Nom du coordinateur / Coordinator's name	Thomas Fernique
Acronyme / Acronym	QuasiCool
Titre de la proposition de projet	Refroidissement des quasicristaux : des pavages aléatoires aux pavages apériodiques
Proposal title	Quasicrystals cooling: from random tilings to aperiodic tilings
Comité d'évaluation / Evaluation committee	SIMI 2
Type de recherche / Type of research	☒ Recherche fondamentale / Basic research ☐ Recherche industrielle / Industrial research ☐ Développement expérimental / Experimental development

Aide totale demandée / Grant requested	230376,27€	Durée du projet / Project duration	48 mois / months

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1 Executive summary

The full title of the proposal QuasiCool is "Quasicrystals cooling: from random tilings to aperiodic tilings". This is a four-year project grouping together seven researchers in combinatorics, probability theory and dynamical systems, with a Ph.D. grant being also asked (to be started the second year). The coordinator of this project, Thomas Fernique, is a CNRS researcher in computer science since october 2008. The aim of this project is to understand from a theoretical viewpoint, namely in terms of *tilings*, the structure and the growth of *quasicrystals*.

Quasicrystals are non-periodic but ordered materials discovered by D. Shechtman in 1982 (what earned him the last chemistry Nobel prize). They are now generally obtained (as crystals) by slowly cooling a melt. From a theoretical viewpoint, the problem is to understand which quasicrystalline structures can be obtained, in order to classify them as does the Bravais-Fedorov classification of crystalline structures.

Tilings are covering of a space without overlap by compacts called *tiles*. In the early 60's, it has been discovered that some non-periodic tilings of the plane can be completely characterized only by specifying the way tiles can be neighboor, that is, by *local constraints*. Such tilings are said to be *aperiodic*. The connection with quasicrystals was quickly done after they were discovered, with local constraints modeling finite range interactions. However, the existence of aperiodic tilings does not ensure that they can be really (*i.e.*, easily) obtained. This led scientists to study an alternative model of quasicrystals, namely random tilings. This model however recently turned out to be limited, as some real quasicrystals look much more like aperiodic than random tilings.

That is where our project comes into the picture. We model the cooling of quasicrystals by a process where local transformations called *flips* are stochastically performed on an initial random tiling, with a flip being all the more probable as the resulting tiling locally looks more aperiodic. Understanding the convergence rate – hence the realism – of this process is a major objective of our project. The two other major objectives of our project are strongly related: classify aperiodic tilings (the "target" of the process) and understand random tilings (the initial point of the process).

2 Context, position and objectives of the proposal

2.1 Context, social and economic issues

The discovery of the first quasicrystal in 1982 by Dan Shechtman, which earned him the 2011 Nobel prize in chemistry, opened a new broad field of research. Experimental research aims to produce new types of quasicrystals and to investigate their properties, while industrial research looks forward for promising usage of these new materials. But both are tributary of basic research, which is still in its infancy. There is indeed yet no classification of which structures of quasicrystal can be obtained – as, for example, the Bravais-Fedorov classification of possible crystal structures or the periodic table of the chemical elements of Mendeleev. Such a classification would hopefully be of great help to guide experimental research (as some element theoretically predicted by Mendeleev were only later discovered). Moreover, the growth of

quasicrystals is poorly understood: some quasicrystals which could theoretically exist have still failed to be experimentally grown, and no theory explains this.

2.2 Position of the project

Our project focus on the problems of structure and growth of quasicrystals. The approach is theoretical, with quasicrystals being modeled by tilings. This basic research project is actually a logical sequel to a two-year multidisciplinary exploratory project ("Projet Exploratoire Pluridisciplinaire") granted in 2009-2010 by the CNRS, entitled StochasFlip (for "Stochastic Flips"), which involved roughly the same team (with little change – see team description in section 5.1). The aim of this previous project was mainly to set up a formal research project by conducting simulations and stating corresponding conjectures. We are now in a position to carry out this research project.
Let us mention connections with three previous ANR-funded projects (the last two involved people from this project, see Section 5.3): CrystalDyn (coordinator: Jean-René Chazottes), EMC (coordinator Bruno Durand) and SubTile (coordinator: Pierre Arnoux). The nature of these connections is detailed in the next section.
Motivated by the study of quasicrystals, this research project has clearly to do with the physics of condensed matter. We are however mathematicians and theoretical computer scientists, and we want to follow our own approach (let us mention that aperiodic tilings – which are now widely used to model quasicrystals – have been discovered before quasicrystals by mathematicians and computer scientists). Of course, this does not at all preclude contacts with physicists. For example, we plane to attend to the conference Aperiodic'2012, promoted by the International Union of Crystallography, which brings together mathematicians, physicists, chemists and crystallographers. We have also already successfully proposed to Nicolas Destainville – professor in physics which is concerned with tiling – to be, so to say, our "external expert" in physics.
Our project also has connections with numerous european and international research projects, although those have different goals and approaches. We namely plane to interact (at least) with the research groups leaded by Michael Baake (Bielefeld – Germany, specialized in diffraction theory and random tilings), Fabio Martinelli (Roma – Italy, specialized in mixing times of Markov chains in statistical physics problems), Chaim Goodman-Strauss (Fayetteville – US, specialized in aperiodic substitutive tilings) or Michael Schraudner (Santiago – Chile, specialized in dynamical systems and ergodic theory).

2.3 State of the art

The birth of aperiodic tilings

In the early 60's, the logician Hao Wang was interested in the so-called *domino problem* ([90]): given a finite set of unit squares with colored edges (the *tiles*), can we decide whether these tiles can be used (each tile can be used as many time as needed) to *tile* the plane, *i.e.*, to cover it without overlap with the *local constraints* that adjacent edges have matching colors being satisfied. His idea was to try to tile larger and larger finite squares, until either a non-tileable square is found, or a square whose left and right (resp. top and bottom) edges match, *i.e.*, which can be used to tile periodically the plane. But what if there exists an *aperiodic tile set*, that is, a tile set which does tile the plane, but only in a non-periodic fashion? Wang conjectured that there is no such tile set, but one of its student, Robert Berger, found one in 1964 and used it to prove the undecidability of the domino problem by reduction to the Halting problem,

with Turing machine computations being simulated by tiles ([9]). The terminology is not firmly fixed, but let us here say that a non-periodic tiling is *aperiodic* if there is some finite tile set and finitely many local constraints, so that only tilings with the same finite patterns can be formed (in particular, this forbids periodic tiling). Aperiodicity is thus stronger than non-periodicity (indeed strictly stronger, as easily shown by a counting argument). The aperiodic tile set found by Berger is large (20426 tiles) but was sharply reduced in 1971 by Arthur Robinson ([79]). A few number of other small aperiodic tile sets were later found (a detailed account of the quest for small aperiodic tile sets can be found in [48]) – with maybe the most celebrated one being due to Roger Penrose ([72], see Fig. 1).

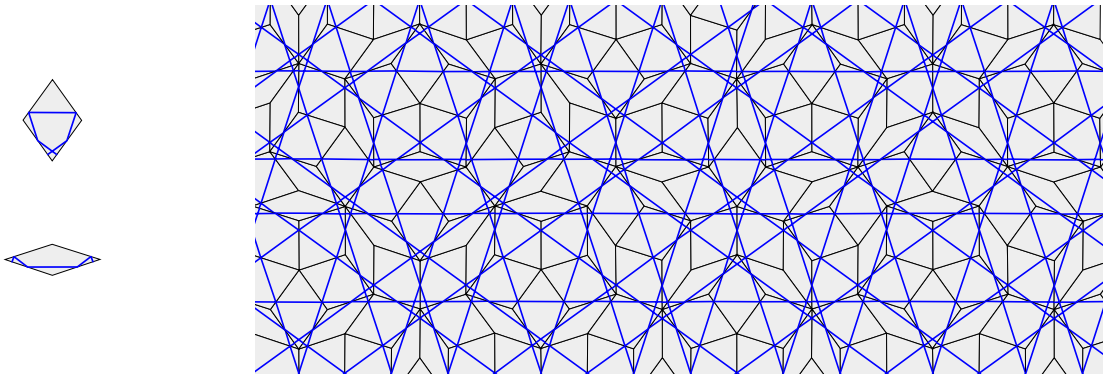


Figure 1: The tiles are a fat and a thin rhombi on which line segments are drawn (Penrose tiles, left). The local constraint is that line segments must form lines (called *Ammann bars*). Tilings of the whole plane exist and are all non-periodic – they are the *Penrose tilings* (right, partial view).

Hierarchy and computation

The first aperiodic tilings were all *hierarchical*, that is, invariant by a transformation – usually called *substitution* – which inflates each tile and replaces it by a set of original size tiles. Hierarchy indeed forbids periodicity: a translation which would leave invariant the tiling should do so at any level of the hierarchy, and could therefore not be finite. This led to ask whether aperiodicity is a general propery of hierarchical tilings – and this question is the backbone of the ANR project SubTile mentioned in Sec. 2.2. The answer turned out to be generally positive ([17, 43, 47, 70]), yielding infinite families of aperiodic tilings.

The hierarchical structure of aperiodic tilings was also used to embed Turing machine computations – the key ingredient of the proof of the undecidability of the domino problem. This led to study tilings as a model of computation – this is the backbone of the ANR project EMC mentioned in Sec. 2.2, which yielded surprising and powerful results ([3, 4, 35–39]).

In this context, the goal is to understand the expressive power of aperiodic tile sets. In particular, the size of these sets mainly remains an issue of secondary importance.[1]

The birth of quasicrystals

The scientific interest in aperiodic tilings – which were for a long time considered as recreational mathematics – was greatly renewed by the outstanding discovering of *quasicrystals* in 1982 ([83]). Quasicrystals (the term was proposed in 1984 in [66] and officially recognized only in

[1] Let us however mention the beautiful aperiodic tile set of size 14 found by Jarkko Kari ([55], see also [23]), which simulates a dynamical system topologically conjugated to an irrational rotation on the torus $\mathbb{R}/\mathbb{Z}$.

1992) share with crystals an *ordered* structure – revealed by sharp peaks in their X-ray diffraction diagram – but differ by their non-periodicity – revealed by so-called "forbidden symmetries" in their X-ray diffraction diagram. The connection with aperiodic tilings was quickly done, with the tiles modeling particularly stable cluster of atoms, and the finite range energetic interactions between atoms being modeled by local constraints on tiles. In this context, the size of aperiodic tile sets matters. Indeed, the larger a tile set is, the less realistic are the stable clusters of atoms which it aims to model. Thus, rather than finding the largest classes of aperiodic tilings, the issue now becomes finding classes of simple aperiodic tilings (that is, tilings by small aperiodic tile sets). In this way, the most promising results have been obtained for so-called $n \to d$ *tilings*.

Simple aperiodic $n \to d$ tilings

Let $n > d > 0$ and fix n pairwise non-colinear d-dimensional vectors $\vec{v}_1, \dots, \vec{v}_d$. A $n \to d$ tiling is a tiling of $\mathbb{R}^d$ whose tiles are parallelotopes generated by any d of the $\vec{v}_i$'s. For example, the Penrose tiling (Fig. 1) is a $5 \to 2$ tiling, while Fig. 3 depicts $3 \to 2$ tilings (aka *dimer tilings*).
It is convenient to provide an alternative viewpoint on $n \to d$ tilings. Let $\vec{e}_1, \dots, \vec{e}_n$ be the canonical basis of $\mathbb{R}^n$. Given a $n \to d$ tiling, let us arbitrarily map one of its vertex to $\vec{0} \in \mathbb{R}^n$, and then each tile generated by $\vec{v}_{i_1}, \dots, \vec{v}_{i_d}$ onto the d-dimensional face of a unit hypercube of $\mathbb{Z}^n$ generated by $\vec{e}_{i_1}, \dots, \vec{e}_{i_d}$, with two tiles adjacent along an edge $\vec{v}_i$ being mapped onto two faces adjacent along an edge $\vec{e}_i$. This defines (up to the choice of the vertex mapped to $\vec{0}$, *i.e.*, up to a translation) the *lift* of the tiling. This allows us to see $n \to d$ tilings as digital d-dimensional manifolds in $\mathbb{R}^n$. For example, the $3 \to 2$ tilings depicted on Fig. 3 can easily be seen as digital surfaces in $\mathbb{R}^3$ (piles of cubes).
Furthermore, if there exist a d-dimensional space $E \subset \mathbb{R}^n$ and a real $w \geq 1$ such that the lift of a $n \to d$ tiling entirely lies into the "slice" $E + [0, w)^n$, then this tiling is called a *plane tiling* of *slope* E and *width* w. Plane $n \to d$ tilings can be seen as digital d-dimensional spaces. For example, De Bruijn has proven in 1981 that the Penrose tiling (Fig. 1) is a unit width plane $5 \to 2$ tiling whose slope has Grassmann coordinates $(\varphi, 1, -1, -\varphi, \varphi, 1, -1, \varphi, 1, \varphi)$, where φ is the golden ratio ([24]). Unit width plane tilings are also called *cut and project tilings* ([45]).
We can now rephrase our question in this formalism: which plane tilings are aperiodic? More precisely: can we find an algebraic characterization of the slopes of aperiodic plane $n \to d$ tilings? The first general results in this way (beyond particular cases as the Penrose tiling or the Ammann-Beenker tiling [2]) were obtained in 1988 by Leonid Levitov ([67]). He provided a necessary condition on a two- or three-dimensional slope E for the existence of a finite collection of patterns, said to be *forbidden*, so that the only tilings where none of these patterns appears are the unit width plane tilings of slope E (that is, the tilings with the same finite patterns as the unit witdh plane tiling of slope E). He also provided a sufficient condition on E for the existence of forbidden patterns which allow only bounded width plane tilings of slope E. Let us stress that forbidden patterns are very simple local constraints (there is no edge colors propagated through the tiling). These results were then extended by several researchers ([18, 60–65, 84, 85]), but no complete algebraic characterization has yet emerged.

Growing aperiodic tilings

Beyond the problem of the structure of quasicrystals, there is the problem of their growth. The most natural way to proceed is to add one tile at time on random sites of the boundary of the grown patch, so that no local constraint is violated. However, the non-determinism of such a growth is inherent in the case of aperiodic tilings (this is, *e.g.*, an easy consequence of [34]). Joshua Socolar proposed in [86] (see also [71]) a very interesting modified process for the

Penrose tilings, where each tile is added on a site either with probability one if this is the only tile which can be added on this site, or with a small probability $\varepsilon > 0$ otherwise. He showed that the smaller ε is, the larger one gets a patch of a Penrose tiling before an error occurs. But the growth rate increases exponentially in $1/\varepsilon$! Actually, it was shown that any aperiodic tile set can form *deceptions*, that are arbitrarily big patches which do not violate the local constraints but cannot be extended to tilings of the whole plane ([40], see Fig. 2). In other word, such a

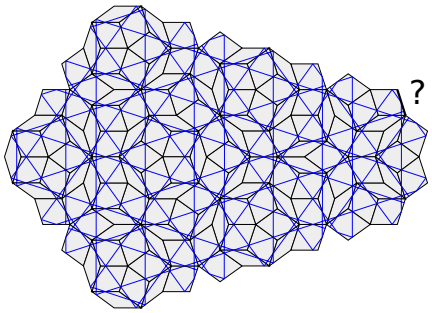


Figure 2: Either of the two Penrose tiles can be added along the emphasized edges (upper right corner) without violating the local constraints. However, only one choice leads to a patch which can then be extended to tile the whole plane.

process seems to inherently create errors which are only later discovered. As dire as that result may sound, some hope may be in the recently flourishing research on *self-assembly*, where a temperature parameter allows some control on the order tiles are added (see, *e.g.*, [7]). The application of self-assembly to aperiodic tilings remains however a largely uncharted research field.

The random tiling alternative

The first quasicrystals were obtained by very rapid cooling of a melt (*quenching*). They thus most likely have a structure stable at high temperature which would had be "frozen" by the quenching. Now, a general thermodynamic principle states that stability of a system is governed by the minimization of its free energy $F = E - TS$, where E is its interaction energy, S its entropy and T the temperature. At low temperature, this corresponds to minimize the interaction energy, that is, in terms of tilings, to satisfy the local constraints – this is the aperiodic tiling approach discussed above. But at high temperature, this corresponds to maximize the entropy. The (configurational) *entropy* of a tiling is usually defined as the logarithm of the number of different tilings that can be obtained by a rearrangement of its tiles (one gets the *entropy per tile* by dividing by the number of tiles in the tiling). This suggests an alternative approach to explain the structure of quasicrystals, which had been proposed soon after the discovery of quasicrystals ([41]): do the tilings of maximal entropy have a quasicrystalline structure? Note that tilings are here always considered up to rearrangements of tiles – one speaks about *random tiling ensemble* (see, *e.g.*, [50, 78]). Hence, the above question shall reads: does a tiling chosen uniformly at random in a random tiling ensemble of maximal entropy has with high probability a quasicrystalline structure? Or, in other words, do *typical* tilings of maximal entropy model quasicrystals?

Actually, the question of how looks like a typical tiling is prior to the discovery of quasicrystals. One can namely cite the work of Kasteleyn in 1961, who computed the entropy of some particular tilings ([56]). One of the most celebrated results is the *artic circle* theorem, proven in 1995 by James Propp and collaborators ([22, 51], see Fig. 3). This result has been nicely generalized

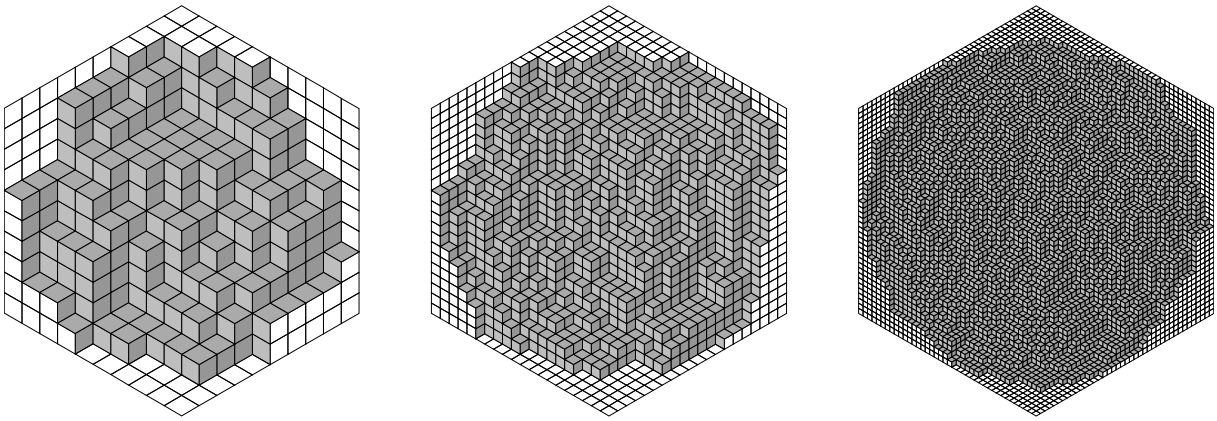


Figure 3: The boundary of the "frozen zone" (white tiles) of random $3 \to 2$ tilings of larger and larger hexagonal domains converges in probability towards a circle – called the "arctic circle" (from left to right).

by Andreï Okounkov and collaborators ([58, 59]) – it is actually one of the main results which earned him the 2006 Fields medal. The situation is even more complicated beyond the $3 \to 2$ case, and most of the known results (in particular due to Nicolas Destainville and collaborators, see [28, 30, 33, 91–93]) are numerical. Nevertheless, these results strongly suggest that typical tilings could have almost quasicristalline structure, with large-scale order being more or less preserved. In particular, X-ray diffraction does not make a big difference between random and aperiodic tilings. Random tilings thus seem explaining the structure of quasicrystals almost as good as aperiodic tilings do.
Now, what about the growth problem? The question is here somewhat different: instead of growing a particular aperiodic tiling, we "simply" need to grow one of the many, many tilings in a random tiling ensemble of maximal entropy. Numerous simulations suggest that this could be easier ([52–54, 87, 89]), although no rigorous result has yet been obtained.

Random or aperiodic tilings?

Recent progress of the experimental research, though, challenged the random tiling model. While first quasicrystals were obtained by quenching, the actual ones are now obtained by slow cooling (Bridgman–Stockbarger technique). Moreover, the development of high-resolution transmission electron microscopy (HRTEM), which yields a much deeper insight than X-Ray diffraction into quasicrystals, showed that slow cooling can produce much better quasicrystals than fast cooling (Fig. 4). The figure is thus a bit schizophrenic. On the one hand, random tilings seem better modeling the growth of quasicrystals and their structure at high temperature. On the other hand, aperiodic tilings seem better modeling the quasicrystal structure at low temperature. This discrepancy was the starting point of the two-year multidisciplinary exploratory project StochasFlip (for "stochastic flips"), which involved most of the participants of our team (see Section 5.3) and recently finished.

StochasFlip

The leading idea of the project StochasFlip was to model the slow cooling of quasicrystals by stochastic local transformations on an initial random tiling, with the more violated local constraints being corrected by a transformation, the higher is the probability of this transformation to be performed. In other words, starting at high temperature from an entropically-stabilized tiling (a random tiling), energetically-driven local transformations are stochastically performed,

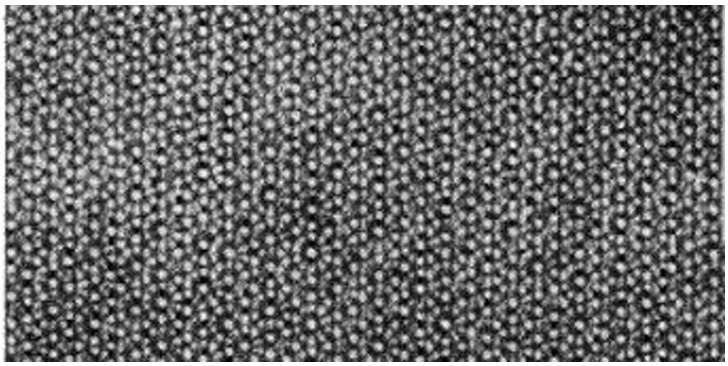


Figure 4: HRTEM reveals the quasi perfect aperiodic structure of modern quasicrystals.

until an energetically-stabilized tiling is obtained (an aperiodic tiling). This idea was exposed to the sixth International Conference on Aperiodic Crystals, organized under the auspices of the Commission on Aperiodic Crystals of the International Union of Crystallography ([12]). More precisely, the initial random tiling is a finite patch of a $n \to d$ tiling, the local transformations are the so-called *flips* (see below), and the final "aperiodic" tiling is a finite patch of an aperiodic $n \to d$ plane tiling. The cooling process is thus a discrete time Markov chain on a finite space, and our main concern are asymptotics of its convergence rate when the space size goes to infinity. The cooling has been proven to be rapid when the Markov chain is time-homogeneous in the most simple cases ($2 \to 1$ and $3 \to 2$ tilings, see [13, 44]). Simulations for $4 \to 2$ and $5 \to 2$ tilings (Fig. 5) show a still rapid cooling, but no rigorous result have yet been obtained in these much more difficult cases. The case of $n \to d$ tilings for larger n or d remains largely unexplored.

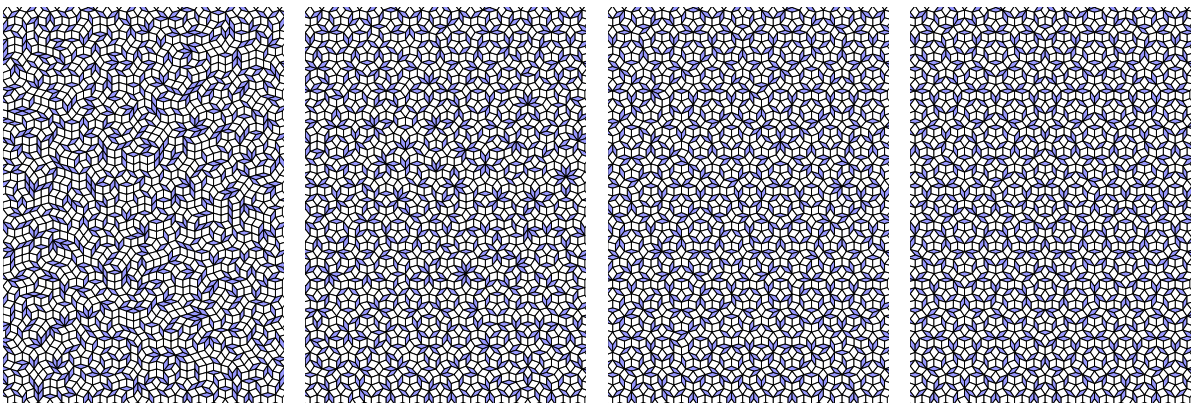


Figure 5: The cooling of a $5 \to 2$ random tiling rapidly yields a Penrose tiling (from left to right).

Flip spaces

Whenever a vertex x of a $n \to d$ tiling belongs to exactly $d+1$ tiles, one gets a new tiling of the same region by translating each of these tiles by the vector which belongs to the d other tiles (Fig. 6). This local transformation on $n \to d$ tilings is the above mentioned *flip*; it generalizes a notion introduced by William Thurston in [88] in the particular case of domino tilings. Flips naturally endow each random tiling ensemble with a structure of graph: tilings are vertices,

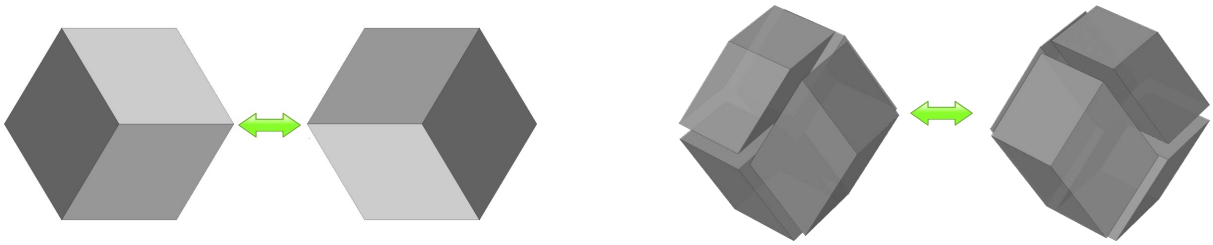


Figure 6: A flip swaps three rhombi for $d = 2$ (left), four rhomboedra for $d = 3$ (right, exploded view).

with each tiling being connected to the tilings which can be obtained by performing a flip. We call *flip space* this graph. Some properties of its structure are already known. It is connected for $n \to 2$ tilings ([57], see also [14]), but not always for $n \to d$ tilings with $d \geq 3$ ([31, 32]). It has a structure of distributive lattice for $3 \to 2$ tilings ([73]), of graded poset for $4 \to 2$ tilings ([21]). Some deeper insight in the fine structure of this graph has also been obtained in [11, 29]. The comprehension of this structure is crucial in order to study the convergence rate of the above defined cooling process, and there is still much work to be done for this purpose. Let us mention, to conclude, that in the case of a process where flips are equiprobable, a bound on the convergence rate (or mixing time) has recently been obtained ([20], see also [68, 94] for a slightly different chain). This corresponds however rather to the evolution of the random tiling ensemble at high temperature than to the cooling we are interested in.

2.4 Objectives, originality and novelty of the project

Our project has three main general objectives:

1. algebraic characterization of aperiodic planar $n \to d$ tilings, depending on the power of the considered local constraints (basically: the number of colors used by matching rules);
2. algebraic characterization of the random $n \to d$ tilings of maximal entropy and characterization of their typical properties (*e.g.*, number of flips to reach an aperiodic tiling);
3. asymptotics of the convergence rate of the cooling process for $n \to d$ tilings.

We are aware that the two first objectives can sound much too ambitious. The first one has indeed been investigated for around 50 years by many scientists, while the second one aims to find a broad generalization of a result which recently earned a Fields medal! But these objectives do not follow a zero-one law: numerous partial results can be obtained. In particular, each objective on $n \to d$ tilings can be splitted in as many cases as there are values of n and d (the complexity of such "sub-objectives" is expected to grow with n and d). The third objective is much more original and offers a new challenge – but bounding convergence rates of Markov chains is generally a hard task!

3 Scientific and technical programme, project organization

3.1 Scientific program, project structure

Our program is structured in five connected tasks:

1. "flip spaces" studies the structure flips endow random tiling ensembles with;
2. "self-assembly" aims to model the growth of random or aperiodic tilings;
3. "random tilings" studies the starting point of the cooling;
4. "aperiodic tilings" studies the ending point of the cooling;
5. "cooling" aims to explain the slow cooling of quasicrystals (our main goal).

In addition, there is a task dedicated to the coordination of the project. Fig. 7 summarizes these tasks, as well as their connections (which are detailed in Sec. 3.3).

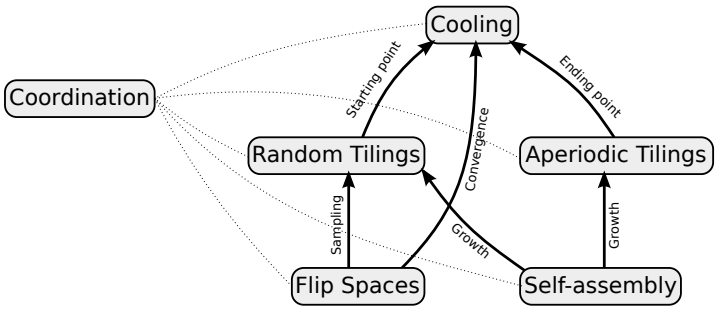


Figure 7: Structure of the project QuasiCool.

3.2 Project management

The project management is detailed in the description of the coordination task (Task 0, below).

3.3 Description by task

3.3.0 Task 0: Coordination

Involved: Thomas Fernique

Our project involves people from different universities in different cities – namely Marseille, Paris, Lyon and Orléans. Train connections between these cities are highly efficient, and strong bonds between participants already exist.[2] Nevertheless, the coordination is of course more challenging than if we would all be in the same place. To meet this challenge, we plane to create a web site which will be collectively maintained (namely a *wiki*, as it was done by the coordinator for the projects SubTile and Stochasflip) and to organize twice a year meetings bringing all the participants together – and possibly a few external people to give a talk and discuss with. Smaller meetings (*e.g.*, between participants to a common task) will also be regularly held.

[2]In particular, Th. Fernique was already the coordinator of the two-year project Stochasflip, which involved O. Bodini, D. Regnault, É. Rémila and M. Sablik. Also, N. Bédaride, Th. Fernique and M. Sablik have together organized in Marseille in februar-march 2010 a five-week conference with 280 participants.

3.3.1 Task 1: Flip spaces

Involved: Éric Rémila, Olivier Bodini, Thomas Fernique

This task studies graphs obtained by endowing random tiling ensembles with the flip operation (flip spaces). This is essential to get sharp bounds on the convergence rate of our cooling process (Task 5). This is also useful for random sampling of tilings, in order to numerically investigate random tiling ensemble properties (Task 3). As for any basic research project, it is hard to forecast which result will be obtained. Let us give some precise examples of questions that we will investigate:

- How tight is the bound of [11] on the number of flips between two tilings?
- Does the expansion factor of flips spaces match the *expander sampling walk lemma* ([1, 46])?
- Which three-dimensional flip spaces are connected? What if we extend the notion of flip?
- Do flip spaces remain connected when some flips[3] are forbidden?

3.3.2 Task 2: Self-assembly

Involved: Florent Becker, Éric Rémila, Thomas Fernique

The aim of this task is to model the growth of random or aperiodic tilings by self-assembly, that is, with tiles being added one at a time (and a temperature parameter which allows some control on the order tiles can be added). The main problems we will consider are:

- the self-assembly of substitutive tilings;
- the self-assembly of plane tilings depending on their width;
- the self-assembly of random $n \to d$ tilings.

These problems have yet been only numerically considered, and providing rigorous results is very challenging, except maybe in some easier case (*e.g.*, $n \to 1$ or $3 \to 2$ tilings).

3.3.3 Task 3: Random tilings

Involved: Olivier Bodini, Mathieu Sablik, Thomas Fernique

The cooling process we want to study (Task 5) starts from a random tiling of maximal entropy. But characterizing such tilings need a significant amount of work. This work falls to Task 3. The main problems we will consider are:

- algebraic characterization of the slopes of plane $n \to d$ tilings which maximize the entropy;
- random sampling of $n \to d$ tilings by flips (with bounds on the convergence rate);
- numerical and theoretical investigations of properties of typical random $n \to d$ tilings of maximal entropy (*e.g.*, width, energy, arctic circle like theorem *etc.*).

[3] For example, those with a low probability in the cooling process, see Task 5.

3.3.4 Task 4: Aperiodic tilings

Involved: Mathieu Sablik, Nicolas Bédaride, Thomas Fernique

The local constraints which characterize aperiodic tilings are a key ingredient in the cooling process we are interested in, since the probability of each random flip strongly relies on them (see Task 5). We thus first need to study these local constraints. In particular, we want to

- prove that $n \to d$ plane tilings are aperiodic if and only if they have computable slopes;
- find an algebraic characterization of the slopes of simple aperiodic $n \to d$ plane tilings (or, at least, find new interesting necessary and/or sufficient conditions on these slopes);
- better understand how aperiodicity (in particular hierarchical aperiodicity) is enforced by local constraints, in order to sharply reduce the complexity of these local constraints;
- investigate which $n \to d$ tilings are aperiodic beyond the planar ones.

3.3.5 Task 5: Cooling

Involved: Damien Regnault, Olivier Bodini, Thomas Fernique

This task aims to model and explain the slow cooling of quasicrystals. This is actually the main purpose of our project. The idea is to randomly perform flips on an initial random tiling of maximal entropy (Task 3), with the temperature decreasing until zero – the process then stops. Each random flip is performed with a probability which depends on the variation of the number of violated local constraints it changes, that is, the energy variation. More precisely, this probability is $\min(1, \exp(-\Delta E/T))$, where ΔE is the energy variation and T the temperature. This is thus, at fixed temperature, the Glauber dynamics for the Gibbs distribution. And when the temperature decreases, this is a classical *simulated annealing* process. However, simulations carried out as part of our project StochasFlip indicate that this cooling process converges much faster than the bound given by general results on simulated annealing (polynomial versus exponential convergence rate). To establish rigorous results in this way, we are guided by the following main questions:

- What is the mixing time at fixed temperature T (in particular when $T = \infty$ or $T = 0$)?
- Which *cooling schedule*[4] does minimize the convergence rate towards an aperiodic tiling?
- What if the initial random tiling cannot be transformed into an aperiodic tiling?[5]

3.4 TASKS SCHEDULE, DELIVERABLES AND MILESTONES

The schedule of the different tasks is represented on Fig. 8 (the coordination task, not represented, obviously runs during the whole project). Since each task can be decomposed in as many subtasks as there are types of considered tilings, the dependancies between the tasks (represented by directed edges on Fig. 7) can be accordingly decomposed. This allows to carry out tasks in parallel – up to small shifts due to the dependencies between subtasks.

[4]The cooling schedule (or simulated annealing schedule) specifies how the temperature varies with time.
[5]This happens, for example, when both tilings have different tile proportions that flips cannot equal.

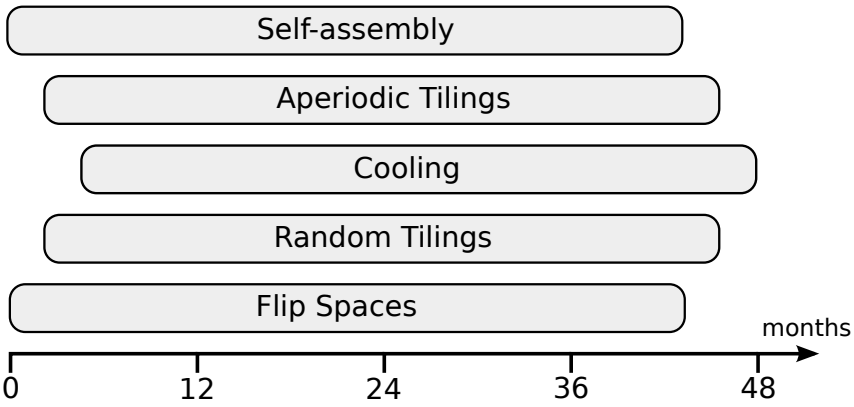


Figure 8: Schedule of the tasks of the project QuasiCool.

4 Dissemination and exploitation of results. Intellectual property

As usually in basic research, we plane to disseminate our results in publications of research articles in international scientific journals, as well as in oral communications in international conferences. A list of these publications will be maintained on the webpage of the project.

We moreover plane to organize two international conferences on topics closely related to our project. The first one, to be held rapidly after the beginning of our project, shall give us the opportunity to get a deeper understanding of the latest results in the domain and to start collaborations with renowned scientists. The second one, to be held at the end of our project, shall give us the opportunity to spread the outcome of our project to the scientific community.

We also plane more original actions as creating short tutorial videos that shall be uploaded on video-sharing websites, and making aperiodic tile sets (using cardboard, wood or acrylic glass) that shall be used in workshops of science popularization (*e.g.*, "Maths en Jeans" or "Fête de la science"). Such actions intend to spread the essence of some fundamental concepts of our project (*e.g.*, aperiodicity) beyond the restricted circle of specialists.

5 Team description

5.1 Partners description & relevance, complementarity

The project QuasiCool has seven participants (two mathematicians and five computer scientists). They all have a significant experience of the questions arising in the task there are involved in.

Flip spaces Éric Rémila studied flips on tilings for some time and has already numerous publications on the subject ([21, 26, 27, 69, 81]). Recent collaborations [10, 11, 14, 16] with Olivier Bodini and/or Thomas Fernique led to study more general flip spaces. They are thus in the perfect situation to pursue this work.

Self-assembly Florent Becker defended in 2008 his Ph.D. on self-assembly. He has published two papers on the subject ([5, 6]) and one in collaboration with Éric Rémila ([8]). They

already started to work on the new subject of the self-assembly of aperiodic tilings (namely the Robinson tiling), and are thus in a position to tackle this question in our project.

Random tilings The expertise of Olivier Bodini in analytic combinatorics allowed him to recently find the first polynomial-time sampler for random tiling according to their size ([15]). Together with the expertise of Mathieu Sablik in probability theory, this shall be of great help in order to tackle the issues raised by our project.

Aperiodic tilings Mathieu Sablik recently obtained powerful results on aperiodic tilings via a computational approach ([3, 4]). He also brings his expertise in dynamical systems (see, *e.g.*, [25, 49, 82]). Mathieu Sablik and Thomas Fernique also independently showed how to locally describe a wide class of substitutive tilings ([17, 43]). Nicolas Bédaride recently went on tilings ([19]), where he brings his expertise in geometry. They currently already regularly meet in order to extend these results in the direction of our project.

Cooling Damien Regnault defended in 2008 his Ph.D. on asynchronous cellular automata, that are specific discrete time Markov chains. He obtained several results on the mixing time of these chains ([42, 74–77, 80]). Then, together with Thomas Fernique and Olivier Bodini (within the project Stochasflip), the techniques used on cellular automata were extended to some tilings to get the first theoretical results on the cooling of quasicrystals ([12, 13, 44]). They are thus in the perfect situation to extend these results to more general tilings.

5.2 Qualification of the project coordinator

Thomas Fernique is the most natural coordinator for the following reasons:

- he knows well all the participants (at least one year spent with each one at the same place);
- as a full-time researcher (since october 2008), he can spend much time to the coordination;
- he was the coordinator of the project StochasFlip, which was the precursor of this project;
- the former point, as well as the serie of lectures on the subject he gave to the Ph.D. students of the University of Moscow in spring 2011, allowed him to mature this project.

5.3 Qualification and contribution of each partner

The following table summarizes the involvment of the participants (total: 196 person.month):

Nom	Prénom	Emploi actuel	Discipline	Personne × mois	Rôle/Responsabilité dans le projet (4 lignes max.)
Becker	Florent	MdC	Informatique	24	Expertise: Self-assembly Involved in Task 1
Bédaride	Nicolas	MdC	Mathématiques	12	Expertise: Geometry of tilings Involved in Task 4
Bodini	Olivier	Pr	Informatique	24	Expertise: Random tilings Involved in Tasks 1,3,5
Fernique	**Thomas**	**CR CNRS**	**Informatique**	**36**	**Coordinator.** **Involved in Tasks 0–5**
Sablik	Mathieu	MdC	Mathématiques	24	Expertise: Aperiodic tilings Involved in Tasks 3,4
Regnault	Damien	MdC	Informatique	16	Expertise: Mixing times Involved in Task 5
Rémila	Éric	MdC	Informatique	24	Expertise: Flip spaces Involved in Tasks 1,2
		Ph.D. Student		36	To be preferably involved in Task 4

Most of the participants are also involved in other projects, as indicated by the table below.

Nom de la personne participant au projet	Personne × mois	Intitulé de l'appel à projets, Source de financement, Montant attribué	Titre du projet	Nom du coordinateur	Date début & Date fin
N. Bédaride	36	ANR JCJC 2010	LAM	A. Hilion	2011/2014
O. Bodini	6	PEPS Maths-ST2I	Stochasflip	Th. Fernique	2010/2011
	24	ANR Blanc 2010	Magnum	M. Soria	2011/2014
	24	ANR Blanc 2006	Gamma	F. Bassino	2007/2010
Th. Fernique	6	PEPS Maths-ST2I	Stochasflip	Th. Fernique	2010/2011
	24	ANR Blanc 2008	Subtile	P. Arnoux	2009/2012
	12	ANR Blanc 2008	EMC	B. Durand	2009/2012
	12	ANR Blanc 2007	Lareda	B. Vallée	2007/2009
M. Sablik	6	PEPS Maths-ST2I	Stochasflip	Th. Fernique	2010/2011
	12	ANR Blanc 2008	Subtile	P. Arnoux	2009/2012
	24	ANR Blanc 2008	EMC	B. Durand	2009/2012
D. Regnault	6	PEPS Maths-ST2I	Stochasflip	Th. Fernique	2010/2011
É. Rémila	6	PEPS Maths-ST2I	Stochasflip	Th. Fernique	2010/2011
	12	ANR-Blanc 2009	MINT	A. Rusinowska	2009/2013
	12	ANR-Blanc 2006	MecaMerge	É. Rémila	2007/2010
	24	ANR-Blanc 2008	SubTile	P. Arnoux	2009/2012

Note that the projects EMC and SubTile, which involve some of us, last until the end of 2012. There could thus be a short overlap with this current project (depending when the grant is afforded). We however decided to present our project now, for at least two reasons. First, waiting for the next year to present our project would let most of us several months without any grant. Second, the maturation of our project has now reached a critical point that makes it natural to be started now, branching out from the projects EMC and SubTile. Let us also mention that the project Magnum (which continues the project Gamma) can bring us via O. Bodini powerful technics in analytic combinatorics and random sampling, that shall be especially useful (task 3).

6 Scientific justification of requested ressources

Equipment

None.

Staff

We ask 105848, 64€ – the cost of a complete Ph.D. at the University Paris 13.

We indeed would like to hire a Ph.D. student to work within our ambitious project. A first reason is that there is a lot of work to be done, and a full-time participant shall help us very much. A second reason is that the coordinator of the project, Thomas Fernique, spent the last year at the french-russian laboratory Poncelet, in the Independant University of Moscow (Russia), where he met many gifted students very interested in doing a Ph.D. in France, or between France and Russia (cotutelle). This idea is encouraged by the head of the Poncelet lab., Michael Tsfasman – it is indeed a very good way to set up a collaboration between France and Russia.

As regards the scientific part, this Ph.D. could going in several directions of our project, but a preferential way would be the one explored by the "Moscow school" ([18, 60–65, 67]), which

works in the framework of algebraic geometry in order to get very simple aperiodic $n \to d$ tilings. Precisely, a challenging problem could be to show how the width of an aperiodic $n \to d$ tiling can be decreased by adding as few as possible new local constraints (in Levitov terminology: how weak matching rules can be transformed into strong matching rules). This perfectly fits the objectives of Task 4 and opens a wide range of non-trivial questions.

Subcontracting

None.

Travel

We ask a total of 96800€ for travels. This amount breaks down as follows:

- Invitations of international researcher for short stays (one week) of intensive collaboration. Such stays are yearly planed, and the cost of each is estimated at 2500€.
  Cost: $4 \times 2500 = 10000$€
- The cost of travels of the participants of our project to attend international conferences or schools (in particular to present their results) is estimated at 3000€ for 12 person-months.
  Cost: $3000 \times 196/12 = 49000$€
- We need around 200€ for each participant (7 plus one Ph.D. student) for each of the bi-annual internal meetings we intend to hold.
  Cost: $200 \times (7+1) \times 2 \times 4 = 12800$€
- Last, as explained in Sec. 4, we want to organize two international conferences during our project. For each, we would like to invite five renowned international scientists to give lectures that would benefit to the whole community.
  Cost: $2 \times 5 \times 2500 = 25000$€

Internal expenses

None.

Other expenses

We ask a total of 18867€ for other expenses. This amount breaks down as follows:

- We need to buy specialized books that are not (or not easily) accessible to participants. We count on five books at around 70€ each for 12 person-months.
  Cost: $5 \times 70 \times 196/12 = 5700$€
- Laptops are essential to us, in particular to present our results abroad. We estimate the cost of the upgrade or maintenance of our computer equipment at 1500€ for 36 person-month (this includes, *e.g.*, one laptop for the Ph.D. student).
  Cost: $1500 \times 196/36 = 8167$€
- The original actions we plane to disseminate some fundamental concepts of our project beyond the retricted circle of specialists (see last paragraph of Sec. 4) will lead us to turn to professionals (*e.g.*, laser cutting of aperiodic tiles).
  Cost: ~ 5000€

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8 CV, Resume

One page per member, coordinator first, then in alphabetical order.

Surname, First Name	**Fernique, Thomas**
Webpage	http://www.lipn.univ-paris13.fr/~fernique/
Age	30
Curriculum	
2011–Now	Junior CNRS researcher at the LIPN (Univ. Paris 13)
2010–2011	Junior CNRS researcher at the Poncelet lab. (Moscow)
2008–2010	Junior CNRS researcher at the LIF (Univ. Marseille)
2008	Post-doctoral fellow, Univ. Novosibirsk (Russia)
2004–2007	Ph.D. student at the LIRMM (Univ. Montpellier)
2001–2005	Student at the ÉNS Lyon
Other Activities	
2011	Involved in Maths en Jeans, Lycée français de Moscou
2010	Member of the organizing committee of the Math-Info thematic semester (februar–july, CIRM, Marseille)
2004–2005	Invited at Poncelet lab., Moscow, Russia

Total number of publications: 19

Selected publications

1. O. Bodini, Th. Fernique, M. Rao, and É. Rémila. Distances on rhombus tilings. *Theor. Comput. Sci.*, 412(36):4787–4794, 2011.
2. O. Bodini, Th. Fernique, and D. Regnault. Crystallization by stochastic flips. *Journal of Physics: Conference Series*, 226:012022, 2010.
3. O. Bodini, Th. Fernique, and D. Regnault. Stochastic flips on two-letter words. In M. Golin and R. Sedgewick, editors, *Proceedings of the 7th Workshop on Analytic Algorithmics and Combinatorics*, pages 48–55. SIAM Journal on Computing, 2010.
4. Th. Fernique and N. Ollinger. Combinatorial substitutions and sofic tilings. In J. Kari, editor, *JAC*, pages 100–110. Turku Center for Computer Science, 2010.
5. Th. Fernique and D. Regnault. Stochastic flips on dimer tilings. In M. Drmota and B. Gittenberger, editors, *21st International Meeting on Probabilistic, Combinatorial, and Asymptotic Methods in the Analysis of Algorithms*, pages 205–218. DMTCS, 2010.

Surname, First Name	**Becker, Florent**
Webpage	http://www.univ-orleans.fr/lifo/Members/Florent.Becker/
Age	28

Curriculum

2009–Now	Assistant professor (MdC) at the LIFO (Univ. Orléans)
2008–2009	Post-doctoral fellow, Univ. Berlin (Germany)
2005–2007	Ph.D. student, ÉNS Lyon
2002–2006	Student at the ÉNS Lyon

Total number of publications: 7

Selected publications

1. F. Becker, É. Rémila, and N. Schabanel. Time optimal self-assembly for 2D and 3D shapes: the case of squares and cubes. In A. Goel, F. C. Simmel, and P. Sosík, editors, *DNA Computing*, pages 144–155. Springer, 2009.
2. F. Becker. Transformations and preservation of self-assembly dynamics through homotheties. In C. Martín-Vide, F. Otto, and H. Fernau, editors, *LATA*, volume 5196 of *Lecture Notes in Computer Science*, pages 101–112. Springer, 2008.
3. F. Becker. Pictures worth a thousand tiles, a geometrical programming language for self-assembly. *Theor. Comput. Sci.*, 410(16):1495–1515, 2009.
4. F. Becker, S. Rajsbaum, I. Rapaport, and É. Rémila. Average binary longlived consensus: Quantifying the stabilizing role played by memory. In A. A. Shvartsman and P. Felber, editors, *SIROCCO*, volume 5058 of *Lecture Notes in Computer Science*, pages 48–60. Springer, 2008.
5. F. Becker. Transformations and preservation of self-assembly dynamics through homotheties. In C. Martín-Vide, F. Otto, and H. Fernau, editors, *LATA*, volume 5196 of *Lecture Notes in Computer Science*, pages 101–112. Springer, 2008.

Surname, First Name	**Bédaride, Nicolas**
Webpage	http://junon.u-3mrs.fr/bedaride/
Age	35
Curriculum	
2007–Now	Assistant professor (MdC) at the LATP (Univ. Marseille)
2005–2007	Teaching & research assistant (ATER), Univ. Marseille
2001–2004	Ph.D. student, Univ. Marseille
2001	Master thesis of mathematics, Univ. Marseille
2000	Agrégation de mathématiques
Other Activities	
2011	Member of the organizing committee of the conference *Laminations and symbolic dynamics* (april, CIRM, Marseille)
2010	Member of the organizing committee of the Math-Info thematic semester (februar–july, CIRM, Marseille)

Total number of publications: 9

Selected publications

1. N. Bédaride and A. Hilion. Geometric realizations of two-dimensional substitutive tilings. arXiv:1101.3905v2.
2. N. Bédaride and J. Cassaigne. Outer billiard outside regular polygons. *J. London Math. Soc.* 2011: jdr010v1-jdr010.
3. N. Bédaride and E. Domenjoud and D. Jamet and J. L. Remy. Number of balanced words for a given length and height. *Discrete mathematics and theoretical computer sciences*, 12(3):41–62, 2010.
4. N. Bédaride. Directional complexity of the hypercubic billiard, *Discrete mathematics*, 309:2053–2066, 2009.
5. N. Bédaride and P. Hubert. Billiard complexity in the hypercube. *Annales de l'institut Fourier*, 57(3):719–738, 2007.

Surname, First Name	**Bodini, Olivier**
Webpage	http://www.lipn.univ-paris13.fr/~bodini/
Age	41
Curriculum	
2011–Now	Full professor (Pr) at the LIPN (Univ. Paris 13)
2006–2011	Assistant professor (MdC) at the LIP6 (Univ. Paris 6)
2003–2005	Assistant professor (MdC) at the LIRMM (Univ. Montpellier)
2001–2002	Teaching & research assistant (ATER), ÉNS Lyon
2000–2001	Teaching & research assistant (ATER), Univ. Paris 6
1996–1999	Ph.D. student, Univ. Paris 6
Other Activities	
2010	Member of the organizing committee of ALEA'10
1995–1999	Involved in Maths en jeans (+creation of the website in 1999).

Total number of publications: 30

Selected publications

1. O. Bodini, Th. Fernique, M. Rao, and É. Rémila. Distances on rhombus tilings. *Theor. Comput. Sci.*, 412(36):4787–4794, 2011.
2. O. Bodini, Th. Fernique, and D. Regnault. Crystallization by stochastic flips. *Journal of Physics: Conference Series*, 226:012022, 2010.
3. O. Bodini, Th. Fernique, and D. Regnault. Stochastic flips on two-letter words. In M. Golin and R. Sedgewick, editors, *Proceedings of the 7th Workshop on Analytic Algorithmics and Combinatorics*, pages 48–55. SIAM Journal on Computing, 2010.
4. O. Bodini, É Fusy, and C. Pivoteau. Random sampling of plane partitions. *Combinatorics, Probability & Computing*, 19(2):201–226, 2010.
5. O. Bodini and É. Rémila. Tilings with trichromatic colored-edges triangles. *Theor. Comput. Sci.*, 319(1-3):59–70, 2004.

Surname, First Name	**Regnault, Damien**
Webpage	http://www.ibisc.fr/~dregnault/
Age	29

Curriculum

2010–Now	Assistant professor (MdC) at the Ibisc (Univ. Évry-Val-d'Essone)
2009–2010	Teaching assistant (ATER) at the LIF (Univ. Marseille)
2005–2008	Ph.D. student, ÉNS Lyon
2002–2006	Student at the ÉNS Lyon

Total number of publications: 12

Selected publications

1. O. Bodini, Th. Fernique, and D. Regnault. Crystallization by stochastic flips. *Journal of Physics: Conference Series*, 226:012022, 2010.
2. O. Bodini, Th. Fernique, and D. Regnault. Stochastic flips on two-letter words. In M. Golin and R. Sedgewick, editors, *Proceedings of the 7th Workshop on Analytic Algorithmics and Combinatorics*, pages 48–55. SIAM Journal on Computing, 2010.
3. Th. Fernique and D. Regnault. Stochastic flips on dimer tilings. In M. Drmota and B. Gittenberger, editors, *21st International Meeting on Probabilistic, Combinatorial, and Asymptotic Methods in the Analysis of Algorithms*, pages 205–218. DMTCS, 2010.
4. D. Regnault, N. Schabanel, and É. Thierry. On the analysis of "simple" 2D stochastic cellular automata. *Discrete Mathematics & Theoretical Computer Science*, 12(2):263–294, 2010.
5. D. Regnault, N. Schabanel, and É. Thierry. Progresses in the analysis of stochastic 2D cellular automata: A study of asynchronous 2d minority. *Theor. Comput. Sci.*, 410(47-49):4844–4855, 2009.

Surname, First Name	**Rémila, Éric**
Webpage	http://perso.ens-lyon.fr/eric.remila/
Age	52
Curriculum	
1994–Now	Assistant professor (MdC) at the LIP (Univ. Lyon)
1997	Habilitation thesis (HDR), Univ. d'Auvergne
1991–1994	(PRAG), IUT Roanne
1992	Ph.D., Univ. Lyon
1983	Agrégation de mathématiques
Other Activities	
1999–Now	Organisation of 7 conferences (includeing four international ones)

Total number of publications: 73

Selected publications

1. O. Bodini, Th. Fernique, M. Rao, and É. Rémila. Distances on rhombus tilings. *Theor. Comput. Sci.*, 412(36):4787–4794, 2011.
2. O. Bodini, Th. Fernique, and É. Rémila. A characterization of flip-accessibility for rhombus tilings of the whole plane. *Inf. Comput.*, 206:1065–1073, 2008.
3. F. Chavanon and É. Rémila. Rhombus tilings: Decomposition and space structure. *Discrete Comput. Geom.*, 35:329–358, 2006.
4. É. Rémila. The lattice structure of the set of domino tilings of a polygon. *Theor. Comput. Sci.*, 322(2):409–422, 2004.
5. O. Bodini and É. Rémila. Tilings with trichromatic colored-edges triangles. *Theor. Comput. Sci.*, 319(1-3):59–70, 2004.

Surname, First Name	**Sablik, Mathieu**
Webpage	http://www.latp.univ-mrs.fr/~sablik/
Age	33
Curriculum	
2009–Now	Assistant professor (MdC) at the LATP (Univ. Marseille)
2006–2008	ATER, ÉNS Lyon
2003–2006	Ph.D. student, Univ. Marseille
2002	Agrégation de mathématiques
1999–2003	Student at the ÉNS Lyon
Other Activities	
2010	Member of the organizing committee of the Math-Info thematic semester (februar–july, CIRM, Marseille)

Total number of publications: 14

Selected publications

1. N. Aubrun and M. Sablik. Multidimensional effective S-adic systems are sofic. preprint,
2. N. Aubrun and M. Sablik. Simulation of recursively enumerable subshifts by two dimensional SFT. to appear in *Acta Appl. Math.*, 2012.
3. M. Delacourt, V. Poupet, M. Sablik, and G. Theyssier. Directional dynamics along arbitrary curves in cellular automata. *Theor. Comput. Sci.*, 412(30):3800–3821, 2011.
4. B. Hellouin de Menibus and M. Sablik. Self-organization in cellular automata: A particle-based approach. In G. Mauri and A. Leporati, editors, *Developments in Language Theory*, volume 6795 of *Lecture Notes in Computer Science*, pages 251–263. Springer, 2011.
5. M. Sablik and G. Theyssier. Topological dynamics of cellular automata: Dimension matters. *Theory Comput. Syst.*, 48(3):693–714, 2011.