A Cellular Model for 3-Dimensional Snow Crystallization

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Abstract

Snow crystals are intriguing because they exhibit both symmetry and remarkable diversity. Previous studies have used 2-dimensional models to approximate snow-crystal growth. Here generalizations to three dimensions are considered. In particular, a cellular arrangement of cells is updated according to local rules that involve the identification of receptive cells and averaging values from non-receptive sites. The cellular arrangement is the same as the configuration of water molecules in ice that occurs under ordinary conditions on Earth.

Keywords: Cellular automata, ice crystals, snowflakes

1. Introduction

Snow crystals are fascinating because they have remarkable symmetry while exhibiting diversity that is not easy to explain. However, as early as 1611 Kepler suggested that the symmetry of snow crystals is related to the hexagonal packing of spheres [1], which is remarkably close to being true. Bentley and Humphreys [2], Libbrecht and Rasmussen [3] and Nakaya [4] and many others have photographed thousands of snow crystals giving us a glimpse into their amazing structure. Figure 1 shows several images from [2] that illustrate classic 6-fold growth although we have little sense of their 3-dimensional structure. However, other growth forms, including 3-fold symmetric forms, 12-fold symmetric forms, 3-dimensional needles and capped columns also appear regularly in naturally occurring snow crystals. A few of these are shown in Figure 2. A close inspection of the upper right images in Figure 1 shows that even in figures that appear to have 6-fold symmetry at a glance, there may be subtle features that have only 3-fold symmetry. Other investigators have studied the physical conditions that lead to particular types of crystal growth. In particular, Nakaya [4] dedicated decades to systematically studying their growth, both in the field and in the laboratory. He found that two parameters were essential in explaining the diversity of snow crystals. For his laboratory experiments, those parameters were air temperature and the temperature of a water bath that introduced water vapor into the air. However, it is usually more convenient to think about air temperature and saturation as the two dominant parameters and those can be correlated to the parameters in his experiments.

Cellular automata are local rules applied to a configuration of cells in a uniform manner. The cells values are usually selected from a finite set of allowed values;

however, we will use generalized cellular automata that allow cells to contain real values. Classical applications of cellular automata (some generalized to taking real values) have been made to image processing, image and audio compression, and modeling earthquakes, phase transitions, crystal growth, fluid flow, populations, biologic growth, and computation [5-12]. It seems reasonable that the 3-dimensional growth of snow crystals at a point in space depends largely on the situation in the immediate neighborhood of the point. For cellular models, that corresponds to updating a cell depending upon the state of some local neighborhood of cells. We develop such 3-dimensional models in this paper.

Cellular automata on a 2-dimensional hexagonal arrangement of cells have been used to simulate snow crystal growth with perfect 6-fold symmetry [13]. Earlier versions of that 2-dimensional work appear in Coxe [14] and a variation on quasi-crystalline structures appears in [15]. An early paper dealing with cellular snow crystal modeling is [16]. By varying two parameters, the model in [13] led to growth exhibiting stellar, sector, plate and dendrite patterns. Since that model is 2-dimensional, it was impossible to model needle growth or capped columns which naturally occur. Figure 3 shows an example of the growth of dendrites using that 2-dimensional model.

This investigation considers cellular growth models in three dimensions. We were motivated by the success of the 2-dimensional models and curious to investigate similar models on realistic 3-dimensional lattices. In particular, we choose a cellular arrangement that mimics the 3-dimensional crystalline structure of ice. We then both generalize and simplify the local rule used in [13] for this cellular arrangement. We see 3-dimensional versions of the growth similar to many of those we saw in two dimensions but new

growth forms also appear. In particular, this model exhibits needle growth and growth forms with 3-fold symmetry.

2. The 3-Dimensional Arrangement of Cells

We utilize a cellular arrangement that corresponds to the configuration of the oxygen atoms (the dominant atoms in water molecules) in ordinary ice. While ice crystals with various crystallographic symmetries may be produced in the laboratory, ice occurring naturally at the surface of the Earth is known as Ice-Ih and has the crystallographic structure that we will describe. Detailed descriptions of the structure of ice may be found in [17-18].

Figure 4a shows a convenient simplified model that we can have as a general model for the arrangement of cells and neighbors. The spheres in the image correspond to water molecules (or the oxygen atoms in ice) and the cylinders correspond to hydrogen bonds between neighboring molecules of ice. The spheres correspond to cells in our cellular configuration and which cells are neighbors is shown with the cylinders. Notice that red cylinders and the cells they connect lie in horizontal planes and form hexagons. These planes are called the basal planes in crystallography. Each cell has three neighbors in the basal plane. We will call these the *p*-neighbors of the cells. The configuration of cells in each basal plane is replicated in the perpendicular direction. Each cell also has one neighbor in the direction perpendicular to the basal plane. The connections between those neighbors are shown with green cylinders in the figure. Notice that as one moves around a hexagon in a basal plane, the cells alternate between being attached to the basal plane

above or below the given plane. This perpendicular direction is called the *c*-axis direction in crystallography. We will refer to the neighbor in this direction as the *q*-neighbor.

In actual ice crystals, each cell is tugged slightly out of the basal plane toward its *q*-neighbor. This results in the configuration of cells as seen in Figure 4b. We use this configuration for our three dimensional rendering. However, for purposes of defining our local automata, we need only know that all together, each cell has four neighbors, one of them (the *q*-neighbor) distinguished from the other three. Figure 5 illustrates that simple neighborhood of a cell. Of course, the global arrangement of these neighborhoods is essential to the global symmetry that we will see develop.

3. The Local Rule

Before discussing the 3-dimensional local rule, we will first describe the rule for the 2-dimensional modeling used in [13, 15]. The cells each contain a real number between 0 and 1. A cell is considered ice if it has value 1. A cell is called receptive if it is ice or the neighbor of ice. Informally, we consider material at receptive cells to be bound to the ice crystal and non-receptive material to be free to move around. In the 2-dimensional models, the values in the cells were split into two hexagonal arrays for further processing before those two arrays were recombined. One of those arrays contained the receptive material with zeros in the non-receptive sites. A constant value, γ, where $0 \le \gamma < 1$, was added to each receptive site, the informal idea being that this accounted for some material being available from the third, un-modeled, dimension. The second array contained the non-receptive values and zeros in the receptive sites. This array was processed by averaging the array. Each cell was replaced by an average of its neighborhood with the

center cell having weight one-half and the other cells amounting to the other half. For hexagonal neighborhoods in those 2-dimensional models where each cell has six neighbors, that meant the 6 neighbors each had weight $\frac{1}{12}$ in the average. Finally, the two arrays are added together and any excess over 1 removed so that 1 remains the maximal value. That completes one time step of the cellular evolution which is then iterated. For a typical experiment in that 2-dimensional work, we seeded a single ice cell as 1 in a uniform field of values β at all the other cells. Descriptions and illustrations of how that model develops may be found in [13]. Figure 3 shows the result of the evolution of that 2-dimensional model from a single ice cell when $\beta = 0.35$ and $\gamma = 0.001$.

For the 3-dimensional model we develop here, we also use values between 0 and 1 for our cell values. However, since we now are accounting for all three dimensions, we do not add γ to receptive cells, we simply extend our averaging into the third dimension. We will give the details in the next section. One of our parameters remains the background level. However, to obtain a second parameter, it seems reasonable to bias the averaging weights depending upon whether the neighbors are *p*-neighbors (from the basal plane) or *q*-neighbors (in the perpendicular direction). It turns out that the relative weights of the *q*-neighbor to those for the *p*-neighbors is more important than their relative weights compared to the center site. While we will discuss this in further detail later, our primary class of examples is based upon using the same weight at the center site as for the *p*-neighbors.

4. Variation of Primary Parameters

As described in Section 2 we are modeling on a cellular arrangement where each cell has four neighbors; namely, three *p*-neighbors in the basal plane and one *q*-neighbor in a perpendicular direction. Thus, each neighborhood has 5 cells when the center is included. As in the 2-dimensional case we identify each cell as receptive if the cell or any of its neighbors is ice. The cell is non-receptive otherwise. We split the values in the cells into two arrays. One gives the values at receptive sites (0 elsewhere). Unlike the 2-dimensional case, no further processing (i.e., no added gamma) is done to this array of receptive values. The second array contains the values at the non-receptive sites (0 elsewhere). This array is processed by averaging over the neighborhoods. The non-ice receptive sites will typically receive a non-zero value from this averaging. The weights used in the averaging will vary, but always sum to 1. In this section we will take the center weight to be the same as that for the *p*-neighbors and hence we can specify the averaging scheme by giving the ratio, *r*, of the weight for the *q*-neighbor to that for the *p*-neighbors. In particular, when $r = 1$, the weights used for all five cells are $\frac{1}{5}$ while when $r = 2$, the weights used for the center and *p*-neighbors are all are $\frac{1}{6}$ and the *q*-neighbor takes weight $\frac{2}{6}$. Figure 6 shows an example of a small cellular patch being updated so that a receptive cell becomes ice. While there is not enough data visible to verify the particular computation, it is illustrative of the general scheme being used.

Figure 7 illustrates the result of growth of our model for various *r* and β values. The size of the arrangement of cells was 150 by 150 by 150. A single central cell was turned to ice and evolution ceased when ice reached within three cells of a boundary or if the number of iterations exceeded 5000. Color corresponds to position with *z*-position dominating the change when that is feasible. In any case, the color adds redundant

information, but helps the interpretation of information lost by the projection of the 3-dimensional model into a planar image. The cells are configured as in Figure 4b and ice produced by our automata is rendered using overlapping spheres in the raytracing program POVRay [19]. While the individual spheres are visible, they have been somewhat blended together using POVRay's blob type.

Figure 7 uses a view from the side so that the *c*-axis is vertical in the figure. In the figure we see that small values of *r* tend to produce long crystals with *c*-axis direction growth significant, while large values of *r* produce more planar growth. For *r* larger than 1, we see that as β increases, growth changes from dendrites toward stellar and hexagonal plate forms. In Figure 8 we consider the same variation of *r* and β values with view nearly straight down the *c*-axis. Here the changes from dendrites toward stellar and hexagonal plate forms are even more apparent. The variety of cross-sectional forms for the columnar growth (smaller *r* values) is easy to observe. Note also that several of these forms have (like some of the growth in Figure 2) very obvious 3-fold (but not 6-fold) symmetry. For example, $r = 0.05$, $\beta = 0.25$. Also notice that some of the columns have "waists" as do some of the columnar forms in Figure 2.

Figure 9 shows some of the examples from Figures 7 and 8 in more detail. The capped plates in Figure 2 would seem to result from a change in growing conditions: from columnar growth to plate growth. Notice that when $\beta = 0.6$ and $r = 4$ two horizontal plates appear to be the dominant growth patterns (and a third plate is barely visible). Thus, our model comes close to producing features like capped columns even without changing the growth conditions. When $\beta = 0.65$ and $r = 0.25$ we see a column grow with remarkable vertical uniformity. When $\beta = 0.55$ and $r = 20$ we see some subtle 3-fold

symmetric features reminiscent of the snowflakes in the upper right of Figure 1. When β =0.9 and r = 0.125 we see an almost fractal pattern of growth although the overall extent is closer to a ball in the sense that the growth is similar in the basal and c-axis directions. These fractal structures appear for relatively low r and high β. They do not seem to be a common form of naturally occurring snow crystal although rough sphere-like snow grapple is a common form of snow and similar growth occurred for the analogous 2-dimensional models [13]. More detailed illustrations resulting from this type of growth for additional r and β values appears at [20].

5. Variations

Next we consider the situation where we vary the averaging weight associated with the center cell. Suppose we take the p-neighbors and q-neighbors to have the same weight. Let s denote the ratio of the weight for the center cell to the weight of the other cells. Figure 10 shows the result of using s = 0.25, 1 and 4 when β = 0.15. Notice that these all are similar to images that were seen in Figures 7 and 8; this is consistent with our experience that by varying the ratio r as in the previous section, we see the same qualitative behaviors.

In Figures 8 and 9 we see examples where 3-fold symmetry is apparent. We next show the result of comparing r = 0.05 with β = 0.2 and 0.3 growth with different initial conditions. The top images in Figure 11 show the result of those experiments with the usual single initial cell of ice. The bottom images in the figure show the corresponding growth when six cells forming a hexagon are initially ice. Notice that there is more 6-fold symmetry in the projection, but that in three dimensions the result may still be strongly 3-

fold, as seen in the bottom right where the red corresponds to portions of the growth that are at the bottom. These experiments illustrate the great sensitivity of these growth models.

Figure 12 shows the result of running $r = 0.25$ with $\beta = 0.65$ on a single initial ice cell followed by 30 steps of $r = 20$ with β remaining unchanged. Notice the dramatic capped columns with three primary levels. Similar capped columns appear in Figure 2.

6. Concluding Remarks

The model presented here provides a simple rule for updating a 3-dimensional configuration of cells in order to model snow crystal growth. This model is deterministic and utilizes only two parameters. We see examples of dendrite, stellar and plate growth commonly seen in nature and also seen in previous 2-dimensional models. This 3-dimensional model exhibits new types of growth, including 3-fold symmetric growth, columnar and capped columnar growth. Our model could be made more physical by demanding conservation of mass, for example. However, our efforts in that direction lead to periodic configurations that frustrated robust model design. In the many cases where such models exhibited growth, the growth had grainy feel, like often seen in diffusion limited growth models. Averaging could be used to remove that graininess. However, in our model, averaging is used both for smoothing and transport and we believe that this allows for such a simple model to successful model so many different types of 3-dimensional snow crystal growth.

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Figure Captions:

Figure 1. Some classic 6-sided snow crystals.

Figure 2. Some other snow crystals.

Figure 3. Growth of dendrites from a 2-dimensional model.

Figure 4. Cellular arrangement: (a) simple neighbor model (b) rendering model.

Figure 5. A simplified view of a cell and its neighbors.

Figure 6. The scheme used for updating cells illustrating a receptive cell becoming ice.

Figure 7. Sample growth as β and r vary; side view.

Figure 8. Sample growth as β and r vary; top view.

Figure 9. Some more detailed views.

Figure 10. Varying the center weight for averaging for s = 0.25, 1, and 4 with β = 0.15 has little impact on the qualitative growth forms.

Figure 11. Changing the initial ice configuration from a single cell (top row) to six cells (bottom row) forming a hexagon for r = 0.05 and β = 0.2, 0.3.

Figure 12. Capped columns resulting from changing from r = 0.25 to r = 20 for β = 0.65.