EXCERPTED FROM

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A NEW KIND OF SCIENCE

SECTION 8.2

The Growth of Crystals

fifty or so years, it has almost never been possible to demonstrate that results obtained from such approximations even correctly reproduce what the original mathematical equations would imply.

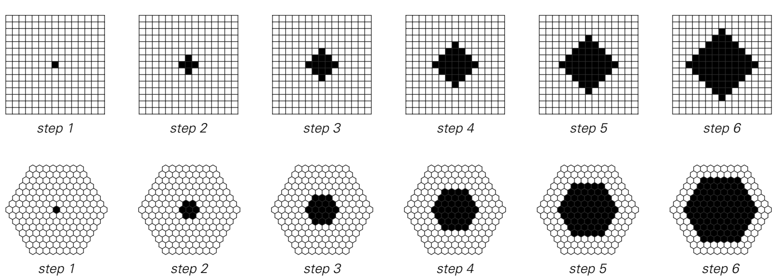
Models based on simple programs, however, suffer from no such problems. For essentially all of them involve only discrete elements which can be handled quite directly on a practical computer. And this means that it becomes straightforward in principle—and often highly efficient in practice—to work out at least the basic consequences of such models.

Many of the models that I discuss in this chapter are actually based on some of the very simplest kinds of programs that I consider anywhere in this book. But as we shall see, even these models appear quite sufficient to capture the behavior of a remarkably wide range of systems from nature and elsewhere—establishing beyond any doubt, I believe, the practical value of thinking in terms of simple programs.

The Growth of Crystals

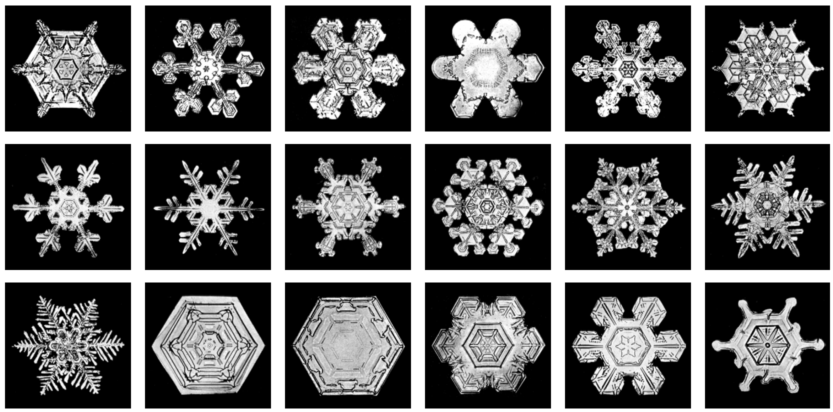
At a microscopic level crystals consist of regular arrays of atoms laid out much like the cells in a cellular automaton. A crystal forms when a liquid or gas is cooled below its freezing point. Crystals always start from a seed—often a foreign object such as a grain of dust—and then grow by progressively adding more atoms to their surface.

As an idealization of this process, one can consider a cellular automaton in which black cells represent regions of solid and white cells represent regions of liquid or gas. If one assumes that any cell which is adjacent to a black cell will itself become black on the next step, then one gets the patterns of growth shown below.



Cellular automata with rules that specify that a cell should become black if any of its neighbors are already black. The patterns produced have a simple faceted form that reflects directly the structure of the underlying lattice of cells.

The shapes produced in each case are very simple, and ultimately consist just of flat facets arranged in a way that reflects directly the structure of the underlying lattice of cells. And many crystals in nature—including for example most gemstones—have similarly simple faceted forms. But some do not. And as one well-known example, snowflakes can have highly intricate forms, as illustrated below.

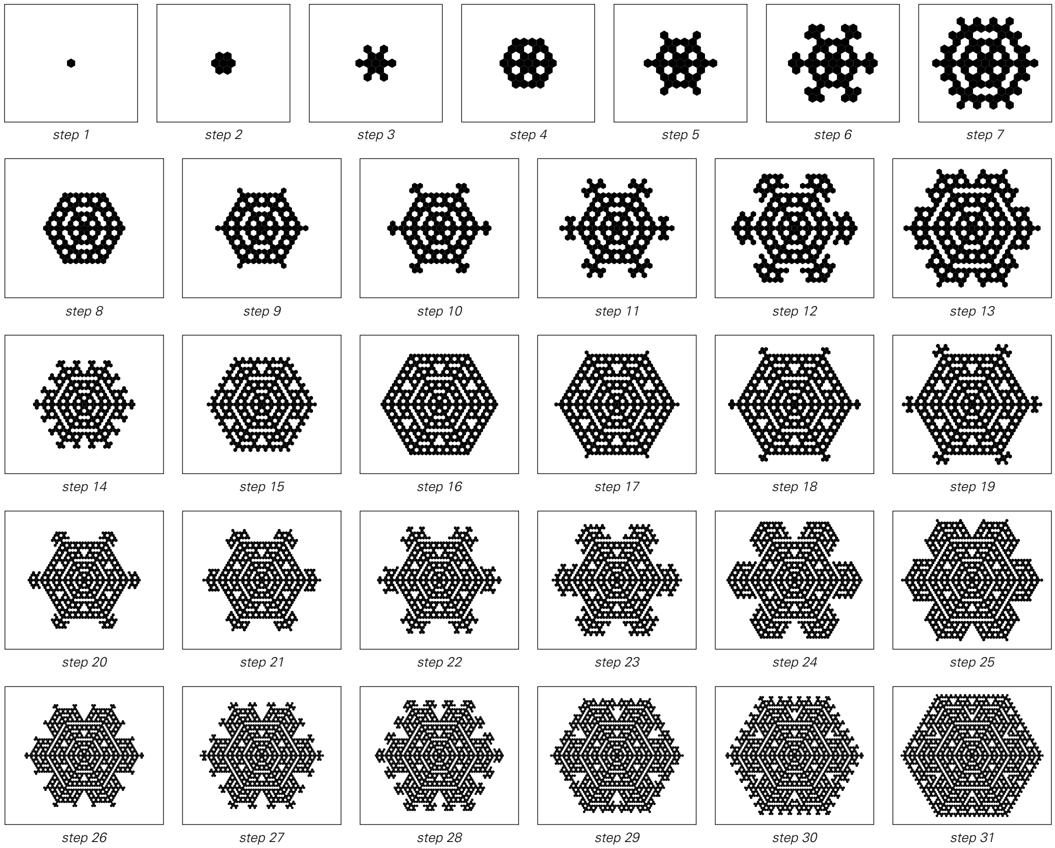


Examples of typical forms of snowflakes. Note that the scales for different pictures are different.

To a good approximation, all the molecules in a snowflake ultimately lie on a simple hexagonal grid. But in the actual process of snowflake growth, not every possible part of this grid ends up being filled with ice. The main effect responsible for this is that whenever a piece of ice is added to the snowflake, there is some heat released, which then tends to inhibit the addition of further pieces of ice nearby.

One can capture this basic effect by having a cellular automaton with rules in which cells become black if they have exactly one black neighbor, but stay white whenever they have more than one black neighbor. The pictures on the facing page show a sequence of steps in the evolution of such a cellular automaton. And despite the simplicity of its underlying rules, what one sees is that the patterns it produces are strikingly similar to those seen in real snowflakes.

From looking at the behavior of the cellular automaton, one can immediately make various predictions about snowflakes. For example,



The evolution of a cellular automaton in which each cell on a hexagonal grid becomes black whenever exactly one of its neighbors was black on the step before. This rule captures the basic growth inhibition effect that occurs in snowflakes. The resulting patterns obtained at different steps look remarkably similar to many real snowflakes.

one expects that during the growth of a particular snowflake there should be alternation between tree-like and faceted shapes, as new branches grow but then collide with each other.

And if one looks at real snowflakes, there is every indication that this is exactly what happens. And in fact, in general the simple cellular automaton shown above seems remarkably successful at reproducing all sorts of obvious features of snowflake growth. But inevitably there are many details that it does not capture. And indeed some of the photographs on the facing page do not in the end look much like patterns produced at any step in the evolution shown above.

But it turns out that as soon as one tries to make a more complete model, there are immediately an immense number of issues that arise, and it is difficult to know which are really important and which are not. At a basic level, one knows that snowflakes are formed when water vapor in a cloud freezes into ice, and that the structure of a given snowflake is determined by the temperature and humidity of the environment in which it grows, and the length of time it spends there.

The growth inhibition mentioned above is a result of the fact that when water or water vapor freezes into ice, it releases a certain amount of latent heat—as the reverse of the phenomenon that when ice is warmed to 0°C it still needs heat applied before it will actually melt.

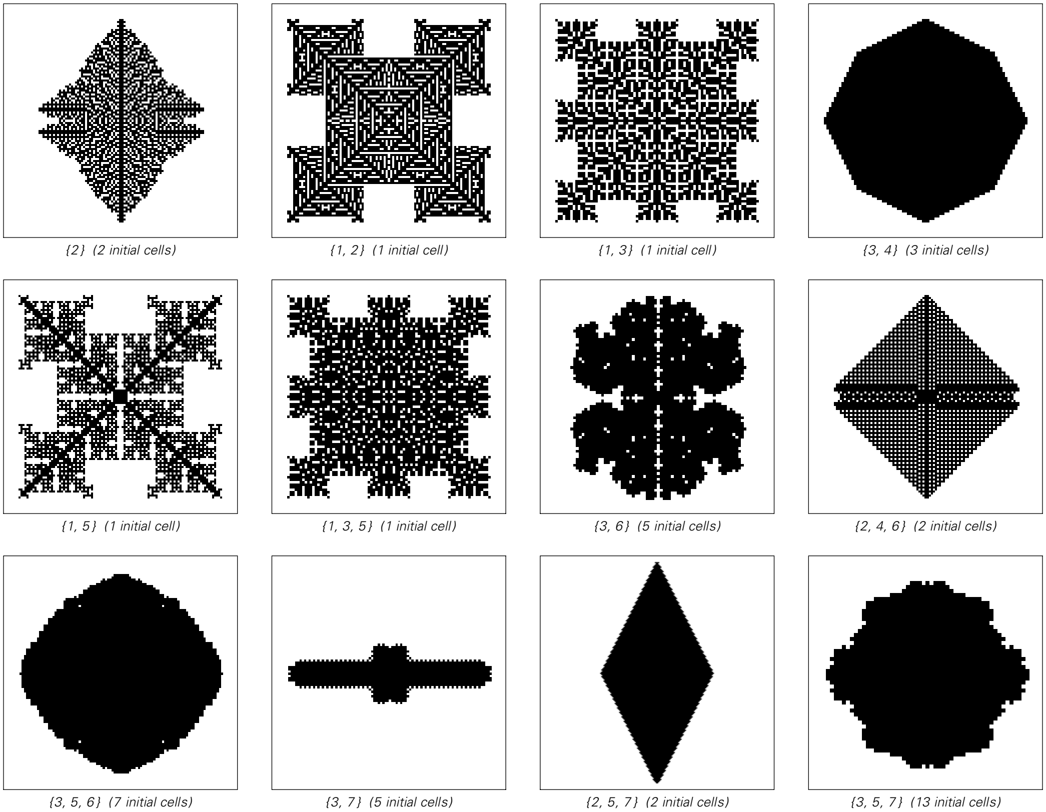
But there are also many effects. The freezing temperature, for example, effectively varies with the curvature of the surface. The rate of heat conduction differs in different directions on the hexagonal grid. Convection currents develop in the water vapor around the snowflake. Mechanical stresses are produced in the crystal as it grows.

Various models of snowflake growth exist in the standard scientific literature, typically focusing on one or two of these effects. But in most cases the models have at some basic level been rather unsuccessful. For being based on traditional mathematical equations they have tended to be able to deal only with what amount to fairly simple smooth shapes—and so have never really been able to address the kind of intricate structure that is so striking in real snowflakes.

But with models based on simple programs such as cellular automata, there is no problem in dealing with more complicated shapes, and indeed, as we have seen, it is actually quite easy to reproduce the basic features of the overall behavior that occurs in real snowflakes.

So what about other types of crystals?

In nature a variety of forms are seen. And as the pictures on the facing page demonstrate, the same is true even in cellular automata with very simple rules. Indeed, much as in nature, the diversity of behavior is striking. Sometimes simple faceted forms are produced. But in other cases there are needle-like forms, tree-like or dendritic forms, as well as rounded forms, and forms that seem in many respects random.



Examples of patterns produced by two-dimensional cellular automata set up to mimic the growth of crystals. The rules in each case take a cell to become black if the specified number of its neighbors (including diagonals) on a square grid are black on the step before. These rules are such that once a cell has become black, corresponding to solid, it never reverts to white again. In each case a row of initial black cells of the specified length was used.

The occurrence of these last forms is at first especially surprising. For one might have assumed that any apparent randomness in the final shape of something like a crystal must always be a consequence of randomness in its original seed, or in the environment in which it grew.

But in fact, as the pictures above show—and as we have seen many times in this book—it is also possible for randomness to arise intrinsically just through the application of simple underlying rules. And contrary to what has always been assumed, I suspect that this is actually how the apparent randomness that one sometimes sees in shapes formed by crystalline materials often comes about.