Math100: Introduction to the Profession

Mathematics and Materials Science

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Mathematics

-- Numbers
-- Geometry, shapes
-- Theorems, equations
-- Solve equations ! Hard…

?

Materials Science

-- Steel and Alloy
-- Carbon material
-- Polymers
-- Crystals ! Microstructure…

How to connect these two fields: Mathematical Modeling

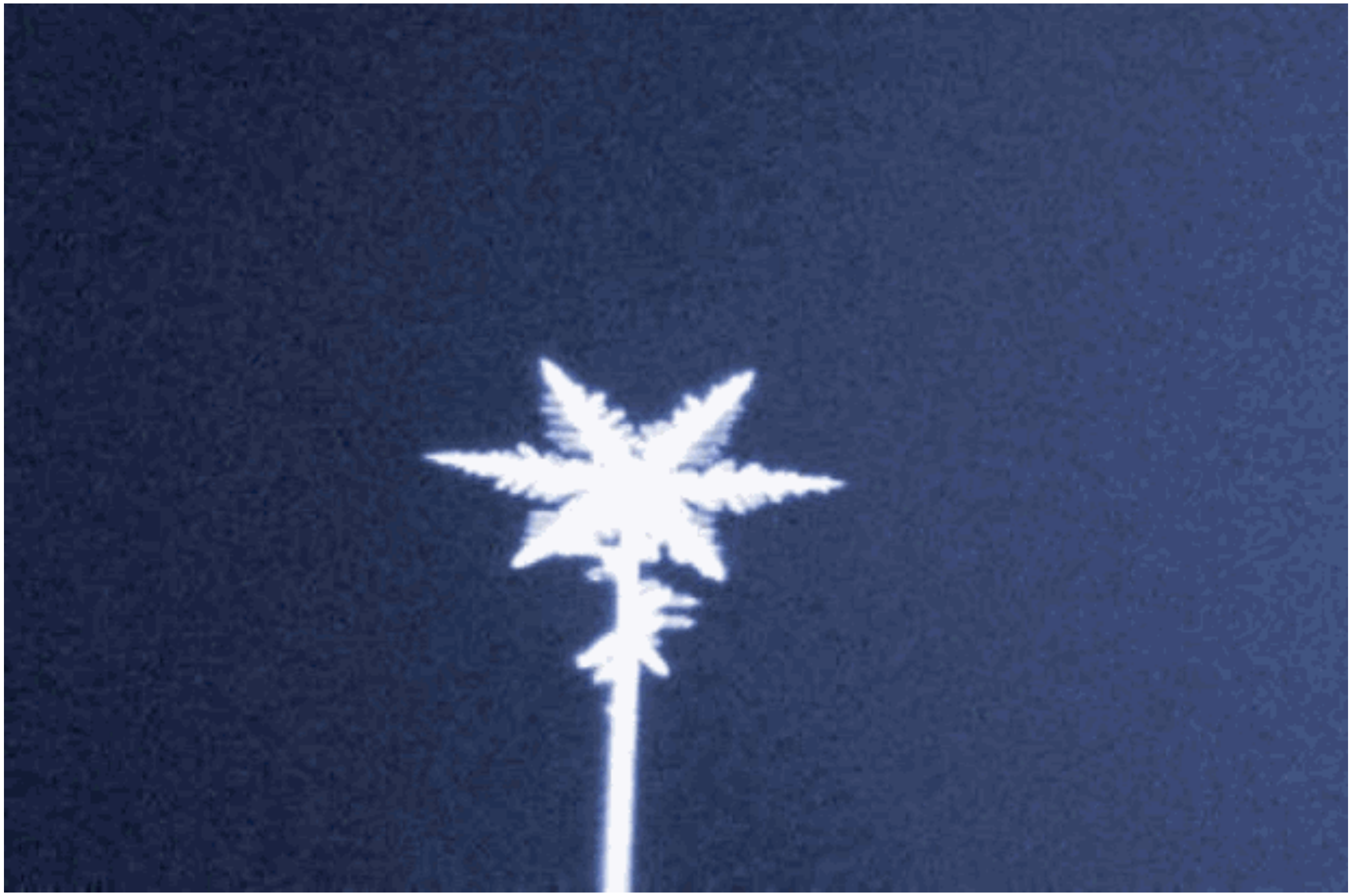
Why use Mathematical Modeling?

Mathematics has the unique ability to model physical and biological systems in ways that enable **prediction and control**

- Identify key processes
- Translate physics into mathematical processes
- Analyze the mathematical system
- Compare results to known physical behavior
- If agree, then move on to make predictions
- If disagree, figure out missed parts and add them back
- Test mathematical predictions by performing new targeted experiments

Circle of discovery

An example: snowflake growth



Snowcrystals.com

What did you observe: ice crystal symmetry

Ice, Ih, the normal form, has a hexagonal crystal structure.

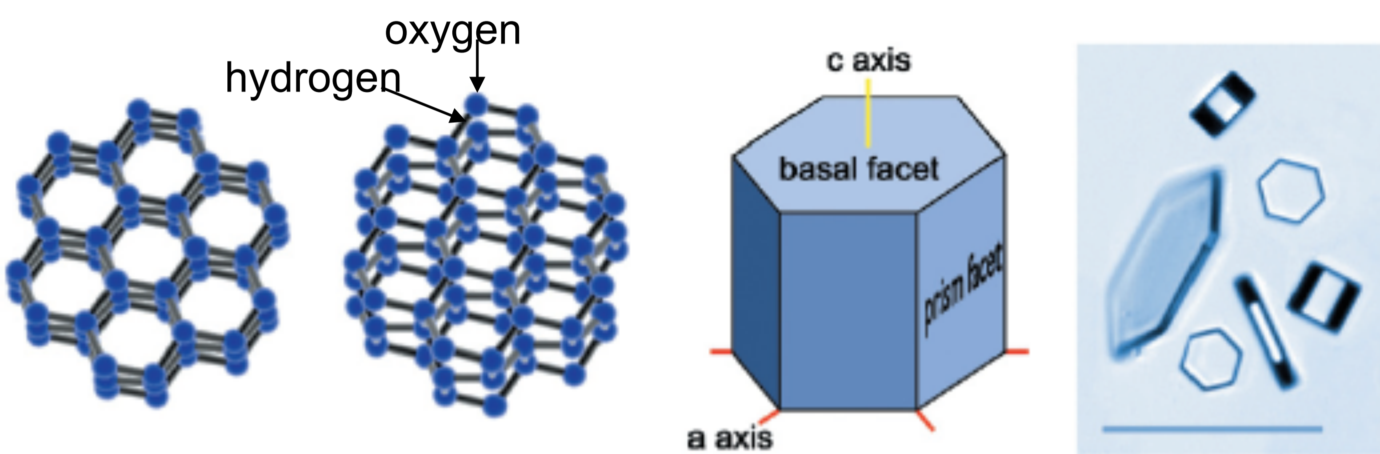
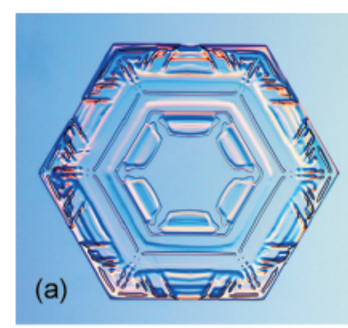


Figure 4. Left: Two views of the crystal structure of ice Ih, showing a lattice of 'puckered' hexagons. Here balls represent oxygen atoms and bars represent hydrogen atoms. Middle: A schematic picture of a simple ice prism, defining the principal crystal axes and facet planes. Right: A mosaic image of some typical small ice prisms grown in the lab, showing different aspect ratios. The scale bar is 100 μm long.

Libbrecht (2005)

Gives ice crystals their natural 6-fold symmetry.



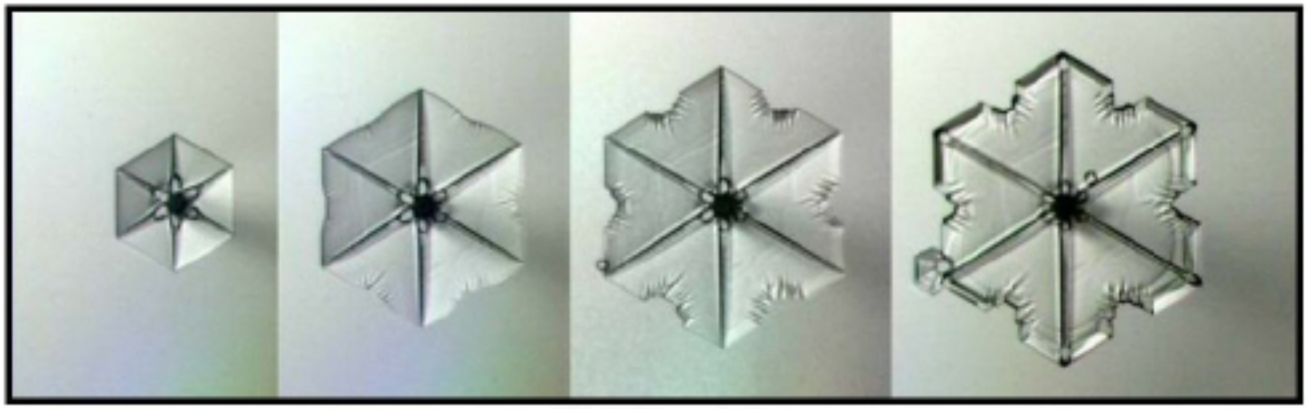
How do ice crystals grow?

- Water molecules diffuse through the vapor.

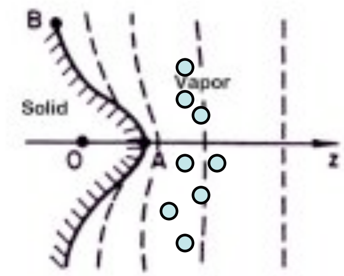
- The molecules are incorporated into the ice crystal lattice. This is typically not instantaneous since they must arrange themselves correctly and the incorporation also depends on the temperature, surface structure, geometry and chemistry. (attachment kinetics)

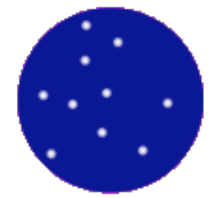
- When the molecules attach to the crystal lattice, they release their heat to the surrounding vapor (latent heat)

A Growth Sequence



(K. Libbrecht)





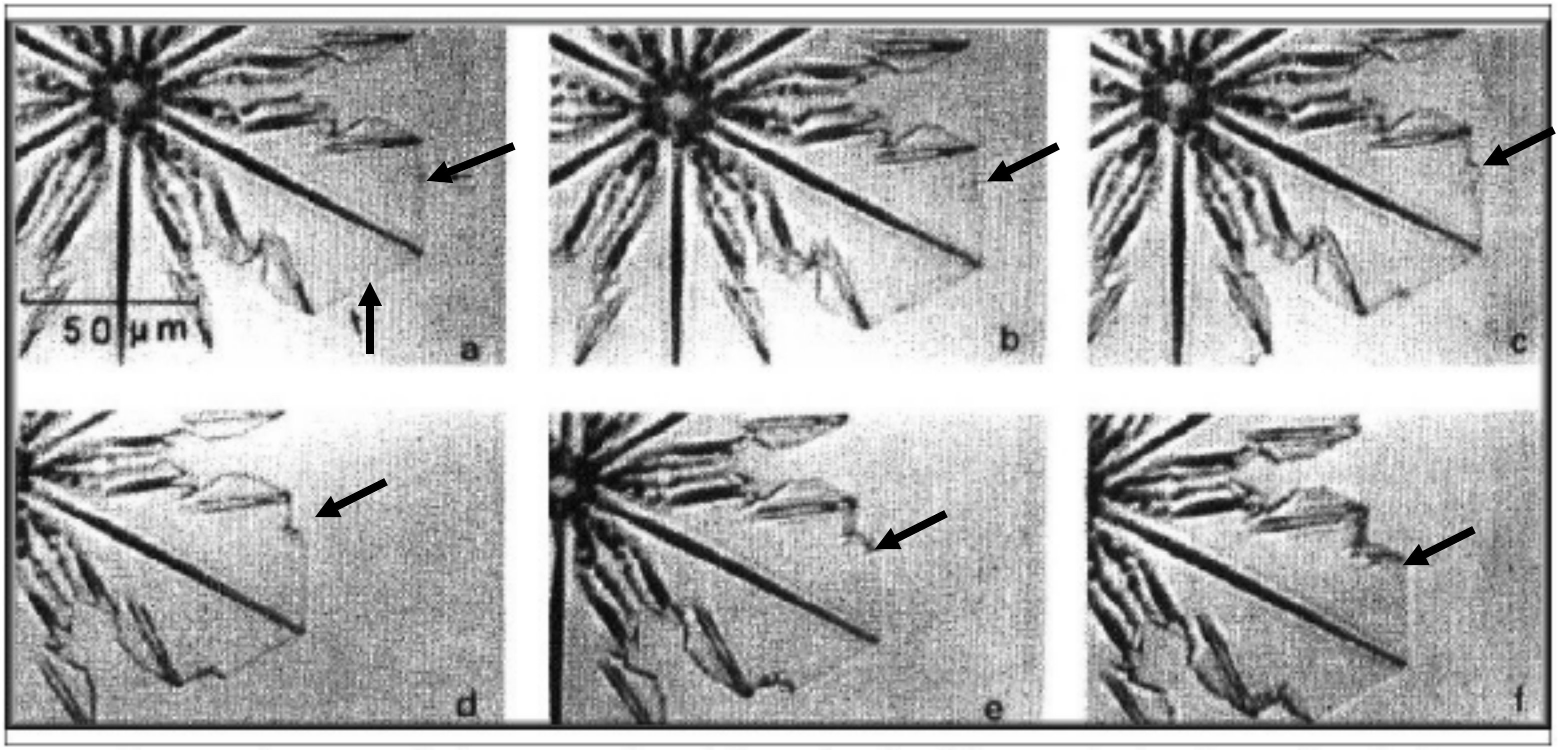
•Growth is limited by rate of diffusion of water molecules to the crystal surface.

•Corners are most accessible to water molecules in the vapor, so attachment tends to happen there first.

•Eventually, the greater attachment rate at the tips causes an instability where the tips grow faster. Further growth, reinforces the tips. (Mullins-Sekerka Instability)

Dendrites

Further instabilities develop to produce dendritic or tree-like structures.



(T. Gonda - S. Nakahara, reprinted from [GN] with permission from Elsevier)

Formation of side-branches. Still controversial!

A Brief History of Snowflakes

- Kepler (1611) wrote a short scientific treatise on snowflakes origins of snow crystal symmetry

  "I do not believe that even in a snowflake, this ordered pattern exists at random."

- Decartes (1637). Described variety of snow crystal morphologies

……

- Wilson Bentley (1931). Vermont farmer. Photographed extensive collection of snowflakes. Credited with establishing idealized snowflake designs as icons of wintertime

History Contd.

- Nakaya (1954). Categorized natural snow crystals under different meteorological conditions. First to grow snow crystals in a controlled environment in the lab.

  "The similarity of the form of the branches is itself a problem that is difficult to explain. There is apparently no reason why a similar twig must grow, in the course of a crystal, from one main branch when a corresponding twig happens to extend from another branch…. In order to explain this phenomenon we must suppose the existence of some means which informs other branches of the occurrence of a twig on a point of one branch."

……

- Libbrecht (2005). A simplified classification of snowflake types (35 types). Down from 80(!)-- Magano-Lee.

Mathematical Modeling

•Very difficult problem (multiple length/time scales).

•In order to obtain a tractible mathematical model, identify key features which will be modeled.

•There is a long history of mathematical models for crystal growth

Range from macroscopic to microscopic

We will begin by considering microscopic models.

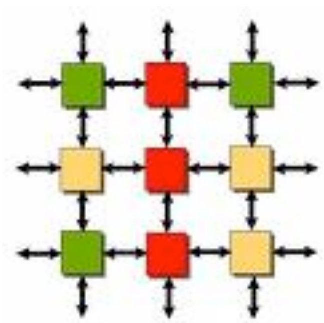
Discrete, Cellular Automata Models

Cellular Automata Modeling

A cellular automaton (CA) is a collection of cells arranged in a grid, such that each cell changes state as a function of time according to a defined set of rules that includes the states of neighboring cells.

The state of each cell changes in discrete steps at regular time intervals. The state depends on (1) its own state at the previous time step, and (2) the state of its immediate neighbors at the previous time step.

Developed originally (1940s) by Stanislaw Ulam (crystal growth) and John von Neumann (self-replicating robot)

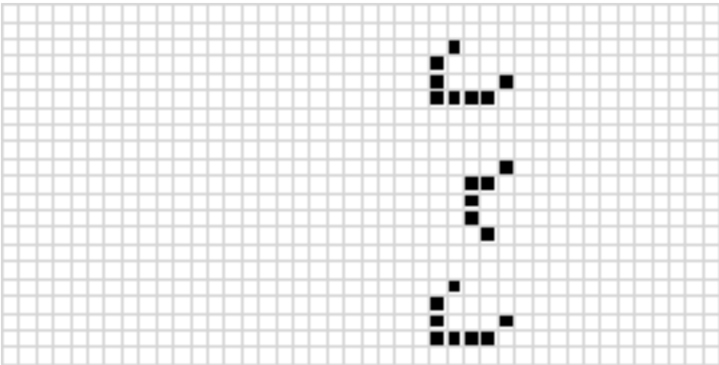


•Featured in Season 2, episode "Bettor or Worse" of the TVShow NUMB3RS

Cellular Automata Contd

- von Neumann (1940s) developed a universal copier. Proved that a particular pattern would make endless copies of Itself.
- John Conway (1980s). Game of life.

A cell is either white or black. If a black cell
Has 2 or 3 black neighbors, it stays black. If
A white cell has 3 black neighbors, it becomes black.
In all other cases, the cell stays or becomes white.



Gliders-- arrangements of cells that move across the grid

http://mathworld.wolfram.com/CellularAutomaton.html

Cellular Automata Contd.

- Wolfram (1980s). Systematic analysis of basic, fundamental class of “elementary” cellular automata. Developer of the software package Mathematica™

Warm-up puzzle: a correct statement

There are 10 kinds of people:
people who know the binary
and people who do not.

Cellular Automata Contd.

<u>“Elementary” Cellular Automata</u> (CA)

- 1 dimensional CA:

- 2 possible states per cell: 1 (black), 0 (white)

- A cell and its 2 neighbors form a neighborhood of 3 cells so there are $2^3=8$ possible patterns for a neighborhood. There are then $2^8=256$ possible rules.

Example of Elementary CA

Rule 30. In binary (i.e. base 2), $30=11110_2$ where the subscript denotes the base

For example, the binary representation:

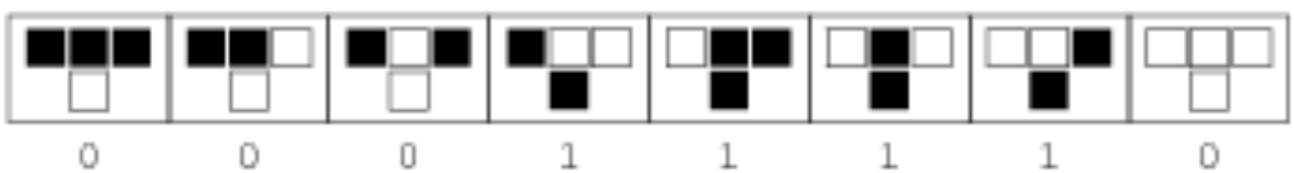
$$10_2 = (1x2^1)+(0x2^0)$$

so, following this reasoning:

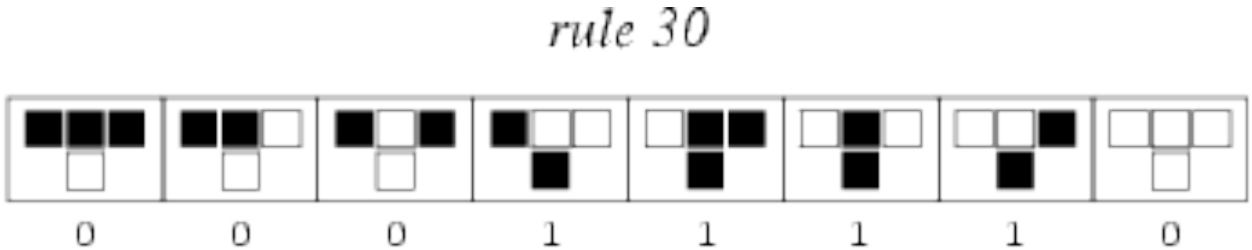
$$11110_2 = (1x2^4)+(1x2^3)+(1x2^2)+(1x2^1)x(0x2^0)$$
$$= 16+8+4+2=30$$

Rule 30:

current pattern
new state for center cell

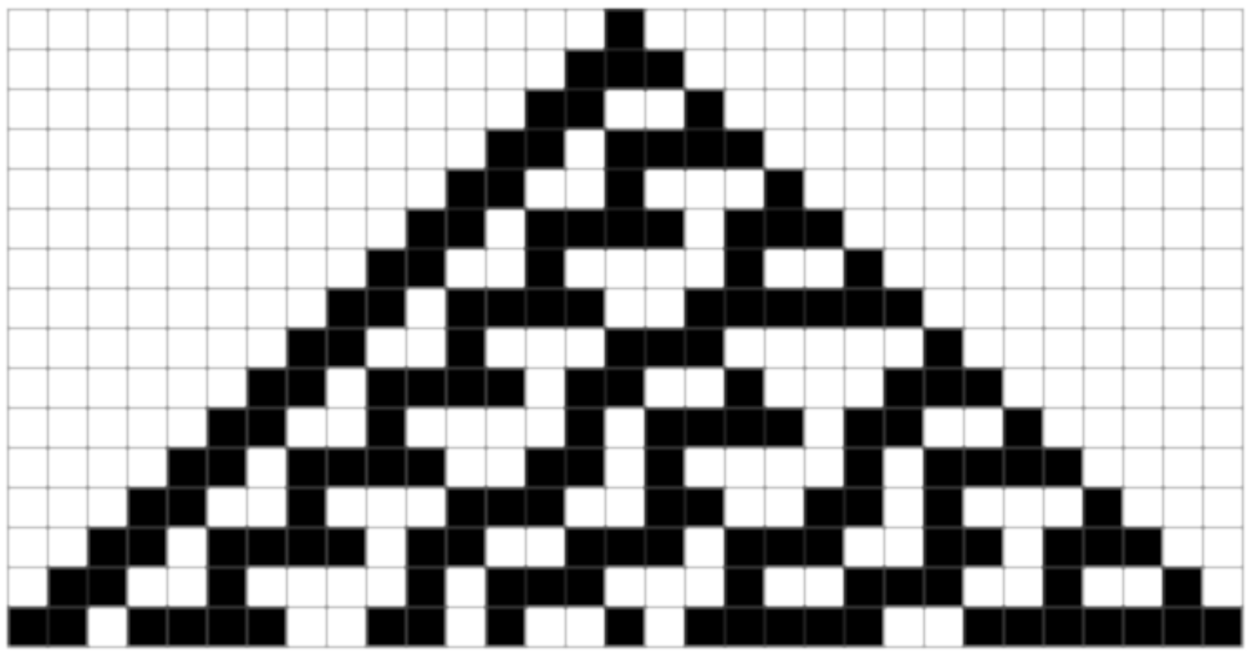


Rule 30 CA Contd.



Neighborhood rule

Time (# steps) increasing



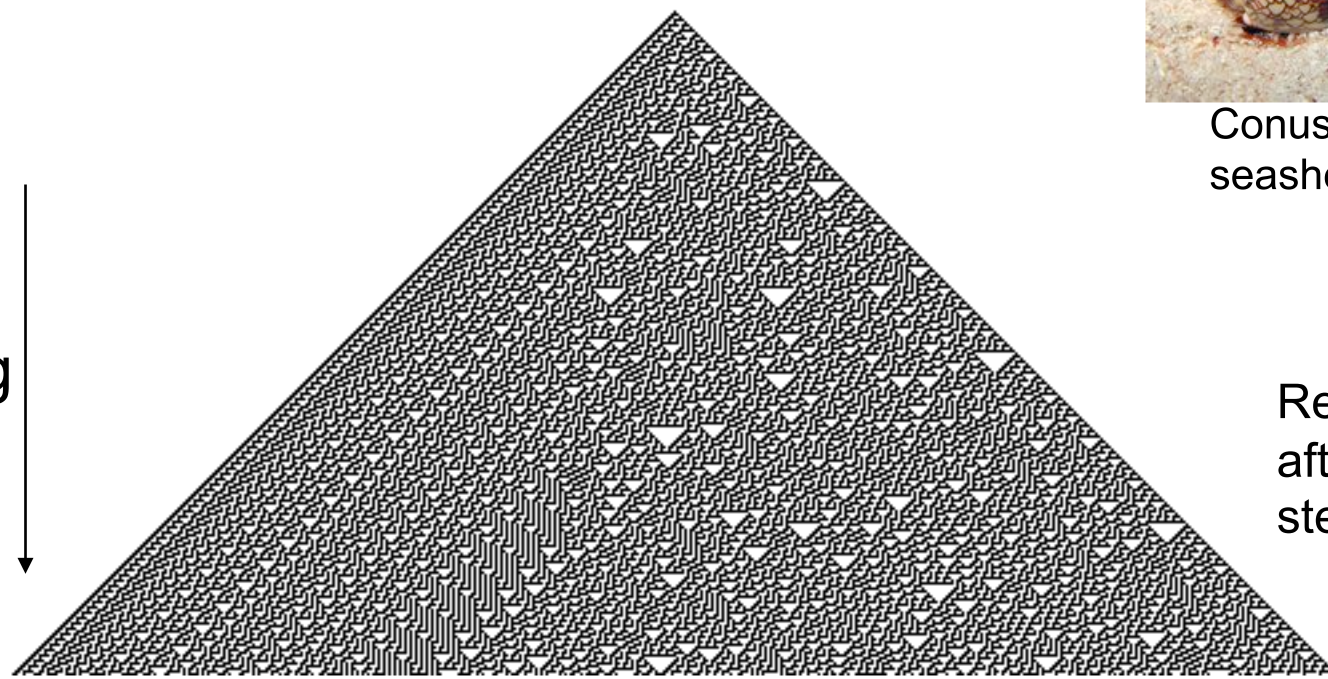
Result After 15 steps

space

Rule 30 CA Contd.

Conus textile seashell

Time (# steps) increasing



Result after 250 steps

space

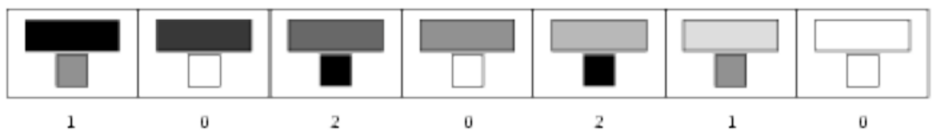
It can be shown that rule 30 is chaotic. Namely, the sequence in the center column does not seem to repeat. (Wolfram, 2002). Indeed, this rule is used as the Mathematica^{TM} random number generator.

More Complicated Rules

k-color, cellular automata. (each cell could have k-possible states)

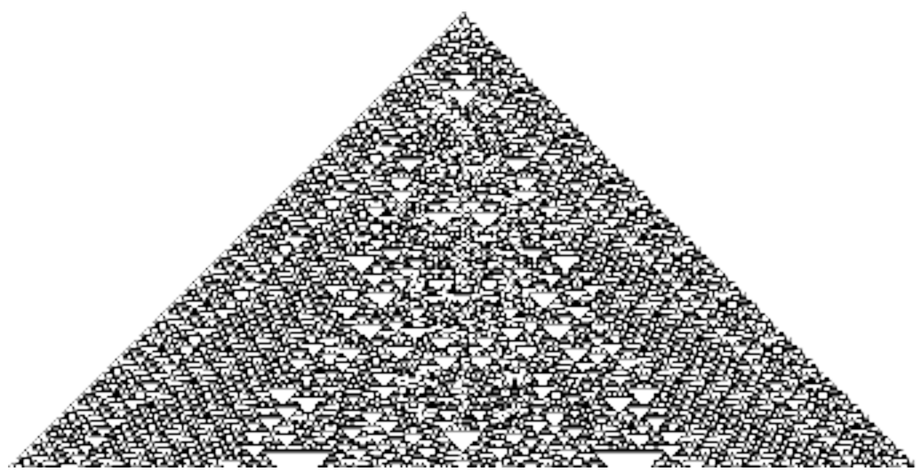
Example with k=3: Black (2), Grey (1), White (0)

(Wolfram, 2002)



(base 3)

time



Result after
300 steps

•Seemingly random pattern.

How to connect to Crystal Growth?

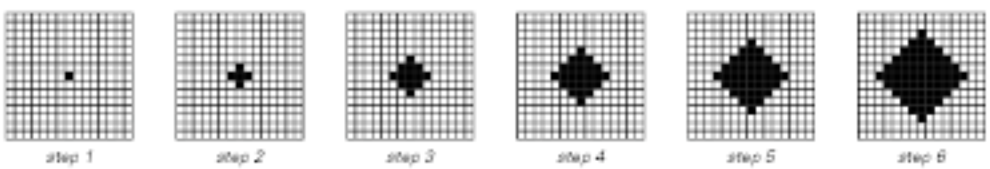
2-dimensional CA.

Consider very simple system.

1=black=solid, 0=white=vapor.

Suppose any cell adjacent to a black cell will become black
On the next step.

This gives:



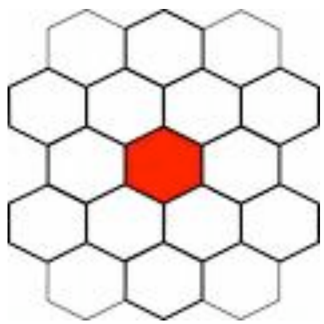
Wolfram (2002)

•Growth of a simple, facetted shape. Not correct symmetry for ice.

(facet is a smooth flat surface)

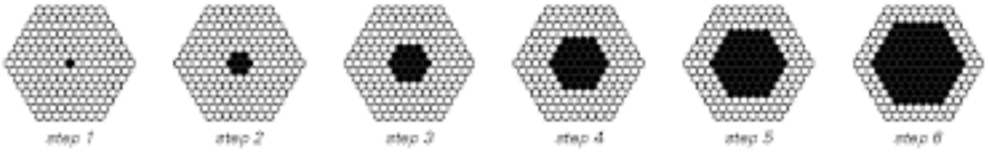
How to Connect to Crystal Growth Contd.

To get correct symmetry for ice, need to change the underlying lattice. Rather than using a Cartesian grid lattice, one may apply the same rule on a honeycomb-like Lattice.



honeycomb

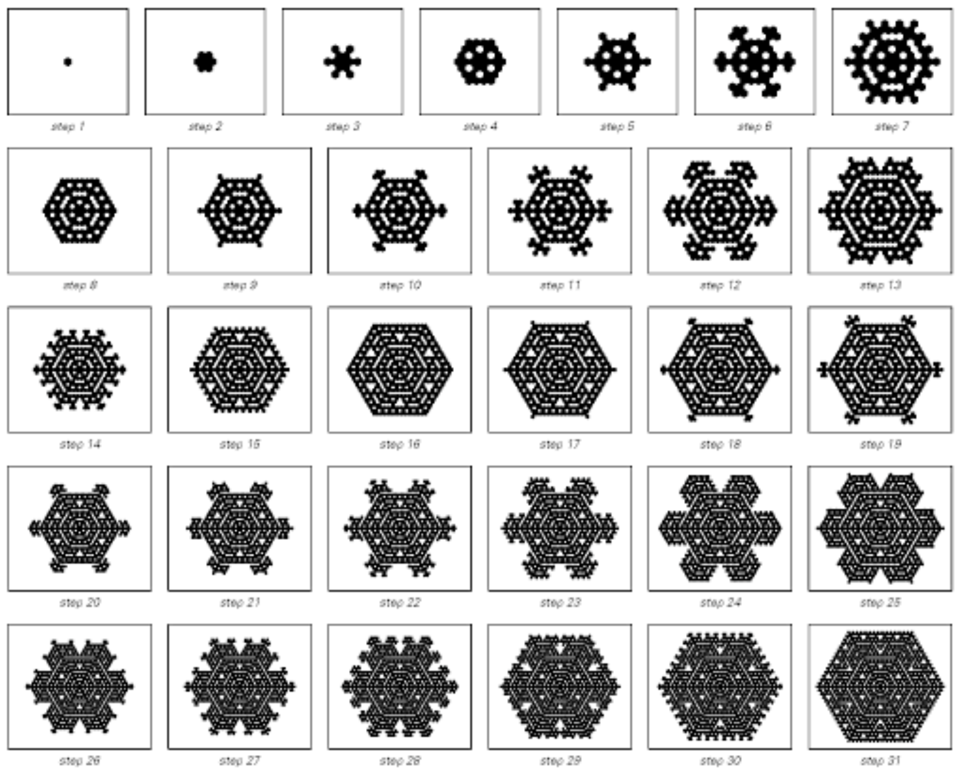
One then gets:



•Growth of 6-fold symmetric facetted shape.

Simple model to account for these features

- Cells become black if they have exactly 1 black neighbor, but stay white if they have more than 1 black neighbor.



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.

Wolfram (2002)

How to Connect to Crystal Growth Contd.

Previous models are highly simplified, as are the corresponding morphologies.

In previous implementation, it was assumed that all cells fill with solid if in contact with the solid.

In reality, not every cell is filled with solid even if it is in contact with the solid.

This is because molecules may not be able to attach readily to the crystal, even if they are adjacent to it (attachment kinetics). Moreover, when a molecule attaches to the crystal, latent heat is released that has an inhibiting effect on the crystallization of nearby molecules.

With anisotropy

$\tau(\theta) = 1 - 15\nu\cos(4\theta),\ \nu{=}0.004 \quad J = 30$