mathrm{Id}_K, h_2 * \mathrm{Id}_K, \ldots, h_p * \mathrm{Id}_K, \mathrm{Id}_H * k_1, \mathrm{Id}_H * k_2, \ldots, \mathrm{Id}_H * k_q\}.$$

3. General combinatorial differential operators

In this section, we recall some of the key notions about general combinatorial differential operators [11]. First, recall that, for any species F, the *derivative of* F, denoted by DF, is the functor

$$DF : \mathbb{B} \longrightarrow \mathbb{B},$$

where, for any finite set U, $DF[U] := F[U^+]$ with $U^+ = U \cup \{*\}$ and where $*$ is an element chosen outside of U.

Example 3.1. Let L be the species of linear orders. Then $DL = L \cdot L (= L^2)$. Indeed, a DL-structure on a set U is a linear order on the elements of U, plus an outside element. This has the effect of "cutting" the DL-structure in two distinct linear orders.

As mentioned in the introduction, Labelle and Lamathe generalized Joyal's differential operators $G(D)$ by introducing more general differential operators of the form $\Omega(X, D)$ that rely on the so-called partial cartesian product and the operation of substitution $T := 1$.

Let $\Omega_1(X, T)$ and $\Omega_2(X, T)$ be a pair of two-sort species. The *partial cartesian product with respect to* T *of* Ω_1 *and* Ω_2 is the functor

$$\Omega_1(X, T) \times_T \Omega_2(X, T) : \mathbb{B} \times \mathbb{B} \longrightarrow \mathbb{B},$$

where, for any finite two-set (U, V) of sort X and T respectively, a $\Omega_1(X, T) \times_T \Omega_2(X, T)$-structure s is a pair $s = (s_1, s_2)$ where $s_1 \in \Omega_1[U_1, V]$ and $s_2 \in \Omega_2[U_2, V]$ with $U_1 \cup U_2 = U$ and $U_1 \cap U_2 = \varnothing$.

Let $G(X, T)$ be a two-sort species. The *substitution* $T := 1$ *in* G is the functor

$$G(X, 1) : \mathbb{B} \longrightarrow \mathbb{B},$$

(also denoted $G(X, T)|_{T:=1}$) whose structures are the $G(X, T)$-structures in which all elements of sort T are unlabelled.

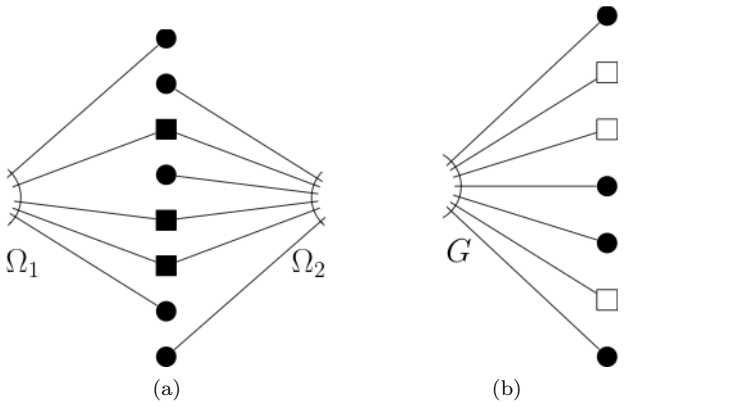


Figure 5: (a) A typical $\Omega_1(X, T) \times_T \Omega_2(X, T)$-structure. By convention, black circles represent labelled points of sort X and black squares represent labelled points of sort T; (b) A typical $G(X, T)|_{T:=1}$-structure. Unlabelled elements of sort T are represented as white squares.

Figure 5 illustrates the notions of partial cartesian product and substitution of a sort by 1. We can now state the definition of general differential operators.

Definition 3.2. *Let* $\Omega(X, T)$ *and* $F(X)$ *be two-sort and one-sort species respectively. One defines* $\Omega(X, D)F(X)$ *by*

$$\Omega(X, D)F(X) := \Omega(X, T) \times_T F(X + T) \mid_{T:=1} .$$

A typical $\Omega(X, D)F(X)$-structure is represented in Figure 6a. As before, labelled elements are represented as black points (•) and unlabelled ones as white squares (□).

Example 3.3. If one sets $\Omega(X,T) = T$, one obtains the ordinary differential operator D. The choice $\Omega(X,T) = \mathcal{C}(X+T)$ corresponds to the operator made of cyclic arrangements of D's and X's mentioned in the introduction. For example, recall that $\mathcal{C}$ is the species of cycles (i.e. circular permutations). Then, Figure 6b shows a typical $\mathcal{C}(X+D)F(X)$-structure on the underlying set $\{1,2,\ldots,9\}$, in conformity with Definition 3.2.

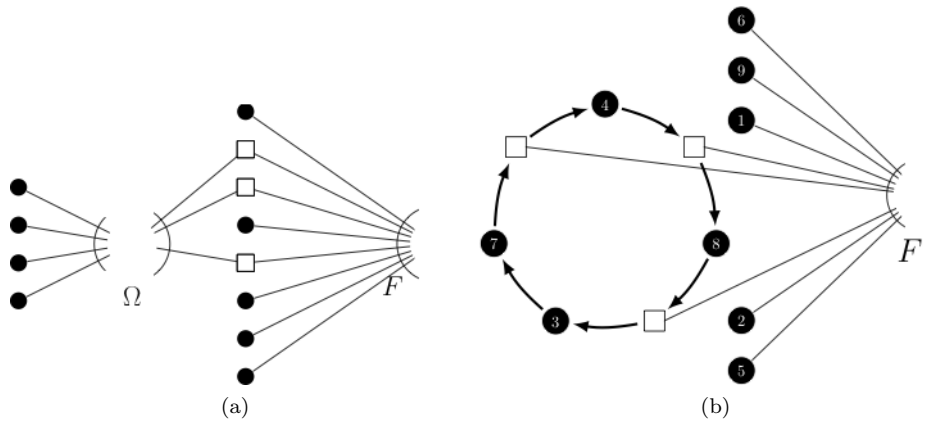


Figure 6: (a) A typical $\Omega(X,D)F(X)$-structure; (b) A $\mathcal{C}(X+D)F(X)$-structure on the underlying set $\{1,2,\ldots,9\}$.

Remark. For the operator $\Omega(X,D)$ to be defined, $\Omega(X,T)$ must be finitary in T, or $F(X)$ must be of finite degree in X. From now on, we assume this is always the case.

The notions of molecular and atomic species can be extended to molecular and atomic differential operators in the obvious way. Indeed, by definition, $\Omega(X,D)$ *is molecular* (resp. *atomic*) if and only if $\Omega(X,T)$ is molecular (resp. atomic).

It is well known that any ordinary one-sort species $F(X)$ can be written, in a unique way up to isomorphism, as a (possibly infinite) linear combination of one-sort molecular species,

$$F(X) = \sum_{H,n} f_H \frac{X^n}{H},$$

where H runs through a system of representatives of the conjugacy classes of subgroups of S_n and $f_H \in \mathbb{N}$ is the number of subspecies of F isomorphic to X^n/H. In the same spirit, any two-sort species $\Omega(X,T)$ can be written in a unique way, up to isomorphism, as a (possibly infinite) linear combination of

two-sort molecular species,

$$\Omega(X,T) = \sum_{K,m,k} \omega_K \frac{X^m T^k}{K},$$

where K runs through a system of representatives of the conjugacy classes of subgroups of $S_{m,k}$ and $\omega_K \in \mathbb{N}$ is the number of subspecies of Ω isomorphic to $X^m T^k/K$. Therefore, to compute $\Omega(X,D)F(X)$, one only needs to know how to compute

$$\frac{X^m D^k}{K} \frac{X^n}{H}. \tag{2}$$

In [11], Labelle and Lamathe stated a fundamental theorem which allows the effective computation of (2). However, only a sketch of the proof was given in their paper. Given its importance for our work, we now give a definition and a lemma that are useful for providing a more detailed proof.

Let A, B and C be finite groups and let $\omega_A : A \longrightarrow C$ and $\omega_B : B \longrightarrow C$ be homomorphisms. The *fibered product* (or *pullback*, see [1]) of A by B over C is the subgroup of $A \times B$, noted $A \times_C B$, defined by

$$A \times_C B = \{(a,b) \in A \times B \mid \omega_A(a) = \omega_B(b)\}.$$

The following lemma states that, to compute the molecular expansion of any species F, one only needs to consider the stabilizer of each element of the set of representatives of F-structures up to isomorphism.

Lemma 3.4. (Molecular expansion of $F(X,T)$ [2]) *Let $F(X,T)$ be any two-sort species. The molecular expansion of $F(X,T)$ is as follows:*

$$F(X,T) = \sum_{m,n \geq 0} \left\{ \sum_{s \Subset F[m,n]/S_{m,n}} \frac{X^m T^n}{\mathrm{Stab}(s)} \right\},$$

where $s \Subset F[m,n]/S_{m,n}$ means that s runs through a set of representatives of the structures on $[m,n] := (\{1,2,\ldots,m\},\{1,2,\ldots,n\})$ up to isomorphism.

We now state and prove the main result of this section.

Theorem 3.5. [11] *For any subgroups $H \leq S_n$ and $K \leq S_{m,k}$, we have*

(i) $\frac{X^m D^k}{K} \frac{X^n}{H} = \frac{X^m T^k}{K} \times_T \frac{(X+T)^n}{H} \mid_{T:=1}$,

(ii) $\frac{(X+T)^n}{H} = \sum_{k=0}^{n} \sum_{\omega \Subset S_{n-k,k}\backslash S_n/H} \frac{X^{n-k}T^k}{\omega H \omega^{-1} \cap S_{n-k,k}}$,

(iii) $\frac{X^a T^k}{A} \times_T \frac{X^b T^k}{B} = \sum_{\tau \Subset (\pi_2 A)\backslash S_k/(\pi_2 B)} \frac{X^{a+b}T^k}{A \times_{S_k} B^\tau}$,

(iv) $\left[\frac{X^a T^k}{A}\right]_{T:=1} = \frac{X^a}{\pi_1 A}$,

where $\omega \Subset S_{n-k,k}\backslash S_n/H$ means that ω runs through a system of representatives of the double cosets $H_1 \sigma H_2$, $\sigma \in S_n$; $\pi_i G = \{g_i \in S_{n_i} \mid (g_1,g_2) \in G\}$, $G \leq S_{n_1,n_2}$; $B^\tau = (\mathrm{Id},\tau)B(\mathrm{Id},\tau^{-1})$; $A \times_{S_k} B$ is the fibered product (pullback) of A by B over S_k.

Proof.

(i) Immediate by Definition 3.2.

(ii) Let $H \leq S_n$. Then, a X^n/H-structure ωH on $[n]$, where $\omega \in S_n$, can be viewed as a $(X+T)^n/H$-structure on $n-k$ elements, $1, 2, \ldots, n-k$, interpreted to be of sort X and k elements, $n-k+1, \ldots, n$, interpreted to be of sort T. Under this view, two such structures ωH and $\omega' H$ are isomorphic if and only if there exists a permutation $\sigma \in S_{n-k,k}$ such that $\sigma\omega H = \omega' H$. Equivalently, there exists $\sigma \in S_{n-k,k}$ and $h \in H$ such that ω' is in $\sigma\omega H$. That is, ω and ω' belong to the same double coset in $S_{n-k,k}\backslash S_n/H$. By virtue of Lemma 3.4, the summation must be taken over $\omega \in S_{n-k,k}\backslash S_n/H$. We conclude by noting that $\mathrm{Stab}(\omega H) = \{\sigma \in S_{n-k,k} \mid \sigma\omega H = H\} = S_{n-k,k} \cap \omega H \omega^{-1}$.

(iii) Let A and B be subgroups of $S_{a,k}$ and $S_{b,k}$ respectively. If $((\alpha_1, \tau_1)A, (\alpha_2, \tau_2)B)$ is a $X^a T^k/A \times_T X^b T^k/B$-structure, then

$$((\alpha_1, \tau_1)A, (\alpha_2, \tau_2)B) = (\alpha_1, \alpha_2, \tau_1)(A, (\mathrm{Id}, \tau_1^{-1}\tau_2)B).$$

This means that $((\alpha_1, \tau_1)A, (\alpha_2, \tau_2)B)$ and $(A, (\mathrm{Id}, \tau)B)$ are isomorphic structures. Furthermore, $(A, (\mathrm{Id}, \tau)B)$ and $(A, (\mathrm{Id}, \tau')B)$ are isomorphic if and only if there exists a permutation $(\alpha_1, \alpha_2, \omega) \in S_{a,b,k}$ such that

$$(A, (\mathrm{Id}, \tau')B) = (\alpha_1, \alpha_2, \omega)(A, (\mathrm{Id}, \tau)B).$$

That is, there exists $(\alpha_1, \alpha_2, \omega) \in S_{a,b,k}$ such that $(\alpha_1, \omega)A = A$ and $(\alpha_2, \omega\tau)B = (\mathrm{Id}, \tau')B)$. Equivalently, there exist ω in $\pi_2 A$ and in $\tau'(\pi_2 B)\tau^{-1}$, which means that $(\pi_2 A)\tau'(\pi_2 B) = (\pi_2 A)\tau(\pi_2 B)$. That is, τ and τ' belong to the same double coset $(\pi_2 A)\backslash S_k/(\pi_2 B)$. Hence, by virtue of Lemma 3.4, the summation must be taken over $\tau \in (\pi_2 A)\backslash S_k/(\pi_2 B)$. Finally, the stabilizer $\mathrm{Stab}((A, (\mathrm{Id}, \tau)B))$ of a structure is given by the set

$$\begin{aligned} & \{(\sigma_1, \sigma_2, \omega) \in S_{a,b,k} \mid (\sigma_1, \sigma_2, \omega)(A, (\mathrm{Id}, \tau)B) = (A, (\mathrm{Id}, \tau)B)\} \\ = \; & \{(\sigma_1, \sigma_2, \omega) \in S_{a,b,k} \mid (\sigma_1, \omega) \in A \text{ and } (\sigma_2, \omega) \in (\mathrm{Id}, \tau)B(\mathrm{Id}, \tau^{-1})\} \end{aligned}$$

which is canonically isomorphic to the group $\{((\sigma_1, \omega_1), (\sigma_2, \omega_2)) \in A \times B^\tau \mid \omega_1 = \omega_2\} = A \times_{S_k} B^\tau$.

(iv) Let s be a $X^a T^k/A$-structure, where $A = \mathrm{Stab}(s)$. Let s_1 be the $\left[X^a T^k/A\right]_{T:=1}$-structure associated to s by unlabelling all its underlying elements of sort T. Then, $\mathrm{Stab}(s_1) = \{\sigma_1 \in S_a \mid \exists \sigma_2 \in S_k, \;\; (\sigma_1, \sigma_2)s = s\} = \{\sigma_1 \in S_a \mid \exists \sigma \in A, \;\; \pi_1\sigma = \sigma_1\} = \pi_1 A$.

□

4. Generating all atomic differential operators

Theorem 3.5 provides a way to effectively compute, with the help of a computer algebra system, the result of the application of a molecular differential operator on a species. However, knowing that every species can be uniquely

decomposed as a sum of products of powers of atomic species, it is enough to consider only the atomic operators to study the effect of general combinatorial differential operators on species.

The aim of this section is to describe and study an algorithm, based on Proposition 2.3 and Corollary 2.4 above, that generates all atomic operators $X^m D^n/H$, for m and n given. Before stating it, recall first that the set of partitions of $\{1, 2, \ldots, m\}$ forms a complete lattice whose minimum element is the "finest" partition $\{\{1\}, \{2\}, \ldots, \{m\}\}$ and maximum element is the "coarsest" partition $\{\{1, 2, \ldots, m\}\}$. Given partitions $p_1, p_2, \ldots, p_k$, $\inf(p_1, p_2, \ldots, p_k)$ is defined as the coarsest partition which is finer than each of the p_i's and $\sup(p_1, p_2, \ldots, p_k)$ is the finest partition which is coarser than each of the p_i's. These operations are available in the open-source mathematical software Sage [14].

Moreover, to each permutation $g \in S_m$ corresponds a canonical underlying partition $\hat{g}$ of $\{1, 2, \ldots, m\}$ obtained by replacing each cycle $c = (i_1, i_2, \ldots, i_v)$ in g by the set $\{i_1, i_2, \ldots, i_\nu\}$ (including the case $\nu = 1$ of one-element cycle). For example, if $m = 8$ and $g = (2, 5)(4, 6, 1)(3)(7)(8)$, then $\hat{g} = \{\{2, 5\}, \{4, 6, 1\}, \{3\}, \{7\}, \{8\}\}$.

Finally, if $g \in S_m$ and $s \subseteq \{1, 2, \ldots, m\}$ is stable under g, that is $g(s) = s$, denote by g_s^* the permutation in S_m defined by $g_s^*(x) = g(x)$, if $x \in s$, and $g_s^*(x) = x$, otherwise.

These preliminaries give rise to Algorithm 1 below.

Algorithm 1

1: Define the subgroup $S_{m,n}$ of S_{m+n} by its four generators $(1, 2)$, $(1, 2, \ldots, m)$, $(m + 1, m + 2)$ and $(m + 1, m + 2, \ldots, m + n)$.
2: Construct a list *list_mol_mn* of all molecular operators $X^m D^n/H$,
3: **for** each H above, given by the generators $g_1, g_2, \ldots, g_i$, **do**
4: Construct the list of partitions $\hat{g}_1, \hat{g}_2, \ldots, \hat{g}_i$ of $\{1, 2, \ldots, m + n\}$;
5: Construct the partition $p = \sup(\hat{g}_1, \hat{g}_2, \ldots, \hat{g}_i)$;
6: **for** k from 1 to $|p| - 1$, **do**
7: **for** each k-subset $\{c_1, c_2, \ldots, c_k\} \subseteq p$, **do**
8: $c = \bigcup_{1 \leq i \leq k} c_i$;
9: **if** $\forall g \in \{g_1, g_2, \ldots, g_i\}$, c is stable under g and $g_c^* \in H$, **then**
10: Delete $X^m D^n/H$ from *list_mol_mn*;
11: **end if**
12: **end for**
13: **end for**
14: **end for**
15: **return** *list_mol_mn* (which now contains all atomic operators for fixed m and n).

Remark. The construction of a list of all molecular operators (Step 2 of Algorithm 1) is not trivial. Indeed, recall that, as stated in Section 2, any molecular two-sort species is isomorphic to a species $X^m T^n/H$, where H is a subgroup of $S_{m,n}$. Since two such molecular species are isomorphic if and only if their

respective subgroups are conjugate in $S_{m,n}$, one must compute a list of all conjugacy classes of subgroups of $S_{m,n}$ in order to obtain all molecular species. For example, one could use the command `conjugacy_classes_subgroups` in Sage [14], which, via GAP [8], returns a list of representatives of the conjugacy classes of subgroups of a given group. Furthermore, Step 3 of Algorithm 1 can be considered as a two-sort implementation of Chiricota's version [4] of Yeh's criterion [15] for one-sort atomic species. Moreover, the complete canonical decomposition of any given molecular operator $X^m D^n/H$ as a product of atomic operators can be obtained through a closer analysis of p and c in Step 3 of Algorithm 1.

Algorithm 1 has been implemented in the Python language using Sage and GAP. We succeeded in computing every atomic operator for $m+n \leq 10$. The source code is available on demand. However, we plan on including it very soon in Sage. Partial results for $m+n=8$ can be found in Table 1.

The performance of Algorithm 1 is clearly dependent on the number of elements in the list *list_mol_mn*. Furthermore, since the number of molecular operators $X^m D^n/H$ is equal to the number of conjugacy classes of subgroups of $S_{m,n}$, the length of *list_mol_mn* is growing fast as m and n increase. In addition, the **for** loop in line 7 computes all 2^p k-subsets of p for $1 \leq k < |p|$. Thus, the time cost of our algorithm is at least exponential.

The computation of the conjugacy classes of subgroups of $S_{m,n}$ is very costly in running time. The creation of a database storing these conjugacy classes is a natural enhancement, available in our implementation.

5. Computations

We computed the lists of atomic operators $X^m D^n/H$ for $m+n \leq 10$. However, due to space constraints, we only include partial results for $m+n=8$ in Table 1.

The first column describes the type (m,n) of atomic operators. For example, $(2,6)$ stands for atomic operators of type X^2D^6/H. The second column describes the number of atomic operators of type (m,n). Finally, the third column contains a partial list of atomic operators of type (m,n). Here, for instance, $\langle (3,4,5)(6,7,8), (1,2)(4,5)(7,8)\rangle$ denotes the subgroup H of $S_{5,3}$ generated by the permutations having cyclic decompositions $(3,4,5)(6,7,8)$ and $(1,2)(4,5)(7,8)$.

It is worth noting that molecular operator of the form XD^n/H where H is a subgroup of $S_{1,n}$ are never atomic for any $n>0$. Indeed, one can easily show that such operators always admit a factorization $X \cdot D/H'$ where H' is the subgroup of S_n isomorphic to H. A similar argument is used to show that $X^n D/H$ is never atomic for any $n>0$.

6. Conclusion

For m and n given, Algorithm 1 computes a list of all atomic operators $X^m D^n/H$. However, due to the large number of elements in $S_{m,n}$, the running

(m,n)	Number of operators	Atomic operators
$(0,8)$	130	$X^0D^8/\langle(1,2)(3,4)(5,6)(7,8)\rangle$ $X^0D^8/\langle(1,2)(3,4)(5,6)(7,8),(1,3)(2,4)(5,7)(6,8)\rangle$ $X^0D^8/\langle(5,6)(7,8),(1,2)(3,4)(5,7,6,8)\rangle$ $\vdots$
$(1,7)$	0	Empty
$(2,6)$	46	$X^2D^6/\langle(1,2)(3,4)(5,6)(7,8)\rangle$ $X^2D^6/\langle(5,6)(7,8),(1,2)(3,4)(7,8)\rangle$ $X^2D^6/\langle(5,6)(7,8),(1,2)(3,4)(5,7)(6,8)\rangle$ $\vdots$
$(3,5)$	6	$X^3D^5/\langle(2,3)(4,5)(7,8),(1,2)(4,5)(6,7)\rangle$ $X^3D^5/\langle(6,7,8),(2,3)(4,5)(7,8),(1,2)(4,5)(7,8)\rangle$ $X^3D^5/\langle(6,7,8),(4,5)(7,8),(2,3)(7,8),(1,2)(7,8)\rangle$ $\vdots$
$(4,4)$	89	$X^4D^4/\langle(1,4)(2,3)(5,7)(6,8)\rangle$ $X^4D^4/\langle(5,6)(7,8),(1,4)(2,3)(7,8)\rangle$ $X^4D^4/\langle(3,4)(5,6)(7,8),(1,2)(5,6)\rangle$ $\vdots$
$(5,3)$	6	$X^5D^3/\langle(3,4,5)(6,7,8),(1,2)(4,5)(7,8)\rangle$ $X^5D^3/\langle(6,7,8),(3,4,5),(1,2)(4,5)(7,8)\rangle$ $X^5D^3/\langle(6,7,8),(2,3,5,4)(7,8),(1,2)(3,5)\rangle$ $\vdots$
$(6,2)$	46	$X^6D^2/\langle(1,2)(3,4)(5,6)(7,8)\rangle$ $X^6D^2/\langle(5,6)(7,8),(1,2)(3,4)(7,8)\rangle$ $X^6D^2/\langle(3,4)(5,6),(1,2)(5,6)(7,8)\rangle$ $\vdots$
$(7,1)$	0	Empty
$(8,0)$	130	$X^8D^0/\langle(1,2)(3,4)(5,6)(7,8)\rangle$ $X^8D^0/\langle(5,6)(7,8),(1,2)(3,4)(7,8)\rangle$ $X^8D^0/\langle(3,4)(5,6)(7,8),(1,2)(5,7)(6,8)\rangle$ $\vdots$

Table 1: Partial results obtained using the implementation of Algorithm 1 in Python using Sage for $m+n=8$

time of our implementation greatly increases as m and n grow.

Future perspectives include solving some algorithmic issues. Namely, the inclusion of our code with the appropriate documentation in Sage for wider visibility and reusability. Furthermore, some interesting features of the Python language, namely iterators and the bisect library, could be used to produce a more efficient implementation of Algorithm 1. In addition, we plan to implement Theorem 3.5 as well as the $\odot$-composition of operators (see [11]). This would allow further studies of the effects of molecular differential operators on species.

Another interesting line of research would be to study the canonical factorization of a molecular operators into atomic ones. Indeed, refining Step 3 of Algorithm 1 yields a non trivial factorization (if it exists) of the operator $X^m D^n/H$ as a product $X^{a_1} D^{b_1}/H_1 \cdot X^{a_2} D^{b_2}/H_2$. The iteration of this process would produce an evaluation tree, from which the canonical atomic factorization is obtained.

Fiore also studies differential operators on species but in the context of structuring typed syntax (see [6, 7]). Therefore, it would be interesting to study atomic and molecular differential operators using tools provided by this theory.

Finally, a natural extension of this paper would be to consider k-sort species ($k \in \mathbb{N}$) that correspond to general combinatorial partial differential operators. The study of such operators is an open subject which would help our understanding of many combinatorial objects.

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