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Paper: **Disorder Disguised as Order**


Topic: Mathematics

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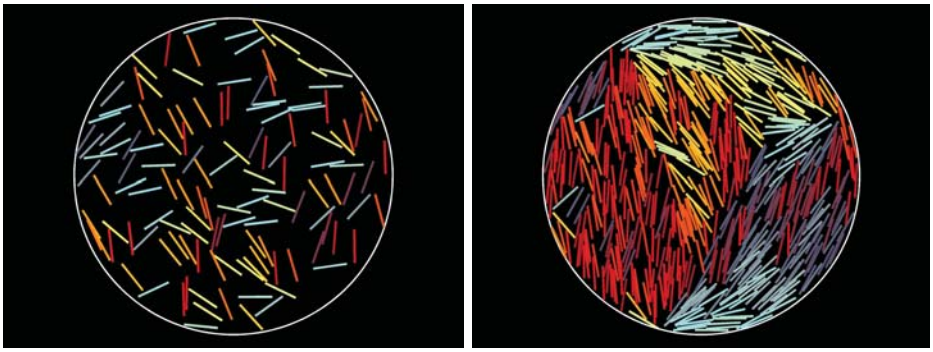
[1] J. Galanis et al, "Spontaneous patterning of confined granular rods", Phys. Rev. Letters 96, 028002 (2006).
[2] M. Ehler, J. Galanis, "Frame theory in directional statistics", Stat. Probabil. Letters, 81, 1046-1051 (2011).

Abstract:
The scientific word "entropy" describes the extent of randomness or disorder found in nature. From our experiences (confirmed by the second law of thermodynamics), disorder, in general, increases. However, entropy can sometimes disguise itself as order to the human eye. We describe this principle and propose an entropy-based approach that opens the possibility of computer generated patterns from spontaneous particle self-assembly.

This approach is based on the idea that there can be multiple types of disorder that compete with each other to achieve the maximum total entropy. For example, rod shaped objects possess two types of disorder: 1) disorder in their position (where they are in space), and 2) disorder in their orientation (which way they are pointing).

The maximum total entropy may not occur when all individual types of disorder are themselves at a maximum. When there are too many rods in too little space, the rods experience significant crowding, and it is not possible for both types of disorder to be high. In fact, the maximum total entropy occurs when positional disorder "wins" and orientational disorder "looses". As a result, rods can be located anywhere in the space but are all pointing in the same direction. It is easier to see the loss of orientational disorder than the gain of positional disorder, giving the false appearance of increased ordering.



We will demonstrate this remarkable effect with rods as well as with other shaped particles by using images and movies from experiments and computer simulations. The images and movies emphasize that disorder can sometimes disguise itself as order to human perception.

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Disorder Disguised as Order: the Science of Randomness

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Abstract

The scientific word *entropy* describes the extent of randomness or disorder found in nature. From our experiences (confirmed by the second law of thermodynamics), disorder, in general, increases. However, entropy can sometimes disguise itself as order to the human eye. We describe this principle and propose an entropy-based approach that opens the possibility of computer generated patterns from spontaneous particle self-assembly.

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1. Can We Identify Disorder?

Most of us have an intuition about disorder or randomness that stems from a variety of experiences, such as the concrete example of rolling dice at a casino, to the enigmatic behavior of the stock exchange, to the banal battle against a messy desk. Despite our hubris, scientific research repeatedly demonstrates that humans are, at best, mediocre at both generating and recognizing randomness (although with the proper training, we can improve our abilities [7]). This need not be cause for despair, as flawed human perceptions of randomness can be turned into an advantage and harnessed as another tool in the generative artist's arsenal of methods.

On a scientific level, the word *entropy* describes the extent of randomness or disorder found in nature. Entropy exists beyond our faulty judgments as a quantity that can in principle be measured and is related to the probability of observing a particular event. Since the probability of a given event is proportional to the number of ways of that event can be generated, you are most likely to observe events that are more probable. The fancy phrase *maximizing entropy* is scientific jargon for *the most probable outcome* (or *the most disordered*).

Based on what we have discussed thus far, we pose the following question:

Which image in Fig. 1 shows maximal entropy (is the most disordered)?

Fig 1: *Two computer generated images of rods in a circular space. Question: Which image is the most disordered? Answer: The image on the right! Read on to understand why.*

Both images in Fig. 1 contain equal numbers of non-overlapping rods, whose position and orientation in the equivalent circular spaces were determined via the same random number generator. The color in these images identifies the direction in which the rods are pointing, clearly highlighting a dramatic patterning difference between the two images. Intuition supports the image on the left as the answer to the question. The rods seem to point haphazardly (randomly) in many directions. In contrast, the image on the right appears structured (ordered), with large groups of neighboring rods that are, at least locally, aligned.

The correct answer, dictated by entropy, is in fact the image on the **right**! How could this possibly be the correct answer? The *trick* in this question resides with our faulty eyes. The **total** entropy in this example is composed of two subtypes of disorder. Our eyes focus readily on one type, entropy in rod orientation, while overlooking the other type, entropy in rod position. To maximize the **total** entropy, these two subtypes of disorder can compete [2,3,5,6]. And obviously in this image, the entropy in rod position *won* while that of orientation *lost*.

This example exposes the very curious and counterintuitive idea that entropy induces particles to *organize* themselves (visually of course, as the particles are in reality maximally disordered). This *self-assembly* process opens the possibility of producing complex and organic patterning that can be simply created with a random number generator. In the remainder of this manuscript, we will elaborate on how entropy can produce *order* as well as the methodology for generating similar images.

2. Basic Probability: Non-Interacting Dice (or a Single Die)

To answer the question from the last section, we start from a familiar place and gradually build the complexity. We begin with dice. Traditionally, a die is a cube shaped object with the numbers 1 to 6 designated on the faces. If the player is not cheating and the dice are *fair*, we know that, with any particular roll, the number that appears on the side facing up is random. In other words, the outcome of a particular roll of the die is not affected by what happened in the previous rolls. We also expect that all the numbers are equally probable, so that the chance of rolling a 1 is the same as a 6, or a 4, etc.

Happily, we do not have to take these assumptions on faith - these properties are readily measurable (to the demise of many cheating gamblers). How is this done? Simple, record the number that appeared for each roll. Figure 2 shows typical examples of such recordings for one, ten, and ten thousand rolls, where a computer both *rolled* a virtual die and recorded the outcome.

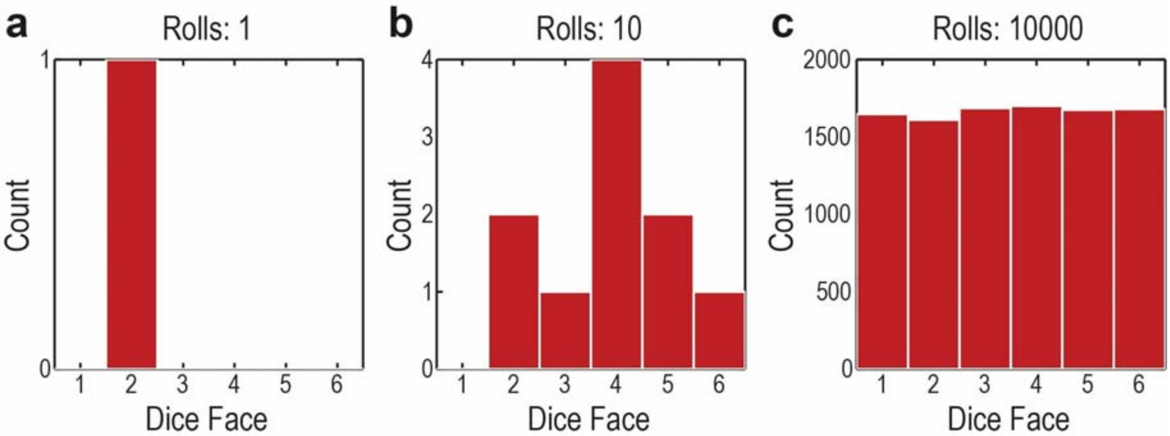

Fig 2: *The behavior of non-interacting dice (or a single die). Recording the number of times each face appeared after one (a), ten (b), and ten thousand (c) rolls. A fair roll of the dice, where all numbers are equally probable, only emerges clearly after a large number of rolls.*

Although we expect that the appearance of all numbers on the die are equally probable, this is not always what emerges from a sample of rolls. The distribution of numbers in Fig. 2(b), for example, is not equal, as the number 4 seems more likely than the other numbers. Moreover, the number 1 has not even shown up at all. Before we denounce the computer for cheating, we must recognize an important point. The true probability distribution only manifests as an outcome of an **excessively** large number of rolls. By inspecting Fig. 2(c), we can feel confident that all numbers on the die are equally probable.

3. Thinking Geometrically: Non-Interacting Rods (or a Single Rod)

We now transpose the ideas from dice to rods in a particular space. Analogous to the roll of a die, we can *toss* the rod into the space. We can pick any space, but for ease of visualization, we choose a two dimensional space. For example, Fig. 3(a) shows a single rod existing in a circle. Instead of thinking in terms of pure numbers as with dice, we must now think geometrically. There are two things that can be random when you toss a rod in a particular space: a) disorder in position (where is the midpoint of the rod located?) and b) disorder in orientation (which way is the rod pointing?).

Similar to our expectations with numbers on a die, we expect that the midpoint of the rod can be located anywhere in the space and that the rod can be pointing in any direction. In other words, we expect an equal probability for all **possible** positions and an equal probability for all **possible** orientations. The word *possible* is used because rod positions and orientations are restricted when considering a *hard* wall, where the rod cannot cross the boundary. The interaction of a rod or rods with boundaries can produce interesting patterning (see, [5] and [6]); however, these effects are beyond the scope of this article. For simplicity, we will focus on what happens everywhere in the space, **except** those areas close to the boundaries, marked by a dashed circle in Fig. 3(a).

Equivalent to dice, we can determine if indeed the outcome of a toss matches our expectations by recording where the rod landed in the space. Figure 3(b) shows the recording of 100 virtual tosses of a rod in a circle by a computer. From these types of recordings, we can measure the probability of various outcomes, recalling from the previous section that we need an excessively large number of tosses to accurately determine the probabilities.

Beginning with positional disorder, we are interested in the location of the rod midpoints, as shown for a particular recording in Fig. 3(c). By eye, it seems that the rod is tossed uniformly throughout the space, but we can be more quantitative by taking a measurement. There are many ways to measure the distribution of the midpoints, and here we choose a simple heuristic method. Using a grid, we partition the circle into tiny boxes and count the number of midpoints in each box. Figure 3(d) readily shows that each box contains about the same number of rod midpoints.

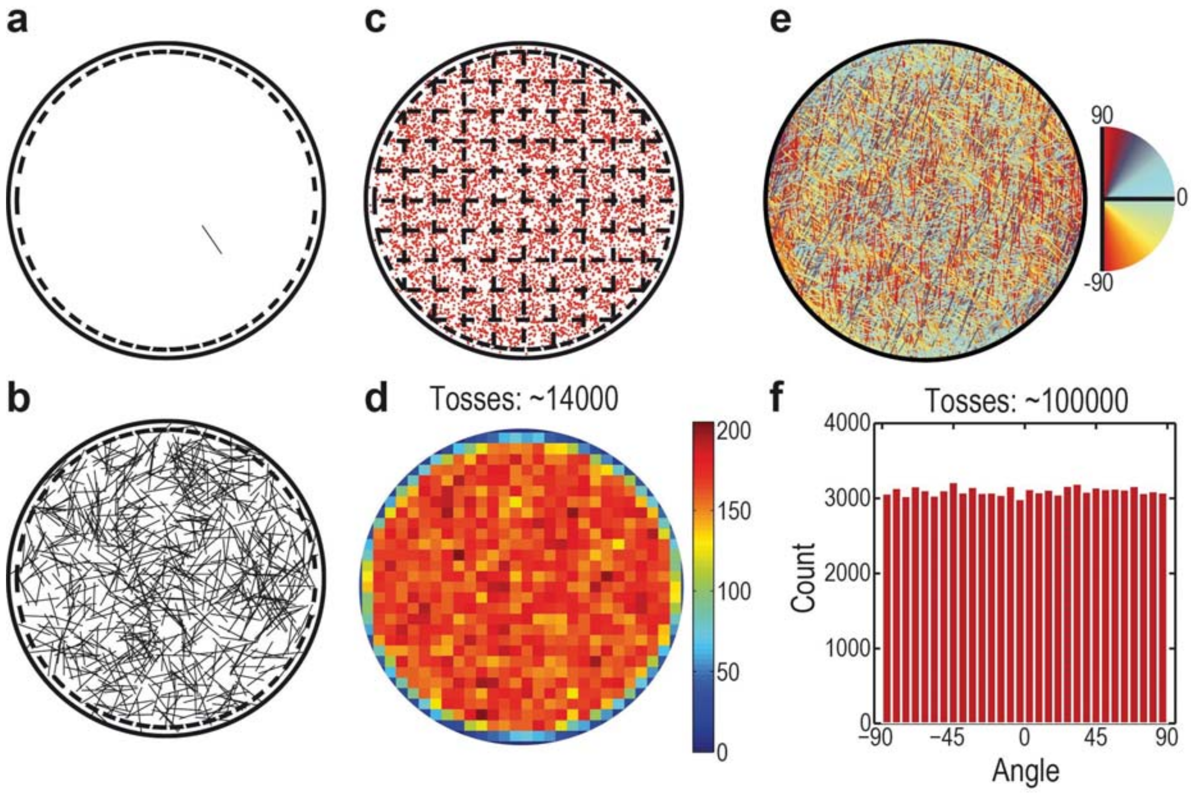

Fig 3: *The behavior of non-interacting rods (meaning they can overlap) or a single rod tossed many times. (a) A single rod in a given space (excluding the boundaries marked by the dashed circle) can have its midpoint located anywhere and its long axis pointed in any direction. (b) An example recording of 100 rod tosses. By looking at just the midpoints of the rods (c), we can divide the space into small boxes (grid) and measure the probability of finding the midpoint in each box. For example, (d) indicates the count in color, showing an equal probability of finding rod midpoints anywhere in the circle. (e) Similarly, we can see by eye that rods are pointing in all directions by coloring the rods depending on their orientation. Graph (f) illustrates the count of rods pointing in each direction.*

Now checking the disorder in rod orientation, Fig. 3(e) shows a recording where color corresponds to the direction a rod is pointing. For example rods are colored blue if they are pointing left and right on the page, and red if they are pointing up and down on the page. Again it appears as if the color variation in the rods is fairly uniform throughout the space; however, we can quantify this with a measurement. We can choose any coordinate axis to define our angles. Here, we chose our reference angles as that in Fig. 3(e). Figure 3(f), shows that the rods indeed have an equal probability to point in any direction.

4. Adding Complexity: Interacting Dice

Thus far, we developed a good understanding about what happens with single objects (one die, one rod). Now lets increase the complexity and have several interacting objects. Suppose you have two dice. And instead of being interested in the number each die gives with a roll, you are interested in the sum of the numbers. By looking at the sum, you have in essence created an interaction between the dice. It is important to remember that the outcome for each individual die is random, as discussed earlier.

However, the interaction (the summed numbers) does not yield an equal probability for all possible outcomes. For example, there is only one way to get the number 2. Both die must roll a 1, or in more compact notation (1,1). In contrast, there are six ways to roll a 7 - the dice can be (1,6), (2,5), (3,4), (4,3), (5,2), and (6,1). Therefore for any given roll of two dice, you are more likely to obtain a 7 than a 2. In other words, the probability of a particular number from the summation is proportional to the number of ways that you can obtain that summed number.

The more dice you have interacting together, the stronger the preference for a small range of numbers compared with the entire range of possible numbers that can be rolled. This effect is easily seen in Fig. 4, where the probability of outcomes are given for two, ten, and one hundred interacting dice. To be more specific, even though it is possible to roll 100 from one hundred dice in a *fair* roll, the chances of you actually obtaining that number are infinitesimally small (one way out of 6^{100} possibilities). In contrast, there are a large number of ways to roll a 350, the most probable number. The number that has the maximum probability is said to have the maximum entropy.

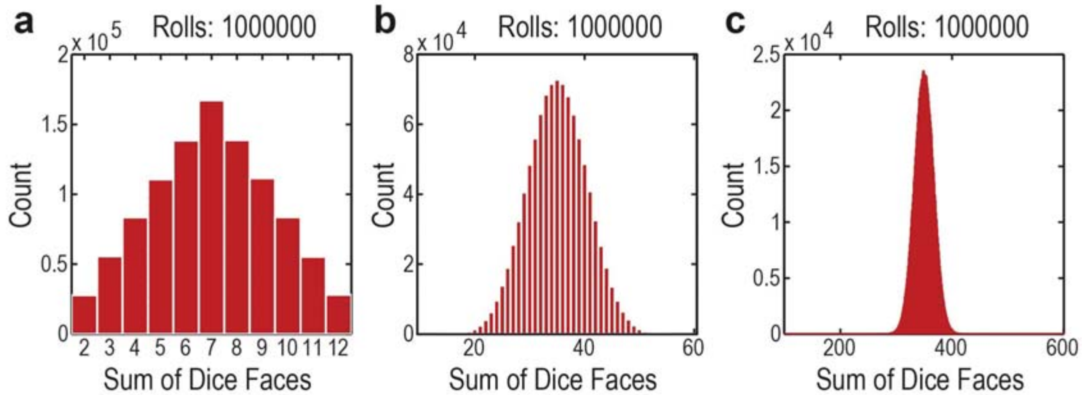

Fig 4: *The behavior of interacting dice. For this interaction, we simply sum the numbers from all the dice for each roll. While the number rolled for each individual die is equal (Fig.2), the inclusion of an interaction (summation) can result in an unequal probability for all possible outcomes, as is shown for the summation of two (a), ten (b), and one hundred (c) dice.*

5. An Answer to the Question: Interacting Rods

We can define a simple interaction between rods by saying that rods cannot intersect, or be located at the same place at the same time. This results in a geometrical restriction between rods. To see how this occurs, let us begin with one rod and fix it in a particular position and orientation. We could have, for example, the rod pointing left-right on the page, similar to the red rod in Fig. 5(a). Now you bring another rod, for example the green rod in Fig. 5(a). You fix the second (green) rod's orientation, but allow it to exist anywhere in the space, provided it does not intersect the first (red) rod. For a particular angle between the two rods, there is a little chunk of the total space that the midpoint of the second rod cannot occupy because the first rod is there. This little chunk of space is called the *excluded area* (or *excluded volume* if the space is three dimensional). Three different examples of *excluded area* are shown as blue boxes in Fig. 5(a) for three different angles between the rods.

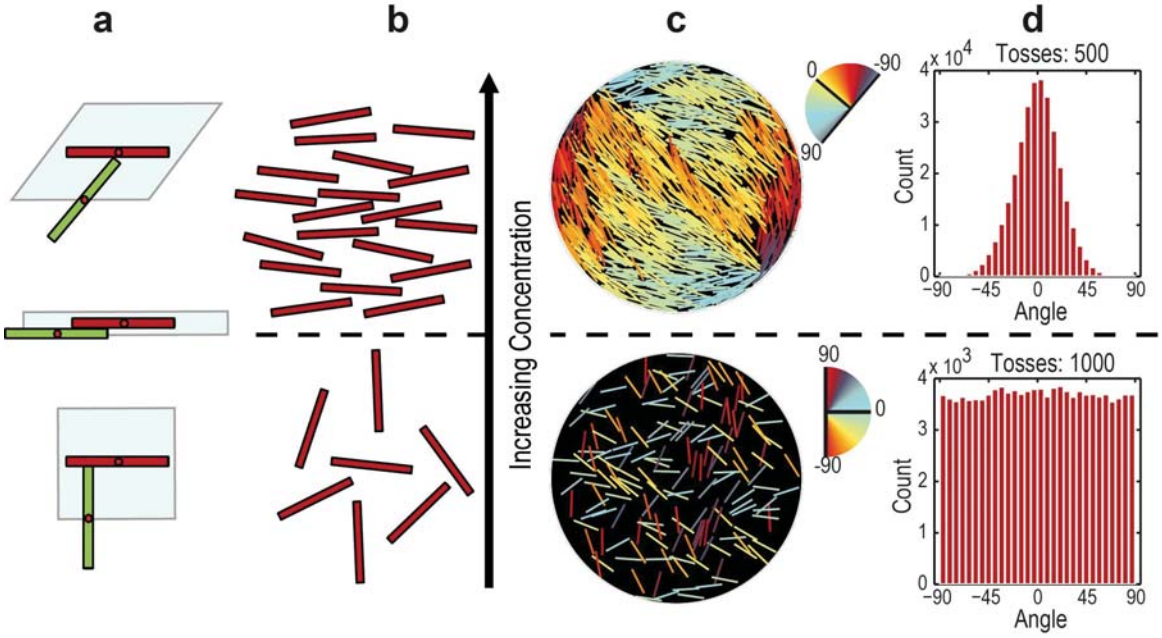

Fig 5: *The behavior of interacting rods. For this interaction, the rods cannot overlap, which creates a space (a, light blue box) that the midpoint of one rod (a, green rod) cannot be located because another rod (a, red rod) is present. The size of this excluded space depends on the angle between the rods, where parallel (a, center) and perpendicular (a, bottom) rod orientations give the least and most, respectively, excluded space. (b) A schematic drawing illustrating that excluded space becomes more important at higher rod concentrations. After a certain concentration (dashed line), rods loose orientational entropy. The change in orientational entropy can be seen in images of rods from simulations (c) and by measuring the probability of finding the rods pointing in a particular direction (d) for high (top) and low (bottom) rod concentrations. The simulations (c) are quasi-two-dimensional, where the thickness out of the page of the circular space is four times the rod diameter.*

In order to understand the implications of excluded area, lets digress for a moment and return to dice. Suppose you engineered a way to modify a die so that, for example, the number 5 was never rolled but the probability for all other numbers remained equal. Unlike the 1/6 probability for rolling a particular number for a regular die, your modified die would have a 1/5 probability for rolling a particular number. Now, you have a better chance at guessing the number that might appear with your modified die. In other words, you have decreased the disorder associated with rolling dice.

The analogous idea with a rod is a restriction in geometry. If you arranged a little section of space in such a way that a rod from a toss never landed there (for example with an excluded area), you have decreased the disorder in the rod position. By looking at Fig. 5(a), you can get a sense from these cartoons that the excluded area depends on the angle between the rods, where the smallest excluded area occurs when both of the rods are parallel to each other (0 degree angle), while the largest occurs when the rods are perpendicular to each other (90 degree angle).

Ah ha! The amount of excluded area (related to positional disorder) is connected to the angle between the rods (related to orientational disorder). Therefore, positional and orientational disorder are linked. In other words if you forced all your rods to point in the same direction (decreasing orientational entropy), you reduce the excluded area and increase positional entropy. And conversely if you imposed an equal probability for all angles of rods (increase orientational entropy), you increase the excluded area and decrease positional entropy. The **total** entropy is, therefore, not simply maximizing the positional and orientational entropies independently, instead both entropies must be considered **simultaneously**.

When would you expect these two types of entropy to compete? Obviously, when there are very few rods in a very large space, the chances of any two rods coming close enough to *feel* each other's excluded area are quite low. Therefore, positional and orientational disorder appear to be both maximized, and it is as if the rods can be approximated as non-interacting rods. A single *toss* of interacting rods in this dilute regime can be seen in Fig. 5(c, bottom). We can use the tools from the previous sections to measure the orientational entropy. Figure 5(d, bottom) show that there is no preference for any particular orientation.

At the other extreme, when a large number of interacting rods are confined to a relatively small space, the rods strongly *feel* each other's excluded area. Positional entropy competes and wins against orientational entropy, and the rods spontaneously align. An example of this extreme is shown in Fig. 5(c, top). Here, the rod alignment is visually striking. But again, we can measure this, as shown in Fig. 5(d,top). For convenience, we chose our reference angle (zero) to be the direction where most of the rods are pointing. It is very obvious that not all angles are equally probable, and that most of the rods prefer to be aligned along the same direction. In between the two extremes in rod concentration, there is a certain concentration where the rods transition in their patterning, depicted schematically by the dashed line in Fig. 5(b).

6. How Do You Obtain the Images?

How do you obtain an image like the one in Fig. 1(right) or 5(c)? These images are, in fact, the product of Monte Carlo simulations. Since there are many excellent tutorials on how to perform Monte Carlo simulations [1,4], we will only outline the essentials here.

We begin by constructing an image like the one in Fig. 1(left). To construct such an image, we start with a space (example, a circle), and we ask the computer to sequentially toss a particular number of rods into the space (randomly pick the location of the rod midpoint and rod orientation) with the rule that rods cannot intersect other rods (or the boundary). In principle, rod arrangements like Fig. 1(left) are a viable configuration for our interacting rod model; however, it was constructed *artificially*. Each rod tossed into the space only interacted with the rods that were already present in the space. For example, the first rod tossed did not interact with any other rod. The second rod tossed interacted only with the first rod. The third rod tossed interacted only with the first two rods, etc. At this point, we do not really know if entropy is indeed maximized or if we are at an extraordinarily unlikely pattern (like rolling a 100 with one hundred interacting dice).

We can solve this problem by asking the computer to now take each rod and randomly move it, with the only criteria that the rods cannot overlap. Now, the rod that is being moved interacts will all the other rods present. Once every rod in the space has been moved (or attempted to move) once, the new configuration can be considered as a new toss. As the computer progresses with an extremely large number of tosses, the rods spontaneously *find* the most disordered arrangement.

7. More Possibilities

Using the specific example of rods, we showed that there may be several subtypes of entropy that contribute to the total entropy. We demonstrated that if the entropy subtypes are linked to together, these subtypes may compete, where one *wins* and the other *looses* in order to obtain the maximum total entropy. Since our eyes cannot detect all forms of entropy equally, it falsely appears as if the total disorder decreases as structure emerges from randomness.

What has been described with rods is by no means limited to just rods. The only requirements are that at least two different types of disorder compete. This situation can be created with various shapes (ex. spheres, rods, wedges), with different sizes of the same shape (ex. big and little spheres), or with combinations of different shaped objects (ex. rods with spheres, Fig. 6). It is not easy to determine what the pattern will be before running the simulation, and in fact, this is an active area of current scientific research. For example, the patterning behavior of rods discussed here is exactly what occurs with liquid crystals and is fundamental to the functioning of LCD based electronics. Aside from exploring unknown intellectual territories and developing technological devices, the movies generated by such methods can be a visually mesmerizing combination of order and disorder.

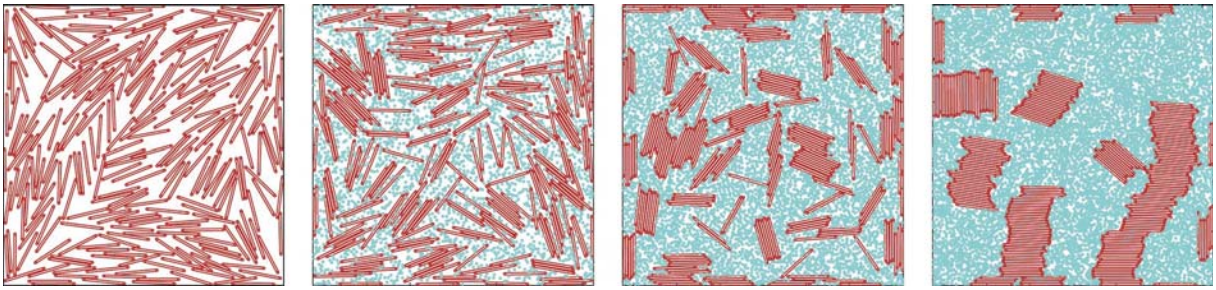

Fig 6: *The competition of various entropies occurs in many places. The images contain mixtures of rods (red) and spheres (blue), where left to right shows zero to increasing numbers of spheres for a constant rod number. As sphere number increases, the entropy of the spheres wins while the entropy of the rods looses in order to obtain the maximum total entropy.*

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