ENUMERATIVE COMBINATORICS AND ALGEBRAIC LANGUAGES

Gérard VIENNOT
UER Mathématiques et Informatique
Université Bordeaux I
33405 TALENCE FRANCE

ABSTRACT - We give a survey of recent works relating algebraic languages with the combinatorics of "planar pictures" (i.e. planar maps, animals, polyominoes, secondary structures,...). Such objects are encoded with words. Applications are in enumeration theory, in connection with statistical Physics, molecular Biology, algorithmic complexity and computer graphics drawing.

- INTRODUCTION -

Let A_n be a finite class of combinatorial objects. The number n will be the "size" of such objects (i.e. number of points or number of edges, of elementary cells,..., see the examples below). Let a_n be the cardinality of A_n and suppose that the generating function $f(t)=\sum_{n\geq 0} a_n t^n$ is algebraic.

An old idea, dear to M.P.Schützenberger [37] [38] is to explain this algebricity by constructing a bijection between A_n and the words of an algebraic (i.e. context-free) language $\mathcal{L}$ defined on an alphabet X by a non-ambiguous grammar. Usually an explicit formula is known for a_n or $f(t)$ by means of classical calculus techniques used in combinatorics (recurrence relations, functionnal equation, Lagrange inversion formula,...). One of the interest in finding such a bijection is in the combinatorial understanding of the objects themselves.

We give below several examples where this methodology has solved open problems in enumerative combinatorics, in relation with molecular Biology and statistical Physics.

From the non-ambiguous grammar of the language $\mathcal{L} \subseteq X^*$, one can classically associate a proper algebraic system in non-commutative power series (see [35] [39]). The unique solution of the system contains the (non-commutative) generating function $L = \sum_{w \in \mathcal{L}} w$ of the language $\mathcal{L}$ coding the combinatorial objects. By sending all the variables x of X onto the variable t , the serie L becomes the generating function $f(t) = \sum_{n \geqslant 0} a_n t^n$, which is solution of an algebraic system (in commutative variables).

The coding appears to be a nice intermediate between the combinatorial level and the analytic level. Each equation of the non-commutative algebraic system is in fact a combinatorial property of the objects themselves.

Apart from solving open enumerative problems, other applications are in the generation and representation of such planar objects. Finding a random animal is an important problem in statistical Physics. Optimization of the running time of the bijection becomes here essential and sophisticated algorithmic methods need to be used.

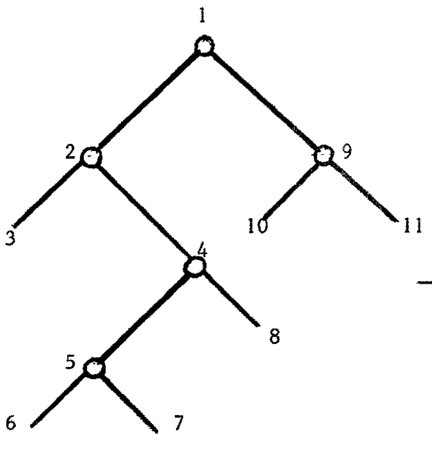
§ 1 - A VERY SIMPLE EXAMPLE : BINARY TREES -

Let $\mathcal{D}$ be the restricted Dyck language on two letters, which will be called here, for short, the Dyck language . It is the set of words w on $X=\{x, \bar{x}\}$ defined by the two following conditions

(1) for every left factor u of $w=uv$, $|u|_x \geqslant |u|_{\bar{x}}$ (number of occurrences),

(2) $|w|_x = |w|_{\bar{x}}$.

It is very classical that the set of binary trees having n internal nodes and $n+1$ leaves is in bijection with Dyck words of length $2n$ (see fig.1).



$\longrightarrow$ $w = x\,x\,\bar{x}\,x\,x\,\bar{x}\,\bar{x}\,\bar{x}\,x\,\bar{x}$

Figure 1. Bijection binary trees- Dyck words (using prefix order).

The (non-commutative) generating function $D = \sum_{w \in \mathcal{D}} w$ satisfies the algebraic equation

$$(3) \qquad D = 1 + x D \bar{x} D.$$

This equation is nothing but to say that every Dyck word is else the empty word, else has a unique factorization $w = xu\bar{x}v$ with u and v in $\mathcal{D}$. By sending the variables onto t, one get the following algebraic equation for the generating function $d(t) = \sum_{n \geq 0} a_n t^n$

$$(4) \qquad d = 1 + t^2 d^2 .$$

Trivial analytic calculus gives

$$(5) \qquad d(t) = \frac{1 - (1-4t^2)^{1/2}}{2t^2},$$

and $a_{2n} = \frac{1}{n+1} \binom{2n}{n}$ the classical Catalan number C_n.

Various families of trees can be enumerated using bijections analogous to the one between binary trees and Dyck words, see for example Goldman [18], Gross [25], Kuich [31] [32].

Another example is the so-called 1-2 trees. They are encoded by what we call Motzkin words, that is words obtained by inserting some letters "a" into a Dyck word (or "shuffle" of Dyck words with words of $\{a\}^*$). The non-commutative equation is

$$(6) \qquad M = 1 + a M + x M \bar{x} M.$$

The number of such words of length n is the Motzkin number M_n. These words will play an important role below.

§ 2 - PLANAR MAPS -

A rooted planar map is displayed on figure 2. Intuitively, a planar graph and its embedding in the plane (in fact the sphere) are given. See [4] or [6] for a more precise definition. Numerous enumerating formulae for planar maps and subclass of planar maps have been given by Tutte and his students during the sixties (an example is [45]). These formulae are deep, surprisingly simple, and the corresponding generating functions are algebraic.

This algebricity has been explained by Cori [4] with some codings with words of algebraic languages. A deep combinatorial theory appears, in relation with equations with operators defined on languages. This work is followed in Cori, Vauquelin [6] where planar maps are encoded by certain words obtained by putting three colors on Dyck words (in a certain manner). This language is not algebraic, but is the difference of two algebraic languages. Such words are in bijection with the so-called well-labeled trees (see [6]). Beautiful improvements and other bijections have been given by Arques [2].

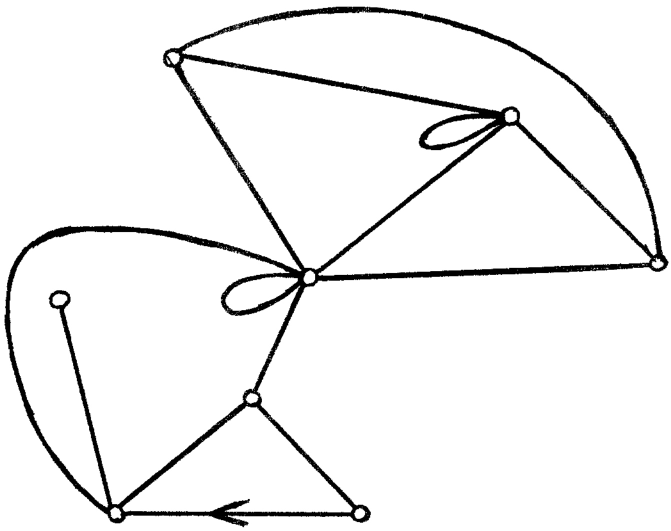


Figure 2. A rooted planar map.

§ 3 - ANIMALS AND POLYOMINOES -

An animal is a set of points of $P=\mathbb{Z}\times\mathbb{Z}$ such that every pair of points of the animal can be related by a path (sequence of points) included in the animal and having elementary steps North, South, East and West, see figure 3.

Let a_n be the number of animals with n points. A major open problem in combinatorics is to find a formula (exact or asymptotic) for this number a_n. This problem is very important in statistical Physics, in connection with percolation theory and thermodynamic models for critical phenomena and phase transitions. Physicists expect the following relations $a_n \sim \mu^n n^{-\theta}$ and $R_n \sim n^{\nu}$ where R_n is the average "radius" of the animals of size n (each of the a_n animals appears with the same probability). The exponents θ and ν are called critical exponents. Particular interests are also for different kind of subclasses of animals (see below).

Animals are sometimes also called polyominoes. Such objects are obtained from animals by replacing each point by an "elementary cell" as shown on figure 6. Polyominoes and animals have been intensively studied in Combinatorics, see for example Golomb [19], Klarner [28] [29], Klarner, Rivest [30].

After the pioneer work of Cori and Vauquelin, another step was done in the use of the algebraic language methodology by Delest,Viennot [10]. A convex polyomino (or convex animal) is a polyomino such that the intersection with every vertical or horizontal line is a connected segment. Knuth asked the question : what is the number of convex polyominoes (see [30]).Klarner, Rivest [30] gave asymptotic formula for the number of such polyominoes having a given area (number of cells). We enumerate them according to the perimeter (number of bonds). After many bijections, such animals can be encoded with words of an algebraic language. The corresponding algebraic system can be solved, with MACSYMA use. Surprisingly, a very simple formula emerges at the end. The number p_{2n} of convex polyominoes with perimeter $2n$ is given by

(7) $p_4 = 1,\ p_6 = 2,\quad \text{for } n \geqslant 0,\quad p_{2n+8} = (2n+11)4^n - 4(2n+1)\binom{2n}{n}.$

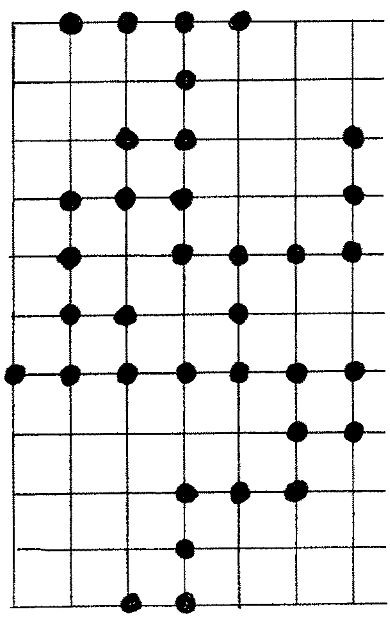


Figure 3. An animal.

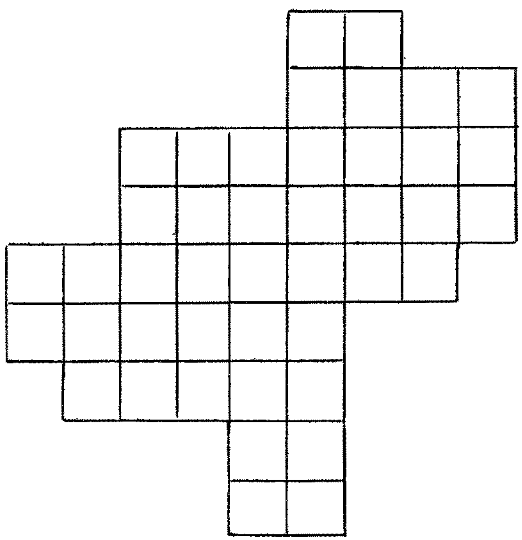


Figure 4. A convex polyomino.

In fact three classes of polyominoes have to be defined, with three coding and three different algebraic systems. One of them requires about 40 equations. A careful use of the algebraic language methodology is needed, with the introduction of substitution operators in languages and multihead finite automata. The words coding these polyominoes are certain Motzkin words, or words close to them.

Since this result, other classes of polyominoes (or animals) have been enumerated. They are respectively the column-convex animals (according to the bond perimeter), Delest [7], the directed column-convex animals (according to the directed percolation perimeter), Delest, Dulucq [8] , and the parallelogram polyominoes (according to the double distribution for the bond and site perimeter), Delest, Gouyou-Beauchamps,Vauquelin [9], see figures 5 and 6. Note that Klarner gives in [28] [29] the generating function for column-convex animals according to the area (number of points in the animals of number of cells in the polyomino) . This result is rederived in [7] with the construction of a bijection with words of a rational language.

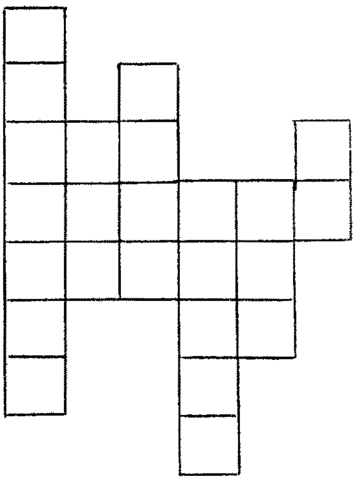


Figure 5. A column-convex polyomino.

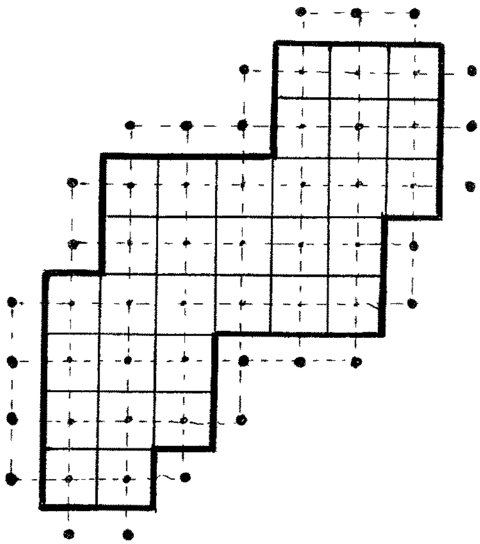


Figure 6. A parallelogram polyomino (with bond and site perimeter)

§ 4 - DIRECTED ANIMALS -

The directed animal problem was posed by Physicists in 1982 and much attention has been given.

A directed animal is a set of points of $P = \mathbb{Z} \times \mathbb{Z}$ containing the point (0,0), called the source point, and such that any other point can be reached by a path contained in the animal and having elementary steps only North or East.

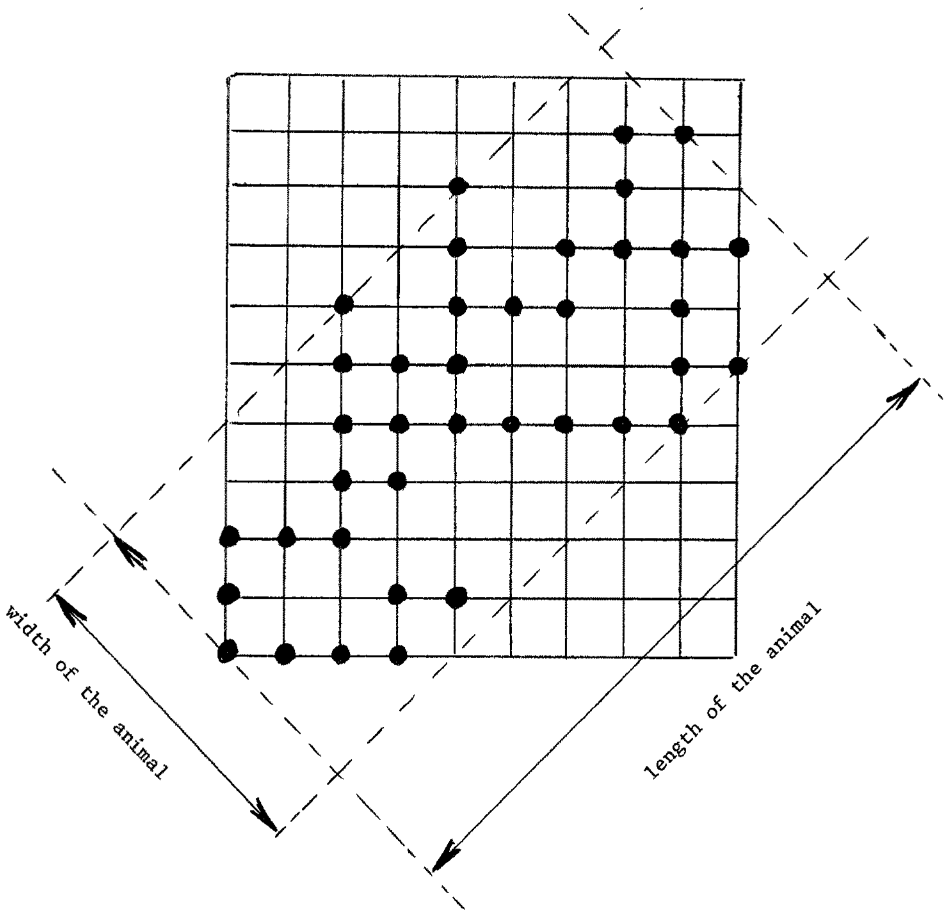


Figure 7. A directed animal.

Let a_n be the number of directed animal with n points. One can define the width and the length of the animal (see figure 7). Let l_n (resp. L_n) the average width (resp. length) of the a_n animals of size n (supposed all equidistributed). Physiscists expect relations of the form

$$(8) \qquad a_n \sim \mu^n n^{-\theta} \quad , \quad l_n \sim n^{\nu_\perp} \quad , \quad L_n \sim n^{\nu_{/\!/}} .$$

Much work has been done in Physics for the computation of the critical exponents θ, $\nu_\perp$, and $\nu_{/\!/}$ by Breuer, Cardy, Janssen, Day, Lubensky, Dhar, Phani, Barma, Family, Green, Moore, Hermann, Stanley, Redner, Coniglio, Yang, Hakim, Nadal, Derrida, Vannimenus. Various physics methods were used (field theory, Flory approximation, renormalisation, exact enumeration up to a given size, transfert matrix method, equivalence with other thermodynamic models,...). This leads to $\theta = \nu_\perp = 1/2$ and $\mu = 3$.

Some exact results have been given by Nadal,Derrida,Vannimenus [34], Hakim,Nadal [26] and Dhar [11] [12].

A complete combinatorial solution is given by Gouyou-Beauchamps,Viennot [23] and Viennot [51]. A survey of the physics and the combinatorial solutions can be found in Viennot [50]. The very surprising fact is that directed animals of size n can be encoded by words on the alphabet $Y = \{a, x, \bar{x}\}$ satisfying condition (1), and of length n-1 . These words are in fact left factors of Motzkin words. The simplicity of the resulting enumeration formula and of the algebraic language is in contrast with the deepness of the bijection between directed animals and left factors of Motzkin words. From these coding one can easily rederive the formulae of [26] and [34] and solve a conjecture of Dhar [11] giving an explicit formula for the average width l_n.

Note that the directed animals growing from (0,0) in the octant $0 \leq x \leq y$ are in bijection with Motzkin words. Also one can define animals on a triangular lattice. They are in bijection with the (enlarged) Dyck words, that is the words satisfying condition (2). The triangular animals growing from (0,0) in the octant are in bijection with the (restricted) Dyck words. All these facts are very deep.

One can define directed animals with several source points, as the so-called compact-source directed animals, see figure 8. The more surprising of all the (surprising) facts about directed animals is that such animals of size n are in bijection with words of length n-1 of $\{a,x,\bar{x}\}^*$, see [23], [50]. The number of these animals is thus 3^{n-1}. This bijection solves some conjectures of Dhar,Phani,Barma [13]

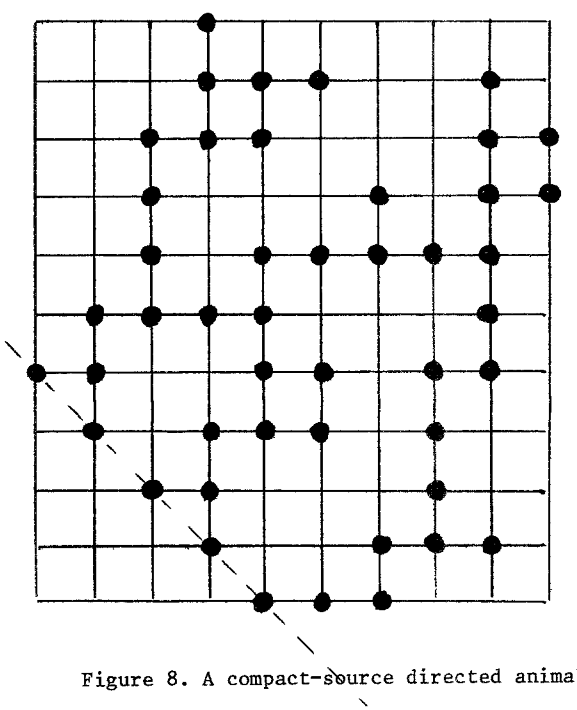


Figure 8. A compact-source directed animal.

§ 5 - SECONDARY STRUCTURES IN MOLECULAR BIOLOGY -

The primary structure of single-stranded nucleic acids (such as RNA, tRNA, mRNA) is the linear sequences of nucleotides (or bases) linked by phosphodiester bonds. Hydrogen bonds fold the molecule into a planar picture called its secondary structure, see figure 9.

Much work has been done in Biology in the prediction of the most stable secondary structure, see for example Tinoco et al. [44]. Of particular importance are ladders and hairpines, that is region containing parallel hydrogen bonds. For energy computation purpose, Mitiko Gô classified hydrogen bonds by a parameter called order.

Waterman restated rigorously this idea in [52]. He defined mathematically <u>secondary structures</u> as a certain class of planar graphs (containing all known RNA secondary structures), and the parameter <u>order</u> (or <u>complexity</u>) of the molecule as an

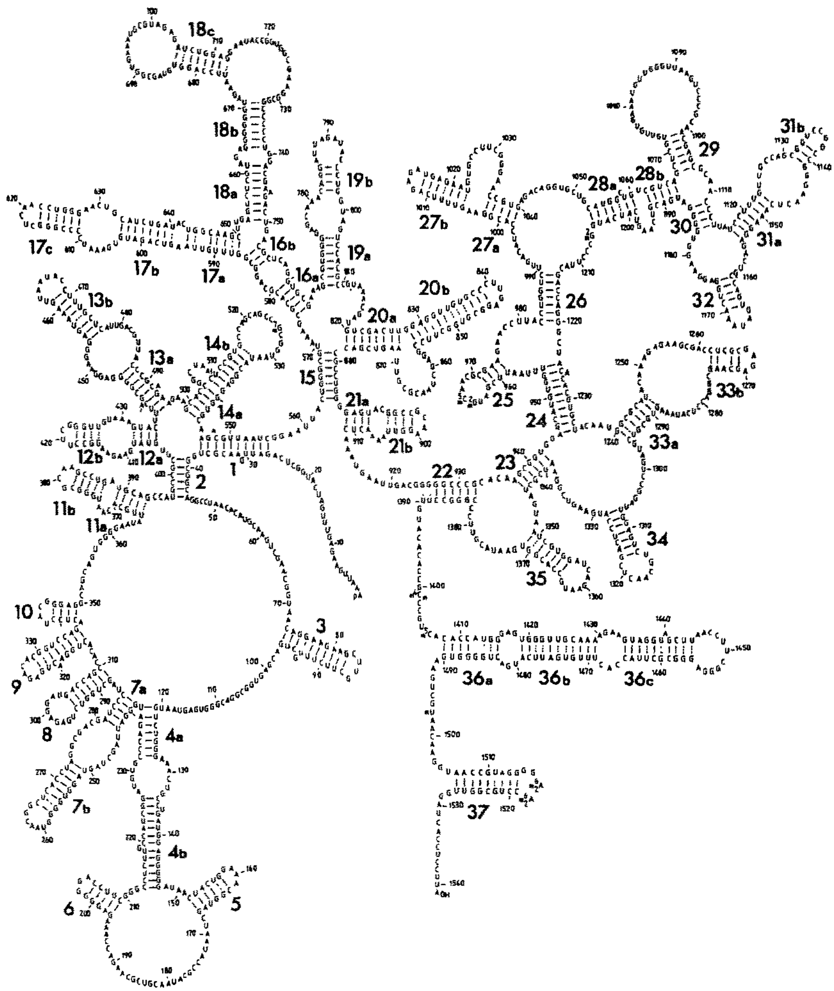


Figure 9. Secondary structure of the 16-S RNA from *Escherichia coli* , from [42].

integer measuring the complexity of the intricate connexions between ladders and hairpines. Waterman raised the question of finding the number $a_{n,k}$ of secondary structures having n bases and complexity k. In particular for k=1, he proves that $a_{n,1}$ is asymptotically of the form λ^n, where λ is the greatest root of the equation $x^3-2x^2-1 = 0$, that is 2.2055... Note that in this context, we are only interested by the planar picture (or map), and not by the particular labelling of the vertices of the graph with four possible bases A,C,G,U.

Secondary structures can easily be encoded with certain Motzkin words. Secondary structures of order k are in bijection with certain words of an algebraic language $\mathcal{L}_k$. The corresponding system for $\mathcal{L}_k$ can be solved recursively if one knows the solution for $\mathcal{L}_{k-1}$. This have been done by Vauchaussade de Chaumont, Viennot [47] [48]. The resolution of Waterman's problem uses not only bijections and the algebraic languages methodology, but also orthogonal polynomials theory and some combinatorial properties of trees and Dyck words with bounded height. The orthogonal polynomials are in connection with bounding the stack of the pushdown automata accepting the words of the algebraic languages. Curiously, some intermediate generating function are used, which are the same as the ones enumerating binary trees having a given Strahler number.

This parameter has been introduced in Hydrogeology and Botanic, see for example Stevens [41], and also appears in Computer Science as the minimum number of registers needed to compute an arithmetic expression, see Flajolet et al. [15] Françon [16], Kemp [27]. The final formula for the generating function of secondary structures of order k is the following

$$\sum_{n\geq 0} a_{n,k}\, t^n = \frac{t^m}{(1-t)Z_1\ldots Z_k} \quad \text{with } m = 5\,.\,2^{k-1}-2 \text{ and} \tag{9}$$

$$Z_1 = 1-2t-t^3\ , \qquad Z_{k+1} = Z_k^2 - 2t^{m+2}\ .$$

§ 6 - SHUFFLE OF DYCK WORDS -

The language formed with words on four letters $x,\bar{x},y,\bar{y}$ obtained by shuffling two Dyck words (one with letters $x,\bar{x}$ the other with letters $y,\bar{y}$), as for example the word $x\, y\, \bar{x}\, x\, y\, x\, \bar{y}\, \bar{y}\, \bar{x}\, \bar{x}$, is no more an algebraic language. This language appears in several codings of various combinatorial objects. An easy calculus proves the following identity (giving the number of shuffle of Dyck words of length 2n)

$$\sum_{k\geq 0} \binom{2n}{2k} C_k\, C_{n-k} = C_n\, C_{n+1} \tag{10}$$

A bijective proof of this identity has been given by Cori et al. [5]. This bijection between shuffle of Dyck words and pair of Dyck words solves a problem given by Mullin in 1966, Mullin [33]. Mullin's problem was written in term of planar maps. The left hand-side and the right hand-side of (10) enumerate certains planar hamiltonian maps. Curiously, in the solution of [5] appears certain permutations : the alternating Baxter permutations on 2n+1, thus enumerated by $C_n C_{n+1}$.

The number of alternating permutations on 2n+1 is well known to be the tangent number. The number of Baxter permutations was given by a difficult analytic proof by Chung et al. [54] . A bijective proof is given by Viennot [41]. In this proof, the alternating Baxter permutations appear in a completely different set of bijections than in [5].

Moreover, the deep combinatorics appearing with shuffle of Dyck words has been recently enriched by the combinatorics of Young tableaux. Gouyou-Beauchamps has proved [20] [21] that the number of standard Young tableaux having at most 4 rows and 2n cells is $C_n C_{n+1}$. Such tableau is displayed on figure 10. Very deep bijections appear, completely different from the bijections defined in [5] and [41]. In particular these Young tableaux are in bijection with words of the language defined by the two following conditions (se [22])

(11) for every left factor u of w=uv, $|u|_x - |u|_{\bar{x}} \geqslant |u|_y - |u|_{\bar{y}} \geqslant 0$,

(12) $|w|_y - |w|_{\bar{y}} = 0$.

The words of length 2n of this language are in bijection with the shuffles of two Dyck words of length 2n. The words of length 2n-1 are enumerated by C_n^2, which is also the number of standard Young tableaux with 2n-1 cells having at most 4 rows. This number is also the number of Baxter alternating permutations on an even number of letters .

11	14				
6	10	13			
3	5	8			
1	2	4	7	9	12

Figure 10. A standard Young tableau with 4 rows.

Note that the number $C_n C_{n+1}$ is also the number of pairs formed by a planar map and one of its spanning tree. An easy bijection can be obtained.

All these facts show that a very deep combinatorics is hidden behind these shuffles of Dyck words.

This combinatorics appears also in connection with some problems about parallelism and concurrency access in data structures, see Flajolet [14] and Françon [17].

§ 7 - GENERATION OF PLANAR OBJECTS -

Such coding of planar objects can be used for different algorithmic purposes, in relation with problems coming from various fields as Computer Graphics, Statistical Physics, Molecular Biology, VLSI,...

For example, coding trees with words and applying recursive generation about these words have been used in Computer Graphics for the generation of synthetic images of trees, see for example Aono [1], Smith [40].

The bijections described above about polyominoes appear to be a first step in the understanding of the combinatorics of pictures formed by union of rectangles on a grid. It would be nice to relate this with VLSI problems. Some connections are described in Chaiken et al. [3] and Van Leeuwen [46].

Coding planar maps with spanning trees and shuffle of Dyck words has been used by Greene [24] for the drawing of planar graphs.

In statistical physics, generating a random animal (or other configurations related to thermodynamic models) is very important. The difficulty is to generate such configurations with the same probability. Monte-Carlo methods can then be used for the evaluation of the critical exponents. Using the coding with words, the problem is reduced to generate a random word of given length of an algebraic language. In the examples considered in this paper, the language is so close to the Dyck or the Motzkin language, that it is possible to generate the words such that each word of given length appears with the same probability.

The critical exponent related to the length of the directed animal is still unknown. From [34], it seems to be very well approximated by 9/11. We think that the coding between directed animal and left factor of Motzkin words can be implemented in linear time. We plan to begin experiments on very large animals (size 10^6).

The coding described in [47] between secondary structures of biological molecules and certains words seems to be useful for the prediction of secondary structures. This problem is important in Molecular Biology, and usually $n \times n$ matrices are used, see for example [44] [52]. In the above example with 16-S molecules, n is 1541. Algorithms manipulating words of length n should be better. Applications for the study of homologies in secondary structures should be of interest.

§ 8 - CONCLUSION -

A remarkable fact about all the various codings of planar objects presented above is that the languages involved are the Dyck language, or the shuffle of the Dyck language with other letters, or the shuffle of two Dyck languages, or other languages "close" to these languages. Thus the Dyck language seems to play a fundamental role in various codings of planarity. We do not know a general explanation of this fact.

An interest of these codings is in the interplay between motivations and considerations coming from Computer Science and Combinatorics (and also Physics) In particular, combinatorists are looking at the languages up to a commutation of the letters. For example, the above secondary structures of order k are encoded by words of an algebraic language, while the (ordinary) generating function is rational. Finding a bijection with words of a rational language is an interesting and deep problem. From the combinatorial point of view, it is really different to consider shuffle of two Dyck words and shuffle of three such words. From the classification of language theory, the difference between two or three stacks is not so relevant.

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