Pólya urns in Philippe Flajolet's work

Introduction to papers [FGP05], [FDP06], [FH08]

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Other related paper by PF: [CF06], [BF11]

1. Pólya urn models

Alice and Bob are collecting coupons but Alice has first choice. Political candidates are so bad that persons who listen to them immediately vote for the opposing candidate. Black and white Welsh sheep change their color as soon as they bleat. Two groups of gunwomen face off, and randomly kill each other. Or even heat chambers, trees that grow with two or three leaves, a father pelican feeding his entrails to his starving young, etc. This list is in no way part of *un Inventaire à la Prévert*[1] but a rapid glance at the metaphoric world Philippe Flajolet developed or assembled, with humor, in order to introduce people to Pólya urn models.

Pólya (or Pólya-Eggenberger) urn models can be succinctly described as follows. Take an urn, initially containing balls of two different colors, say black and white. Randomly pick a ball from the urn, check its color and place it back in the urn. If the drawn ball was black, add α black balls and β white ones into the urn. If the drawn ball was white, add γ black balls and δ white ones. This results in a new random composition of the urn. The urn process consists in iterating this operation, always using the same replacement rules. Time is indexed by natural numbers that represent the number of drawings (so that we interchangeably talk of steps, drawings or time units). Thus, the urn process is entirely defined by the initial composition of the urn, and the replacement matrix

$$\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \tag{1}$$

This definition can of course be extended to any finite number of colors.

The entries of the replacement matrix are integers, and the non-diagonal entries are most often nonnegative. Negative diagonal entries are allowed, but they must then satisfy additional arithmetical requirements (*tenability*) that guarantee that at any time it remains possible to remove balls when the replacement rule requires it.

In addition to these classical assumptions, the three papers this introduction covers make the *balance* assumption: the total number of added balls is the same at any time unit. In other words, there is some integer s such that $\alpha+\beta = \gamma+\delta = s$. This balance condition is one of the key points that allows Philippe Flajolet and his co-authors to connect probabilities and enumeration *via* generating functions and analytic combinatorics.

Philippe Flajolet used to distinguish two main issues with regards to the composition of the urn process: the *slice problem* and the *limit problem.* The first one consists in describing the probability distribution of the composition vector (the k-th coordinate of which is the number of balls of the k-th color) at a given finite time. The second one deals with the almost sure asymptotic behaviour of the urn: one looks for a suitable normalization that leads, for any sequence of random drawings, to some limit when time tends to infinity.

[1] Jacques Prévert, *Inventaire*, in *Paroles*, 1946.

The name of these urn processes comes from György Pólya's papers [EP23] and [Pól30] where he used an urn model to study a contagion problem. However, as mentioned in [FDP06], the earliest contributions are probably due to Jacob Bernoulli and Pierre Simon Laplace. The introductions to both papers [FGP05] and [FDP06] contain a rich description of the historical account on the subject. The books by N. L. Johnson and S. Kotz [JK77] and H. M. Mahmoud [Mah08] also contain details on history and applications of urn models. Roughly said, the following three groups of methods have been considered. All initial approaches were made by *direct enumeration*. Decisive improvements were later provided by *probabilistic methods*. The first general treatment by *analytic combinatorics* is due to Philippe Flajolet and his co-authors in the mid 2000s. They had the idea to consider all trajectories that lead to a given composition of the urn, namely the *histories* to which Section 2 is devoted.

Without delving into the smallest details, it may be worth pausing for a moment to describe a subtle game played by hypotheses and results in the most recent methods.

Flajolet's method provides nice and very precise results on both the slice problem *and* the limit problem *via* a complete parametrization of the urn composition in terms of special functions such as elliptic functions, inverse Abelian integrals on Fermat curves, Jacobian elliptic functions, etc. This allows, in particular, for local limit theorems and very large deviations to be derived. Unfortunately, the method requires solving a differential system, which happens to be only integrable in the general case for small dimensions; this leads the authors to write in [FDP06]: "the global approach that we developed for 2×2 urns admits of no universal generalization in any dimension $d \geq 3$".

Relying on branching process theory, the seminal work on the subject by S. Janson [Jan04] is based on embedding the urn process into continuous time. Available for random replacement matrices in any dimension and without balance assumption, the method provides a large amount of deep results on the limit problem. In particular, it reveals the famous phase transition on the process asymptotics in both discrete and continuous time, depending whether the urn is *small* or *large*.[2] Roughly speaking, small urns have a Gaussian asymptotic behaviour in distribution while large ones admit almost sure limit theorems, with the appearance of non Gaussian limit laws. Of course, the wide generality of the method makes explicit parametrizations out of reach. Besides, it requires that some irreducibility assumption be made on the replacement matrix. For example, [Jan05] presents a special treatment of triangular 2-dimensional matrices.

Irreducibility assumptions are however not required in [Pou08]. This operator approach of the Markov chain in discrete time extends Janson's results on the limit problem to replacement matrices having real entries. Based on structure of moments, this study leads further to a *global* strong asymptotics of the composition vector for large urns. The method applies in all dimensions but it remains valid only for non random and balanced replacement matrices, as in Flajolet's method.

Philippe Flajolet was really interested in the behaviour of urn models in general. Nevertheless, one of the motivations to study urns came from the occurrence of urn models in various problems in the analysis of algorithms and data structures

[2] Write the real parts $\sigma_1, \ldots, \sigma_n$ of the replacement matrix eigenvalues in nonincreasing order. The urn is called small whenever $2\sigma_2 \leq \sigma_1$. Otherwise, it is called large.

or combinatorics. A paradigm is given by the fringe analysis of balanced 2-3 trees. Section 3 is devoted to developing this example.

2. Urn histories

The analytic approach developed by Philippe Flajolet and his co-authors is based on what they named the *histories* of the urn.

Consider coding the urn composition by words whose letters are the ball colors. For example, for a two-color urn, the initial composition is coded by the word

$$W_0 = \mathtt{bbb}\ldots\mathtt{bwww}\ldots\mathtt{w} = \mathtt{b}^{a_0}\mathtt{w}^{b_0}$$

where a_0 and b_0 denote respectively the initial number of black and white balls. A drawing consists then in choosing uniformly at random one letter of this word W_0, say the second one, and in replacing it by the suitable word of the form $\mathtt{b}^x\mathtt{w}^y$. For the replacement matrix (1), in our example, the new composition at time 1 is then coded by the word

$$W_1 = \mathtt{b}\left(\mathtt{b}^{1+\alpha}\mathtt{w}^{\beta}\right)\mathtt{b}\ldots\mathtt{bwww}\ldots\mathtt{w} = \mathtt{b}^{2+\alpha}\mathtt{w}^{\beta}\mathtt{b}^{a_0-2}\mathtt{w}^{b_0}.$$

In this way, the urn process becomes a Markov process taking values in the set of finite words. A *history* of length n of the urn process is then defined by Philippe Flajolet and his co-authors as a sequence $W_0, W_1, \ldots W_n$ of such successive words. Of course, when W_n contains a $\mathtt{b}$'s and b $\mathtt{w}$'s, the composition vector at time n is $\begin{pmatrix} a \\ b \end{pmatrix}$.

The analytic approach of urn processes is developed by then using exponential generating functions of histories. More precisely, the trivariate generating function

$$H\left(x, y, z \;\middle|\; \begin{matrix} a_0 \\ b_0 \end{matrix}\right) := \sum_{n,a,b\geq 0} H_n \begin{pmatrix} a_0 & a \\ b_0 & b \end{pmatrix} x^a y^b \frac{z^n}{n!},$$

is defined in [FDP06], where $H_n \begin{pmatrix} a_0 & a \\ b_0 & b \end{pmatrix}$ denotes the number of histories of length n that lead the process from the initial composition $\begin{pmatrix} a_0 \\ b_0 \end{pmatrix}$ to the final composition $\begin{pmatrix} a \\ b \end{pmatrix}$.

In 2005, the first article *Analytic Urns* [FGP05], published in *The Annals of Probability* is based on the fact that H functions satisfy the partial differential equation (called PDE in the following)

$$\frac{\partial H}{\partial z} = x^{\alpha+1}y^{\beta}\frac{\partial H}{\partial x} + x^{\gamma}y^{\delta+1}\frac{\partial H}{\partial y}. \tag{2}$$

The classical method of characteristics applied to this equation provides solutions that are indirectly expressed in terms of a "fundamental" function ψ defined by an implicit equation. Furthermore, Abelian integrals intervene in the implicit equation that defines ψ, making solutions difficult to handle in this form.

For this reason, the approach is not further considered in the following articles. Indeed, in 2006, the striking and powerful so-called "basic isomorphism" is proven. It comes from two simple rules on generating functions: choosing a ball amounts

to differentiating, while adding a ball amounts to multiplying by a variable. Consequently, as shown in the article *Some Exactly Solvable Models of Urn Process Theory* [FDP06], the H functions have the following fundamental properties.
(i) Multiplicative convolution:

$$H\left(x,y,z\,\middle|\,\begin{matrix}a_0\\ b_0\end{matrix}\right)=H\left(x,y,z\,\middle|\,\begin{matrix}1\\ 0\end{matrix}\right)^{a_0}H\left(x,y,z\,\middle|\,\begin{matrix}0\\ 1\end{matrix}\right)^{b_0};$$

(ii) Ordinary differential system: if x and y are nonzero complex numbers, the functions

$$X(z)=H\left(x,y,z\,\middle|\,\begin{matrix}1\\ 0\end{matrix}\right)\qquad\text{and}\qquad Y(z)=H\left(x,y,z\,\middle|\,\begin{matrix}0\\ 1\end{matrix}\right)$$

are the *solutions to the monomial homogeneous differential system*

$$\begin{cases}X'(z) &= X(z)^{\alpha+1}\,Y(z)^{\beta}\\ \\ Y'(z) &= X(z)^{\gamma}\,Y(z)^{\delta+1}\end{cases}$$

that satisfy the Cauchy conditions $X(0)=x$ and $Y(0)=y$. This ordinary differential system is called ODS in the following.

Once these two main properties are proven, Flajolet's procedure consists in taking a particular case of replacement matrix, solving the differential system by means of explicit—sometimes special—functions and deriving probabilistic consequences. A celebrated example is given in the next section.

3. A paradigmatic example: the $2-3$-tree urn

The fringe analysis of a balanced $2-3$ tree, which is a data structure of computer science used for sorting and searching, leads to the 2-dimensional urn having

$$\begin{pmatrix}-2 & 3\\ 4 & -3\end{pmatrix},$$

as replacement matrix. The corresponding differential system with its Cauchy conditions is

$$\begin{cases}X' &= X^{-1}Y^{3}\\ Y' &= X^{4}Y^{-2}\\ X(0) &= x\\ Y(0) &= y\,.\end{cases}\tag{3}$$

To solve this system, let Z be defined by $Z=X^2$. Then, $Z'=2Y^3$, so that $Z''=6Z^2$. Multiplying this last equation by Z' leads, after integration, to

$$\begin{cases}Z'^2 &= 4Z^3-g_3\\ Z(0) &= x^2\\ Z'(0) &= 2y^3\,.\end{cases}$$

where $g_3=4(x^6-y^6)$. When $g_3\neq 0$, this differential equation is classically solved by elliptic functions: let $\wp(z):=\wp(z;0,g_3)$ denote the doubly periodic Weierstraß function specified by the lattice invariants $g_2=0$ and g_3. Then,

$$Z(z)=\wp(z+z_0)$$

where $z_0 = z_0(x,y)$ is the only complex number in the period parallelogram that satisfies

$$\begin{cases} \wp(z_0) & = x^2 \\ \wp'(z_0) & = 2y^3 \,. \end{cases}$$

Starting from 2 black balls and 0 white ones, which corresponds to the fetish example of [FGP05], the trivariate generating function of histories thus takes the form

$$H\left(x, y, z \,\middle|\, \begin{matrix} 2 \\ 0 \end{matrix}\right) = \wp\left(z + z_0(x,y)\right) \,.$$

It is possible to derive probabilistic consequence from this explicit expression. As in [FGP05], consider for example the probability p_n that, at time n, all balls are black ("extreme large deviations"). In terms of generating functions, this number is

$$p_n = \frac{1}{n+1}[z^n]H\left(0, 1, z \,\middle|\, \begin{matrix} 2 \\ 0 \end{matrix}\right).$$

The corresponding Weierstraß function has invariants $g_2 = 0$ and $g_3 = -4$. The theory of elliptic functions tells us that this function $\wp(z; 0, -4)$ has

$$\Lambda = \omega_1\mathbb{Z} + \omega_2\mathbb{Z}$$

as lattice of periods, where $\omega_1 = 3\rho e^{i\pi/6}$ and $\omega_2 = 3\rho e^{-i\pi/6}$, the constant

$$\rho = \frac{1}{6}B\left(\frac{1}{6}, \frac{1}{3}\right)$$

being named the same way as in [FGP05] (B denotes Euler's Beta function). The two zeroes of $\wp(z; 0, -4)$ in the parallelogram of periods are in this case easily computable: they turn out to be located at ρ and $2\rho = \omega_1 + \omega_2 - \rho$ with respective derivatives -2 and 2. Consequently,

$$\begin{aligned} H\left(0, 1, z \,\middle|\, \begin{matrix} 2 \\ 0 \end{matrix}\right) & = \wp(z - \rho; 0, -4) \\ & = \frac{1}{(z-\rho)^2} + \sum_{\lambda \in \Lambda \setminus (0)} \left[\frac{1}{(z - \rho + \lambda)^2} - \frac{1}{\lambda^2}\right], \end{aligned}$$

the last sum resulting directly from the definition of $\wp$. Note that this result is proven in [FGP05] without solving ODS (3): the author directly deal with PDE (2), the "basic isomorphism" being introduced later in [FDP06]. The last step of the derivation is made by singularity analysis, the poles of $\wp(z; 0, -4)$ being all of order two, located at the points of the lattice Λ as is the case for any Weierstraß elliptic function. This provides very precise asymptotics (complete expansion) of the required number p_n in the scale of powers of ρ.

This is but one example of what can be deduced from the powerful analytic method for 2-dimensional urn processes. Using the structure provided by the differential equations, the following papers [FGP05] and [FDP06] prove many more probabilistic results. These results are valid for all "balanced 2×2 urns with subtraction", *i.e.* with negative diagonal entries. For instance, the number of black balls at time n is asymptotically Gaussian with rate of convergence $O\left(1/\sqrt{n}\right)$ (consequence of Hwang's Quasi-Powers Theorem [FS09, IX.5]). The papers also provide results on the form of moments, large deviation theorem with explicit rate functions, etc.

4. Time reversal effect, duality principle

In [FDP06] and [FH08], Philippe Flajolet and his acolytes use a remarkable time reversal argument in order to treat some non classical urn models with negative off-diagonal coefficients. The main idea consists in a duality principle between a classical urn having R as replacement matrix and the one having $-R$ as matrix.

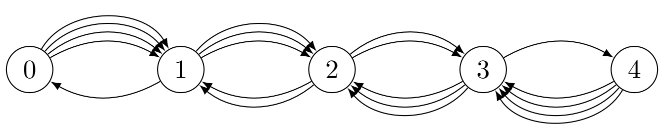
An example of what can be done is detailed in [FH08]. It informally introduces a process in the following way:

> "Say a country consists of a population of N sheep, each of which can, at any given time, be in either one of two states of mind, denoted by A and B. At [any] discrete instant, [...] a randomly chosen sheep in the population bleats in accordance with its current state of mind: if this sheep bleats A[aah], then one of the B-sheep changes to state A ; if this sheep bleats B[eeh], then one of the A-sheep changes to state B. The process stops when unanimity has been reached; that is, all sheep are in one and the same state."

Let M and E be the matrices

$$M = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \qquad E = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}.$$

The sheep process can be viewed as the so-called *Mabinogion* urn having M as matrix replacement. Because of negative off-diagonal entries, this urn is a non classical one. Consider the *dual* urn having E as replacement matrix; it was introduced in 1907 by Paul and Tatiana Ehrenfest "to model particle (or heat) transfer between two chambers". In order to relate these two urns, consider the following directed multigraph, parametrized by a positive integer N: the set of vertices is $\{0, 1, \ldots, N\}$; any possible edge of the form $(j, j-1)$ has multiplicity j while any possible edge of the form $(j, j+1)$ has multiplicity $N - j$. For $N = 4$, the diagram of the multigraph $\Gamma(N)$ is



When k is any vertex and n an natural number, denote by $W_{k,n}^{(N)}$ the number of paths in $\Gamma(N)$ comprised of n steps, starting from vertex 0 and ending in vertex k. As can be elementarily checked, the probability that the Ehrenfest urn starting with N white balls and 0 black ones contains exactly k black balls after n steps of time is

$$\mathbb{P}_{E[N]}\left(0 \to k \text{ black balls in } n \text{ steps}\right) = \frac{W_{k,n}^{(N)}}{N^n}.$$

Similarly, the probability that the Mabinogion urn starting with $k+1$ black balls and $N - k + 1$ white ones ends with 0 black balls after $n+1$ steps of time is

$$\mathbb{P}_{M[N+2]}\left(k+1 \to 0 \text{ black balls in } n+1 \text{ steps}\right) = \frac{N+1}{N+2} \cdot \frac{W_{k,n}^{(N)}}{(N+2)^n}.$$

Mixing the two preceding formulae leads to the *Duality lemma*

$$\mathbb{P}_{M[N+2]}\left(k+1 \to 0 \text{ in } n+1 \text{ steps}\right) = \frac{N^n(N+1)}{(N+2)^{n+1}}\, \mathbb{P}_{E[N]}\left(0 \to k \text{ in } n \text{ steps}\right).$$

The analysis of the Mabinogion urn extinction time is then done from Flajolet's method applied to the Ehrenfest urn, which is parametrized by hyperbolic trigonometric functions.

A similar time reversal argument is given in [FDP06], using the duality between the urns with replacement matrices

$$OK = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \qquad AC = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The *OK-Corral* (non classical) urn is described by:

> "Consider two groups of gunwomen facing each other [...] At each discrete instant, a fighter chosen uniformly at random shoots and kills a member of the opposite group. The problem consists in quantifying the chances for a team to win as well as the number of survivors."

As pointed out by J. F. C. Kingman, this question is a basic one in the mathematical theory of warfare and conflicts. The AC urn, originally introduced by B. Friedman, is also named *Adverse-Campaign* model in [FDP06]:

> "[It models] a propaganda campaign in which candidates are so bad that the persons who listen to them are convinced to vote for the opposite candidate."

The authors conclude the description of this voting model with the humorous remark: "(This is perhaps not such an unrealistic situation!)".

5. Flajolet Urns: how to gather topics and people

No one who talked about urns with Philippe Flajolet can forget the vivid images he used to describe the processes. The curious reader can manage to understand why the urns

$$GCC = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \qquad FP = \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}$$

are respectively the Generalized Coupon Collector's (Alice and Bob both collect images, but Alice gets priority and only gives her duplicates to Bob) and the Father Pelican's—these two models we have evoked at the very beginning of the introduction, are the only ones we have not explained. Both are analyzed in [FDP06].

Thus the definition of a Pólya urn model is very simple to state and to understand: no mathematical background is needed *a priori*, it only deals with balls in a box. But the subject itself still contains many open questions after decades. This "simple" topic is a good illustration of the way Philippe Flajolet did research, and loved to do it.

Urn model is one of the latest subject Philippe Flajolet was interested in; in fact, his work on urn models began in the 2000s. And this may not be a coincidence... Indeed, the radically new point of view he introduced on those models required many of the tools he developed in his long line of past works, but also results from many different mathematical topics. Among them, we can cite the symbolic method in combinatorics, computer algebra, complex analysis of univariate or multivariate generating functions (Mellin transform, singularity analysis, saddle-point method, Riemann surfaces), probability theory, continued fractions, special functions... Philippe Flajolet's work on urns can thus be seen as a synthesis of sorts.

In addition, throughout his career as a researcher, and for urns in particular, Philippe Flajolet never hesitated to seek out scientists working in any outside domain he thought could be relevant. This is very certainly an important aspect of his *grand art*: bridging gaps between topics, and between people, for the betterment of science and its elegance.

6. To be continued...

As mentioned in Section 2, the emergence of the "basic isomorphism" shown in [FDP06] took a few months. The transition between [FGP05] (PDE) and [FDP06] (ODS) is done by an intermediate article of P. Flajolet and E. Conrad, *The Fermat cubic, elliptic functions, continued fractions, and a combinatorial excursion* [CF06]. This article already sets the stage, with the introduction of the following three characters:

$$\text{the urn } \begin{pmatrix} -1 & 2 \\ 2 & -1 \end{pmatrix}, \quad \text{the Fermat curve } x^3 - y^3 = 1 \quad \text{and the ODS } \begin{cases} x' = y^2 \\ y' = x^2 \end{cases}.$$

It contains the first example of the future bridge between the rules of the urn and the expression of the history generating function in terms of a differential system.

Finally, in collaboration with P. Blasiak, specialist in quantum theoretical physics, P. Flajolet unifies involutions, partitions, trees and urns as a wider class of combinatorial structures: gate-diagrams. In their paper *Combinatorial Models of Creation-Annihilation* [BF11], they systematize the key mechanism of the "basic isomorphism": creation and annihilation on the side of combinatorial objects respectively correspond to monomial-multiplication and differentiation on operators (see Fig. 1). This kind of symbolic apotheosis beautifully illustrates one of Philippe Flajolet's favorite motto: "If you can specify it, you can analyze it!".

Beyond the "basic isomorphism", many problems still remain open. We already saw the general non-integrability of the monomial differential system for more than three colors, but even for two colors, the general analysis still has not been completely done. B. Morcrette is seeking to solve the problem in the case where the generating function of the histories is algebraic (see [Mor12] for preliminary results in this direction).

In [HKP07], H. K. Hwang, M. Kuba and A. Panholzer deal with a family of specific examples of urns with negative off-diagonal coefficients, which they call *diminishing urns*, without using the time duality property with respect to classical models. It would be of great interest to determine whether Flajoletical time reversal arguments can be generalized, so as to find an efficient approach of diminishing urns.

Throughout this introduction, we have considered that the replacement rules were fixed; but Pólya urn models with random replacement matrices provide a natural extension to classical ones. Complementary to Janson's work, B. Morcrette and H. M. Mahmoud show in [MM12] that the isomorphism theorem of [FDP06] can be extended to *balanced* urns with random entries. With this framework, exact distributions and possibly asymptotic results can thus be obtained.

Finally, pursuing work initiated by P. Flajolet and B. Morcrette, P. Dumas and B. Morcrette are investigating the case of unbalanced urns (no restrictions on coefficients) using analytic combinatorics. This problem involves partial differential equations which are significantly harder to solve than their deterministic counterparts.

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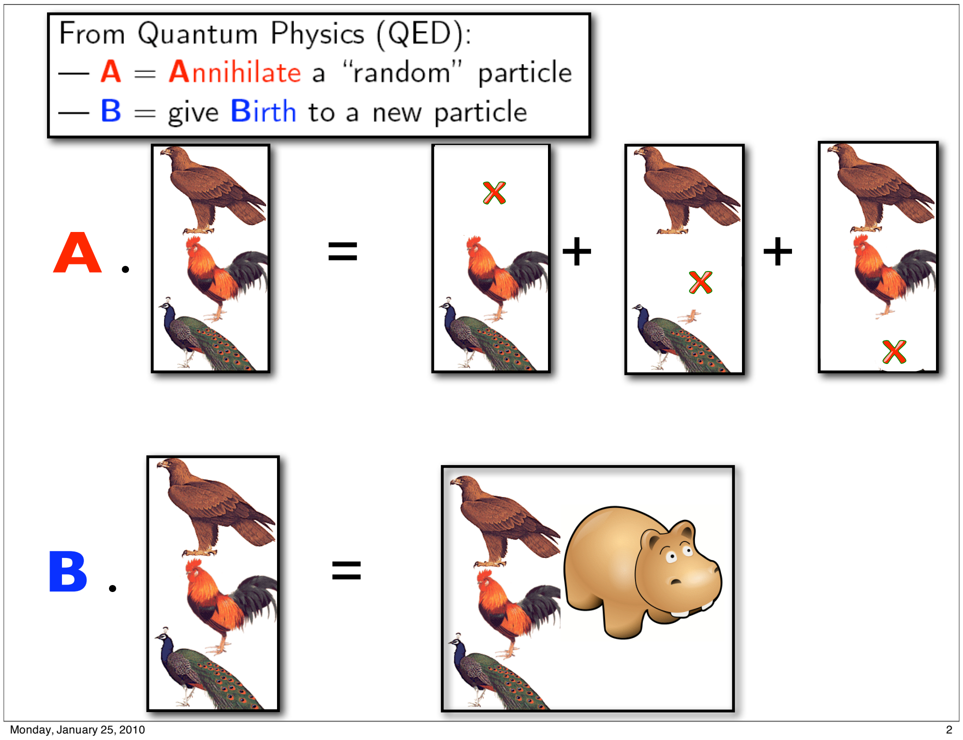

FIGURE 1. Initial slide of Philippe Flajolet's first talk presenting his work with Pawel Blasiak [BF11], to an audience of researchers in combinatorics, in Bordeaux, highlighting the way he harnessed his sense of humor to make the basic ideas of his work memorable to a large audience.