THE EVOLUTION OF A CRYSTAL

Year 2024-2025

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Contents:

Research topic

On a hexagonal grid, we have two types of cells: frozen and non-frozen.

❖ In the next evolution, a non-frozen cell becomes frozen if it is adjacent to 1, 3, 4, 5, or 6 frozen cells. [1]
❖ A frozen cell always remains frozen.
❖ If in the initial evolution (n°0) there is only one frozen cell, what can we say about the subsequent evolutions? Number of frozen cells, diameter, shape...

Approaches and problem solving

Two primary approaches can be identified in modeling the freezing process:

1. **Sequential freezing:** Only one cell is allowed to freeze per iteration, even when multiple cells fulfill the condition. [2]

2. **Simultaneous freezing:** All cells that meet the specified condition freeze at the same time within a single iteration.

These distinct interpretations of the freezing mechanism result in different modeling methodologies and can lead to substantially different system behaviors and outcomes.

I. First approach (sequential freezing)

1. Concepts and constructs

In Sequential Freezing, only one eligible non-frozen cell freezes at a time, and it is randomly chosen. We focused on the Sequential Freezing model, while other groups studied the Simultaneous Freezing model. Both interpretations have applications in physics.

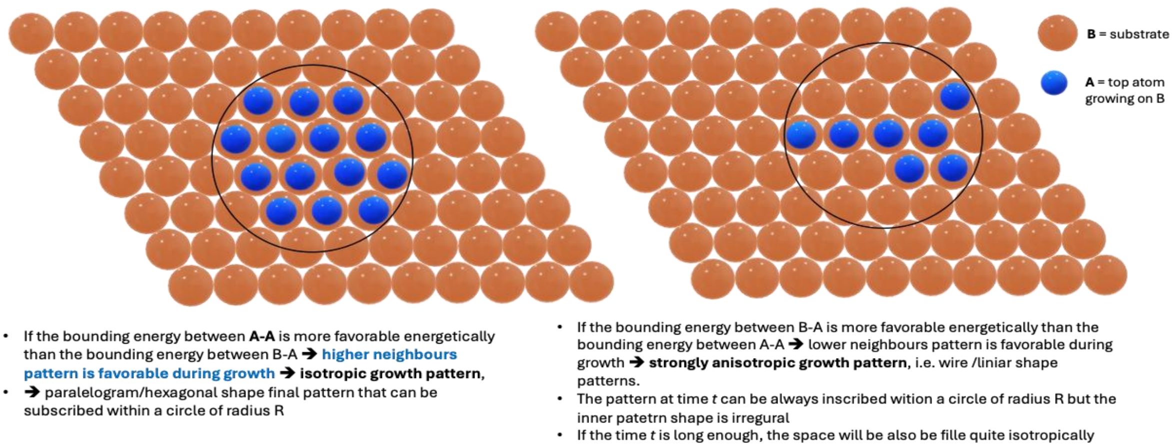


Fig.1 - Isotropic & Anisotropic case

Two main cases of freezing are considered: the Neighbors Case, also called the growing Isotropic Case, and the Random Case, also called the growing Anisotropic Case. In the Neighbors Case, cells with the most frozen neighbors freeze first. Over time, there will be no cells with 4, 5, or 6 frozen neighbors because cells with 3 frozen neighbors are frozen before this happens. The result is a sequence of regular shapes forming after each step. In the Random Case, any eligible non-frozen cell can freeze randomly as long as all conditions are met. Since the Random Case is random, the evolution cannot be predicted except by observing the anisotropic growth. For both cases, the number of frozen cells corresponds to the number of steps. Our analysis focuses on the Neighbors Case, where we observe specific regular shapes forming in predictable patterns. In the Neighbors Case, a step occurs when a single cell freezes, noted by "n." An active step is the first step that forms a new regular shape, and the sequence of frozen cells after this step determines the next shape and the next active step, noted by "s."

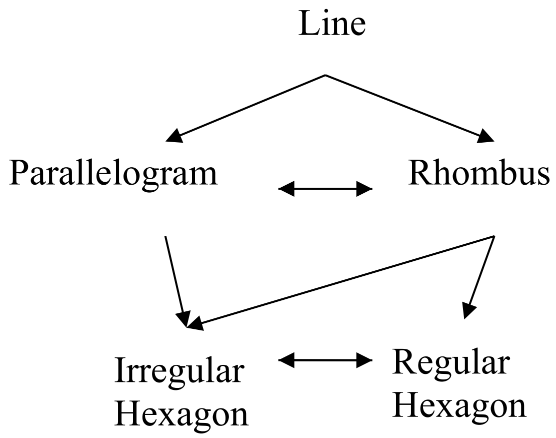


Fig.2 - Scheme of probabilities

The regular shapes that appear in the Neighbors Case are Line, Parallelogram, Rhombus, Regular Hexagon, and Irregular Hexagon. From these, we consider the symmetrical shapes to be most important: Line, Rhombus, and Regular Hexagon. We also often reference the smallest rhombus and the smallest regular hexagon, which are the simplest symmetrical shapes in the grid. While a rhombus is technically a type of parallelogram, we treat them as distinct shapes for clarity. A rhombus has all sides equal, while a parallelogram does not necessarily have this property.

1.1. Subcases Explained [3]

The Line Case

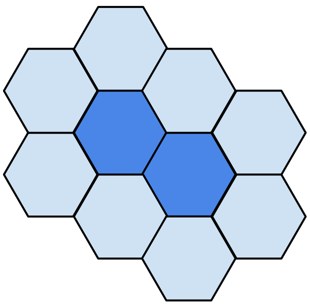


Fig.3 - Result of line case

In this subcase, each step continues in a straight line. There are always six possible directions for the next step, as described in the vectors chapter. Two of these directions continue the line, one forward and one backward. The other four directions can cause the line to evolve into a parallelogram or a rhombus. Once the line transitions into another shape, it cannot return to being a line. The smallest line, consisting of two frozen cells, will eventually evolve into the smallest rhombus.

For example, directions 2 and 5 will keep the shape as a line, while directions 1, 3, 4, and 6 will cause the shape to evolve into a rhombus.

The Parallelogram Case

This subcase can arise from a line case, another parallelogram case, or a rhombus case. Like the line case, there are six possible directions for the next step. Four of these directions either keep the shape as a parallelogram or evolve it into a rhombus. The remaining two directions evolve the shape into an irregular hexagon. Once the shape evolves into a hexagon, it cannot return to a parallelogram. The smallest parallelogram is a rhombus. For example, directions 2, 3, 5, and 6 will continue the parallelogram, while directions 1 and 4 will evolve the shape into either an irregular hexagon or a regular hexagon.

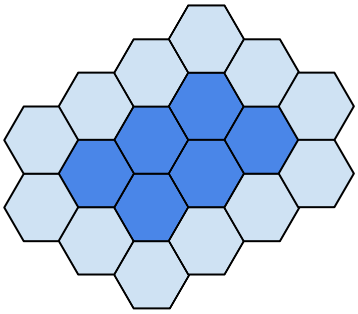


Fig.4 - Result of parallelogram

The Rhombus Case

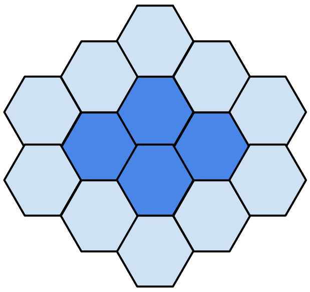


Fig.5 - Result of the Rhombus Case

This case arises from either oscillation between the parallelogram and rhombus cases, or the evolution of the smallest line into the smallest rhombus. The smallest rhombus forms when steps 1, 3, 4, or 6 follow a pattern similar to the line case. For example, alternating between directions 1 and 4 leads to a regular hexagon. Directions 2, 3, 5, and 6 will transition the shape into a parallelogram.

The Irregular Hexagon

This case emerges from a rhombus, parallelogram, or regular hexagon. Each step still has 6 possible directions. Once the shape becomes an irregular hexagon, it cannot revert to a line, parallelogram, or rhombus. From here, it oscillates between regular and irregular hexagons.

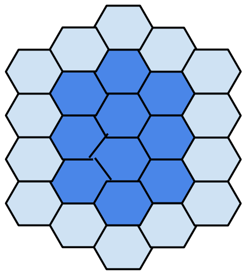


Fig.6 - Result of Irregular hexagon case

The Regular Hexagon Case

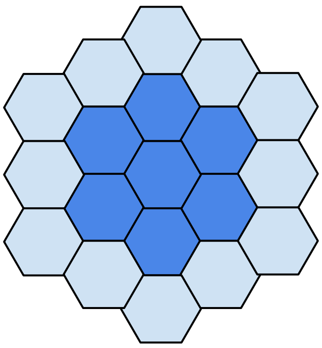


Fig.7-Result of Regular Hexagon Case

This subcase arises from a rhombus or an irregular hexagon. There are 6 possible directions for each step. Once the shape evolves into a regular hexagon, it cannot return to a parallelogram, rhombus, or line. From this point, the shape oscillates between a regular hexagon and an irregular hexagon. For the frozen region to form a regular hexagon, the active steps must be balanced across the three pairs of opposite directions. Consider the direction pairs: d1 (directions 1 and 4), d2 (directions 2 and 5) and d3 (directions 3 and 6).

For example, if two steps are made in each direction (e.g., 154356 or 151356), the hexagon will form regularly. However, an unbalanced sequence such as 121456 will not produce a regular hexagon.

1.2. Some Physics and Chemistry Properties

The shapes and growth patterns of a frozen cluster depend on various physical and chemical factors, including energy, voltage, energy barriers, and diffusion dynamics. If the substrate is uniform and directionally neutral, the cluster tends to adopt a circular or hexagonal shape, reflecting the symmetry of the grid. When the substrate has a bias due to variations in voltage or energy barriers, the cluster can grow in an elliptical shape or form a more complex lattice structure. In an isotropic system, atomic interactions are identical in all directions, which results in uniform growth and a hexagonal or nearly circular shape. In contrast, anisotropic growth occurs when there is a lattice mismatch between materials like graphene and a substrate such as cobalt, which causes different voltages in certain directions. The cluster will preferentially expand in those directions with lower energy, resulting in shapes like ellipses, dendrites, or other complex forms.

Factors Influencing Growth

Substrates like cobalt can induce anisotropic growth in materials like graphene due to lattice mismatches and variations in interface energy. At higher temperatures, atoms move rapidly, promoting uniform growth, while at lower temperatures, growth becomes anisotropic as atoms settle in directions of minimum energy. Edge effects and roughness are more pronounced during anisotropic growth. Isotropic growth tends to favor maximizing the number of neighbors, while anisotropic growth favors minimizing neighbor count.

2. Math and Probabilities

The vector system is used in a 3D framework to explain and demonstrate how steps or actions occur. It also helps in understanding the probability of certain cases. The system includes three axes: Ox, Oy, and Oz. This results in six possible directions: X, Y, Z, -X, -Y, and -Z.

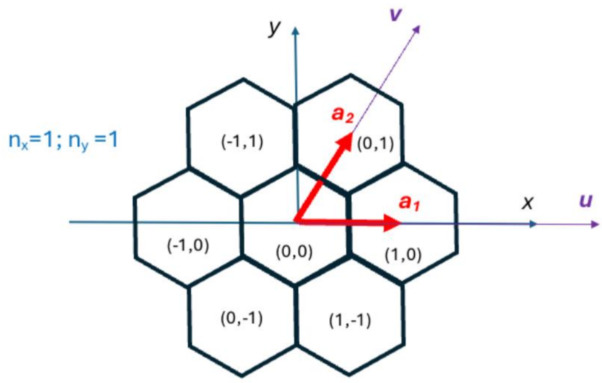


Fig.8 - Vector representation

2.1. Probabilities

Table: Formulas corresponding to each of the growth cases

Growth case	Probability Formula
Line Case	$P = \left(\frac{1}{3}\right)^{s}$
Rhombus Case	$P = \frac{s}{r,r} \cdot \left(\frac{1}{3}\right)^{2r}$
Regular Hexagon Case	$P = \frac{s!}{r! \cdot r! \cdot r!} \cdot \left(\frac{1}{3}\right)^{3r}$

Fig.9 - Tabel of probabilities

1. s is the total number of active steps required for the shape's growth.
2. r is the radius of the shape (i.e., the number of steps in each direction set).
3. $\frac{s!}{r! \cdot r! \cdot r!}$ (for the hexagon) is the multinomial coefficient, representing the ways to distribute steps among the three direction sets. [4]
4. $\left(\frac{1}{3}\right)^{3r}$ (for the hexagon) accounts for the probability of selecting the correct directions.

The table above shows how growth probabilities depend on the structure's symmetry. Line growth, which follows a single direction, has the highest probability due to minimal constraints. Rhombus and hexagon growth require balanced steps in two or three directions, respectively, which limits the number of valid combinations. The use of the multinomial coefficient accounts for how steps can be distributed across directional sets, while the power of $\frac{1}{3}$ reflect the randomness of each step.

2.2. Perfect Growth Probabilities

Table: Probability formula for perfect growth cases

Growth case	Probability Formula
Regular Hexagon Case	$P_{Hex} = \left(\frac{1}{18}\right)^{s}$
Rhombus Case	$P_{Rhombus} = \left(\frac{2}{9}\right)^{s}$

Fig.10 - Table of perfect growth probabilities

Perfect growth occurs when each step follows a precise pattern that maintains symmetry throughout. Because there is no deviation allowed, the probability drops rapidly as the number of steps increases. Perfect hexagonal growth is less likely than rhombus growth due to the greater precision required, with three directional choices compared to two. As size (s) increases, both probabilities decrease exponentially, making larger symmetrical structures increasingly rare. In real-world systems, external factors such as temperature, energy barriers, and substrate properties can influence these probabilities, slightly favoring or inhibiting certain growth patterns.

3. Computer Science and Code

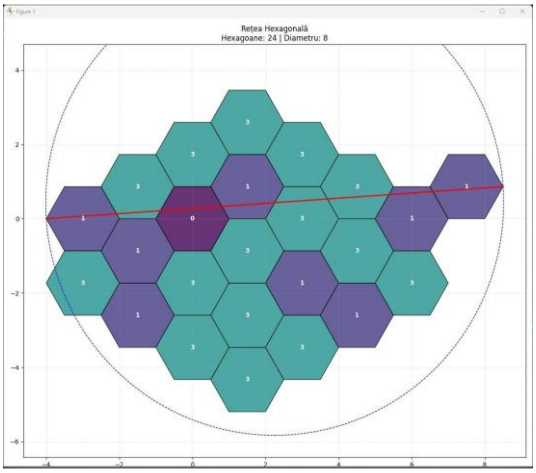


Fig.11 - Python image of running code

This code simulates the growth of a honeycomb lattice, with the ability to either run automatically or interactively based on the user's input. The code includes a **HoneycombLattice** class, helper functions for lattice growth, and two modes of operation: **automatic** and **interactive**.

The calculate diameter method computes the maximum distance between any two hexagons in the lattice by determining the furthest coordinates. The distance is calculated using the absolute difference in each coordinate, and the maximum value is taken among all pairs of hexagons. The diameter is then derived using this maximum distance, applying the appropriate formula to find the length:

AB = $\sqrt{(x_B - x_A)^2 + (y_B - y_A)^2}$.

II. Second approach (simultaneous freezing)

1. Visual side

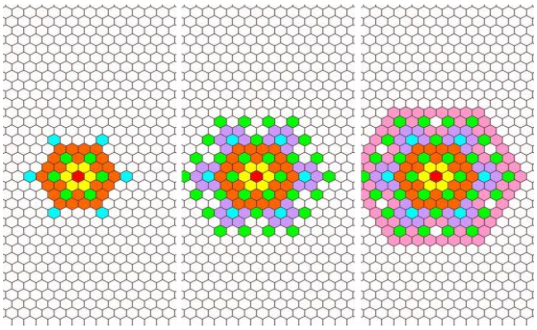


Fig.12 - Example of the crystal's evolution during the first 8 generations

The growth – first generations

At the beginning, there's only one frozen cell. If we add one step, the crystal grows, all the colored cells being frozen. If we add more steps some of the cells will freeze and some will not.

General growing form of the crystal

We could therefore see a pattern, and we tried to understand how often does it repeat.

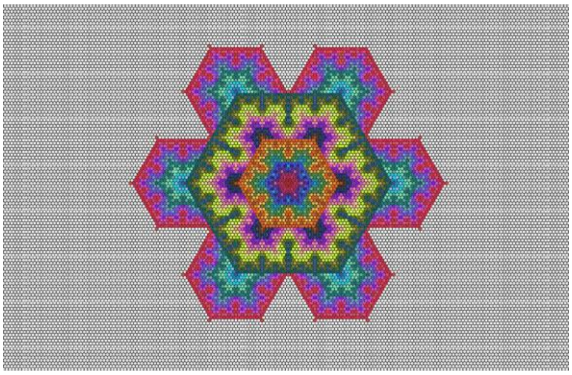


Fig.13 - The crystal

The crystal evolves in a regular manner, forming a hexagon in generations corresponding to powers of two. This happens due to the balance between radial expansion and lateral filling. In early generations, frozen cells propagate more easily along the six principal directions of the hexagonal grid, causing protruding "arms," while gaps persist in between due to some cells only having 2 frozen neighbors (which is not enough to freeze them). Over time, the expansion in these "arms" slows down as they become isolated, while the regions between them accumulate more neighbors and gradually fill in. At generation 2^k, all such delays and irregularities are resolved: every cell within the hexagonal ball of radius 2^k has acquired sufficient frozen neighbors to freeze, and the shape equalizes in all directions. This creates a convex, fully symmetrical figure—a perfect discrete hexagon. Thus, the generations n=2^k serve as structural "reset points" where the automaton temporarily regains exact radial symmetry and regularity. [5]

The crystal - inscribable in a circle

As it grows, the structure remains inscribed within a circle, even when not strictly hexagonal. The evolving shape preserves 6-fold rotational symmetry, with the frozen region expanding uniformly in all six primary directions of the hexagonal grid. While it may not always be a perfect hexagon, the shape remains convex and symmetric, leading to an outer boundary that forms a centrally symmetric polygon. A well-known geometric property asserts that any convex, centrally symmetric polygon with evenly spaced boundary points is inscribable within a circle.

Fig.14 - The crystal remains inscribable in a circle

Even if the shape isn't a regular hexagon, the symmetry and convexity ensure inscribability at every stage. At special generations n=2^k, the shape becomes a regular hexagon, trivially inscribed, but even during intermediate generations, this inscribability persists, maintaining perfect geometric balance throughout. This reflects a controlled, symmetrical expansion that maintains constant geometric balance. The development follows a predictable, infinite pattern, centered around the initial frozen cell.

Physical prototype

In order to better understand the development of the crystal, both research teams first created drawings, followed by 3D printed models, which allowed them to simulate the crystal's growth under certain conditions. Through the drawings, some formulas were discovered, which were later proven arithmetically.

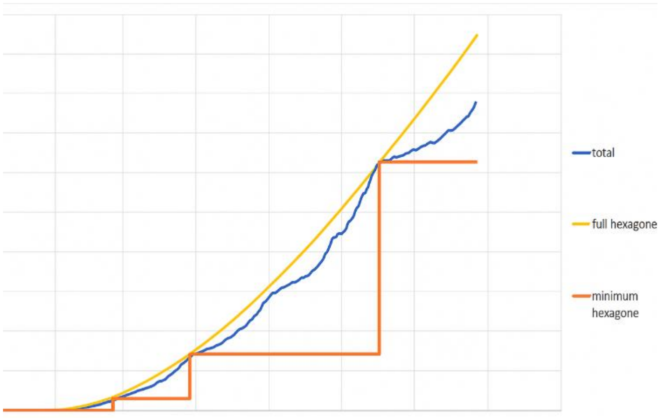
Fig.15 - The 3D printed prototype

2. Mathematic side

The "final formula" target

After understanding the visual manner of the crystal growth, the mathematic way of describing it is by counting the number of the frozen cells, and finding a general formula for the number of frozen cells in a specific generation. There are two ways of doing this:

1. **General number** - counting the general number of frozen cells in a specific generation.
The function describing this growth is clearly exponential but not described by a simple formula (it grows irregular).



blue *- total number of cells in a specific generation*

orange *- total number of cells in the last hexagonal shape of the crystal*

yellow *- total number of cells in the next hexagonal shape (the hexagon in which the crystal can be inscribed)*

Fig.16 - Total number of cells in a specific generation

2. **Number of cells added** - counting only the added cells in each generation.
Unlike the first one, it seems chaotic, without a clear rule, but looking closer there are some patterns. This numeric pattern has a correspondent in the visual pattern, repeating as it gets bigger and bigger.

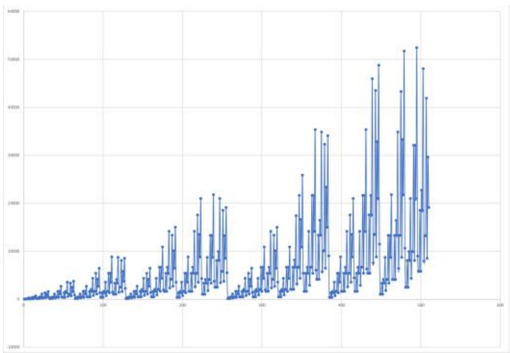


Fig.17 - The number of added cells may seem chaotic

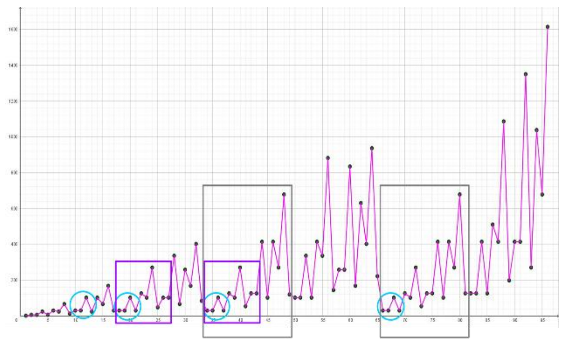


Fig.18 - After every full hexagonal shape, there are some patterns in the number of added cells

Fig.19,20 - The patterns can also be visualized, as the arm of the hexagon along with its branching structure is repeating and becoming bigger after each hexagonal shape and in the table of added and total number of cells. (exp: after each hexagonal shape, the next generation has +6 cells etc.)

time	total added	number added di
2	7	6
3	13	6
4	37	24
5	43	6
6	73	30
7	97	24
8	163	66
9	175	12
10	205	30
11	235	30
12	337	102
13	361	24
14	463	102
15	529	66
16	697	168
17	727	30
18	757	30
19	787	30
20	889	102
21	919	30
22	1045	126
23	1147	102
24	1417	270
25	1465	48
26	1567	102
27	1669	102
28	2005	336
29	2071	66
30	2329	258
31	2497	168
32	2899	402
33	2983	84
34	3013	30
35	3043	30
36	3145	102
37	3175	30
38	3301	126
39	3403	102
40	3673	270
41	3727	54
42	3853	126
43	3979	126
44	4393	414
45	4495	102
46	4909	414
47	5179	270
48	5857	678
49	5977	120
50	6079	102
51	6181	102

After each hexagonal stage of the crystal (in each arm and branch), the number of added cells follows the values shown in the table below. A hexagonal pattern can be observed in generations that are powers of two (highlighted in red), where each line contains the same number of frozen cells. Another noticeable pattern is that after each power-of-two generation, the following lines—except the first—have the same number of frozen cells (highlighted in green), while the last line contains three cells (highlighted in blue).

Generation / Nr. of line[1]	C1	C2	C3	C4	C5	C5	C7	C8	C9	C10
1	1	3	5	7	9	11	13	15	17	19
2		3	3	7	7	11	11	15	15	19
3			3	7	7	7	11	15	15	15
4				7	7	9	9	15	15	15
5					3	9	13	15	15	15
6						7	7	15	15	15
7							7	15	15	15
8								15	15	17
9									3	11
10										7

[1] Relative to the last hexagonal form of the crystal.

All of this indicates that the development of the crystal is also reflected in its smaller branches. The growth appears to follow consistent rules applied at different scales within the crystal.

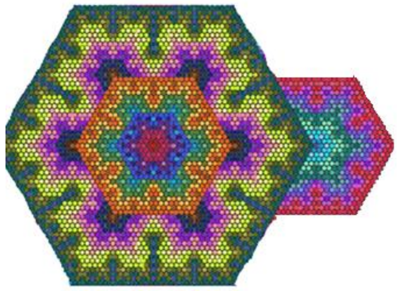


Fig.21 – Each branch grows in a similar way to the large crystal

Formulas

By analyzing the manner in which the crystal grows, certain formulas describing this development can be deduced, formulas that can later be mathematically proven. The fundamental observation is that all the crystal's vertices expand with each generation, which means that the generation number is equal to the radius of the figure[2].

Symbols used:

- g - number of the generation (nr. of steps)
- d - the diameter
- h - number of the hexagonal shape
- A_g - total number of cells in a specific generation
- A_h- total number of cells in the h hexagonal shape

Formulas discovered:

1. $d = 2g - 1$

The diameter is twice the length of the radius, but since it also includes the center point, it can be thought of as two times the radius minus one unit.

2. $g = 2^{h-1} \Leftrightarrow h = log_2 g + 1$

The crystal becomes a hexagon in the power of two generations, but the first hexagon is in generation one (one cell), so the h-th hexagon will have the range of the h−1 power of two. In the same way, if the number of the generation is known, a logarithmic formula can be used to find out the number of the hexagon[3].

3. $A_g = 3 \cdot g^2 - 3 \cdot g + 1 \quad A_h = \frac{3}{4} \cdot 4^h - \frac{3}{2} \cdot 2^h + 1$

[2] The unit of measurement for all calculations is one hexagon.
[3] This formula can be used exclusively for generations that are powers of 2.

When the crystal becomes a hexagon, to determine its area (number of cells), it can be divided into 1 middle cell, and 6 triangular shapes (Fig.20). In each triangular shape, the side is the same as the range of the hexagon minus one (we do not include the middle), so the total number in a triangular shape is $1 + 2 + 3 + \cdots + (g - 1)$, which equals (using the Gauss sum) $\frac{g(g-1)}{2}$, so the total number of cells in the hexagon is $6 \cdot \frac{g(g-1)}{2} + 1$, wich is $A_g = 3 \cdot g^2 - 3 \cdot g + 1$. Using the second formula (for the number of the hexagon and the generation), it can also be determined the area if the number of the hexagon is known.[4]

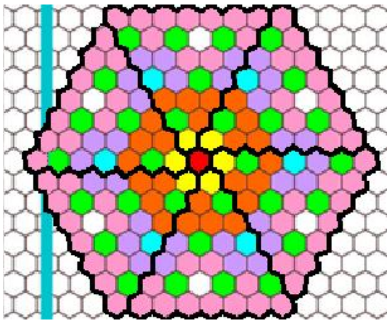
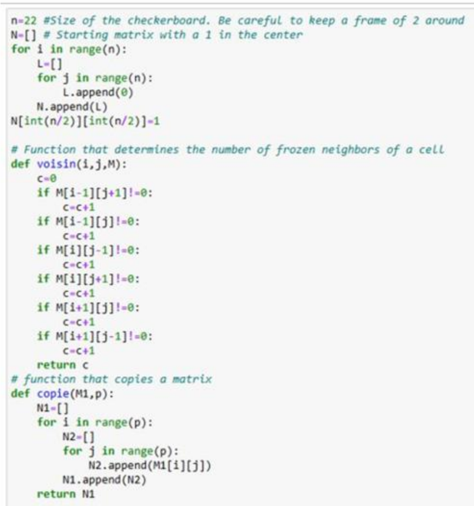


Fig.22 – Dividing a hexagon into triangular shapes

3. Informatic side

French results

The python program has been made in order to automatize each step by a machine. At first, we define a point in the middle of a matrix, which is represented by a list of lists in python, and we check every step if the neighbors can be frozen. If they can freeze, we freeze them and we check if their neighbors can be frozen the next step. Doing this we can calculate the number of hexagons we are having every step. After this we tried to make a visual representation of what the hexagon looks like, so we used the python library Matplotlib to graphically show, with 7 different colors, each step, where a hexagon is represented by a colored point, and the colors are the same if the points are on the same step.



```
n=22 #Size of the checkerboard. Be careful to keep a frame of 2 around
N=[] # Starting matrix with a 1 in the center
for i in range(n):
    L=[]
    for j in range(n):
        L.append(0)
    N.append(L)
N[int(n/2)][int(n/2)]=1

# Function that determines the number of frozen neighbors of a cell
def voisin(i,j,M):
    c=0
    if M[i-1][j+1]!=0:
        c=c+1
    if M[i-1][j]!=0:
        c=c+1
    if M[i][j-1]!=0:
        c=c+1
    if M[i][j+1]!=0:
        c=c+1
    if M[i+1][j]!=0:
        c=c+1
    if M[i+1][j-1]!=0:
        c=c+1
    return c
# function that copies a matrix
def copie(M1,p):
    N1=[]
    for i in range(p):
        N2=[]
        for j in range(p):
            N2.append(M1[i][j])
        N1.append(N2)
    return N1
```

Fig.23 – The Python code

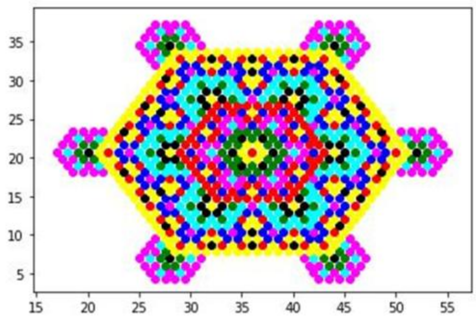


Fig.24 – The Python crystal

[4] This formula can be used exclusively for generations that are powers of 2.

Romanian results

While attempting to understand the underlying problem and model the development of the crystal, we identified a mathematically similar case known as *Conway's Game of Life*. After studying this model, we discovered an adaptation of the game implemented on a hexagonal matrix. Utilizing this open-source implementation, we modified the survival and birth conditions to simulate the specific behavior observed in the crystal's evolution. This computational approach allowed us to explore and visualize the dynamic formation of the crystal in a controlled digital environment.

Conway's Game of Life is a well-known cellular automaton governed by four simple rules that determine whether a cell will be alive or dead in the next generation:

1. **Birth**:
   A dead cell with exactly three live neighbors becomes alive in the next generation.

2. **Death by isolation**:
   A live cell with fewer than two live neighbors dies due to underpopulation.

3. **Death by overcrowding**:
   A live cell with more than three live neighbors dies due to overpopulation.

4. **Survival**:
   A live cell with two or three live neighbors survives to the next generation.

These rules are applied simultaneously to all cells in the grid, determining the state of each cell for the next generation.

4. Conclusions

How to conclude on the evolution of a crystal?
First, a symmetrical pattern repeats ad infinitum when the crystal evolves. Because the structure is inscribable in a circle, we can predict this growth based on the beginning of the structure, its foundations, the first cell! But the whole evolution of the growth is not completely definable.

5. Real life applications/practical side

We can make a parallel with the growing of a snowflake. It's indeed really interesting to learn how both evolutions are similar. As we've said, the crystal starts its growth by one hexagon cell.
A snowflake starts its growth in a cloud. Water vapor freezes around a piece of dust or pollen, this for mis called a seed crystal, and, with water molecule sticking on it, it firstly become a simple hexagon: the hexagonal symmetry of the structure of ice is the result of the way the water molecules arrange themselves when freezing.

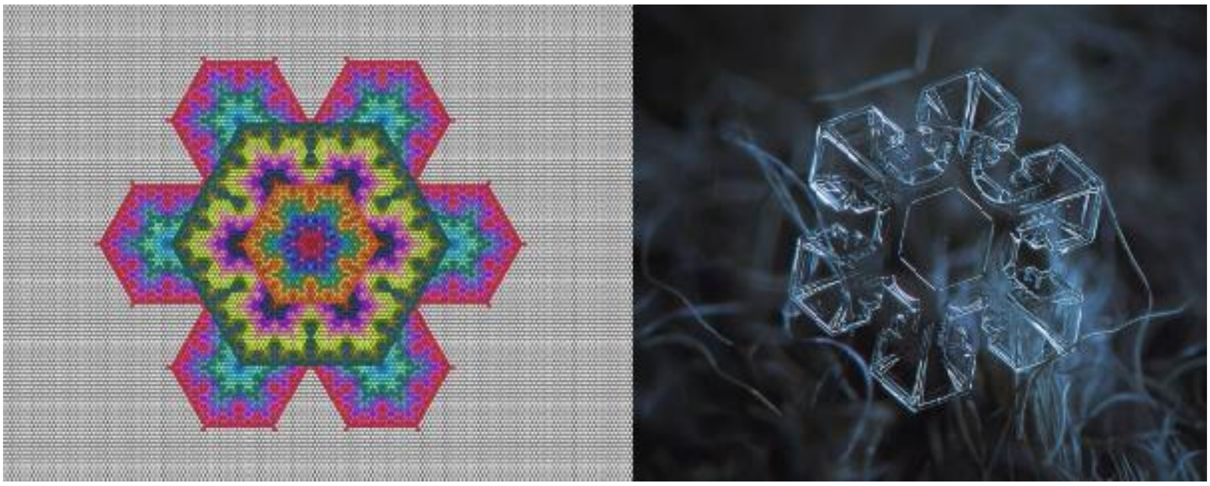


Fig.25 – Similarities between the mathematical and the real model.

In both cases, it continues to evolve by having a hexagonal shape with 6 branches; for the snowflake, the H_2O molecule will be added to each 6 corners of the hexagon. (Each branch will evolve in the same way because they go through the same things at the same time.)
But as our rule is very specific, it's really different for real snowflakes. As there is many different temperatures or humidity in the cloud, but also as the weather is changing on the way of the fall of the snowflake, then many different shapes exist. Because of the different meteorological conditions, snowflakes will never be identical!

General conclusions

Both approaches underscore a fundamental truth: complex structures can emerge from simple rules. Whether it is through analyzing directional vectors and probabilities, or observing recursive patterns and symmetry in growth, the evolution of a crystal offers a beautiful example of order arising from minimal initial conditions. The first study builds a strong analytical framework, while the second enriches it with experimentation, visualization, and analogies to nature. Together, they demonstrate that scientific understanding is most powerful when it combines abstract reasoning with tangible exploration. This synergy not only deepens our grasp of crystalline behavior but also reflects broader principles in mathematics, physics, and even biology.

EDITION NOTES

[1] It should be said why the case of two adjacent cells is excluded.

[2] What happens if more than one cell satisfies this condition? Based on a passage below, it seems that the cell is chosen at random from among those satisfying the condition. This should be made explicit in the definition of sequential freezing.

[3] In the sequel, there are some unproved statements that would deserve at least some intuitive explanation. For instance, why "Once the shape evolves into a hexagon, it cannot return to a parallelogram"? Or, in the case of irregular hexagon, why "it oscillates between regular and irregular hexagons"?

In general, if the frozen cells were numbered progressively, the freezing process and the figures obtained from it would be much clearer.

[4] Here and below, some discussion of how these probabilities are derived would be helpful.

[5] How is this conclusion reached? It appears to be based solely on empirical observations. If so, this should be made explicit; otherwise, some theoretical justification should be provided.