SPATIO-TEMPORAL MODELING OF SNOW FLAKE CRYSTALS USING PACKARD'S CELLULAR AUTOMATA

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Abstract

Cellular automata (CA) modelling is one of the recent advances in spatial–temporal modeling techniques in the field of growth dynamics. Spatio-temporal modeling of growth patterns has gained more importance in the recent years especially in the field of crystal growth, urban growth, biological growth etc. It has become an interest for researchers to study the model on spatial and temporal dynamic behavior. This paper aimed at modeling crystal growth using cellular Automata, which have dynamic capabilities to handle spatio-temporal phenomenon for better and efficient growth process. Cellular Automata models are used to simulate the process of crystal growth and to generate various patterns that the crystals create in nature. CA's do quite easily reproduce the basic feature of the overall behavior that occurs in real world.CA models have been successfully used to simulate different growth behavior of crystals, since cellular Automata and crystals have similar structure.

Index Terms: Crystal *Growth, Snowflake Crystal, Cellular Automata, and Types of crystal*

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1. INTRODUCTION

The spatial dimension plays a key role in many social phenomena. Spatial dynamics refers to the sequence of changes in space and time. The changes which takes place with respect to space is called spatial process, the latter is called temporal process. The spatial and the temporal process are one and the same and they cannot be separated. This spatiotemporal process is used in planning, urban development and issues related to geographical phenomenon. All geographical phenomena are bound to have a spatial and a temporal dimension. The aim of modeling is to abstract and represent the entity being studied. Modeling can be conceptual, symbolic or mathematical, depending on the purposes of the specific application. Modeling can be utilised for analysing, evaluating, forecasting and simulating complex systems to support decision-making. From the perspective of spatial science, modeling must take both the spatial and temporal dimensions.

Model can be represented as "a schematic representation of reality, developed with the goal of understanding and explaining it". Spatial interactions can also be expressed as an *influence* of a location on another, without being explicitly embodied in the form of a measurable exchange or flow. Spatial dynamics are easy to implement when compared to that of temporal dynamics since the change in time should be also be taken into account while modeling. Many techniques were currently used to model spatial and temporal growth especially in the field of crystal growth. 'Crystal' comes from a Greek word meaning clear ice. In the late sixteenth century, Crystal growth has been widely studied for many years. Andreas Libavius, made the theory, which said, "Mineral salts could be identified by studying the shapes of the crystal grains." In 1669, Nicholas Steno observed that corresponding angles in two crystals of the same material were always the same. The first synthetic gemstones were made in the mid-1800s, and methods for making high-quality crystals of various materials have been developed over the course of the past century. Since the mid-1970s such crystals have been crucial to the semiconductor industry. Systematic studies of the symmetries of crystals with flat facets began in the 1700s, and the relationship to internal structure was confirmed by X-ray crystallography in the 1920s.

Crystals form whenever a solid is formed from fluid. Crystals form from vapors, solutions or molten materials, and are built from repeating units. Crystals grow from the outside. Crystal formation is called crystallization. Crystallization means "become crystals". At a microscopic level, crystals consist of regular arrays of atoms laid out much like the cells in a cellular automaton. Crystals always start from a seed such as a grain of dust and then progressively adding more atoms to their surface. Some of the examples are: snowflakes formation from water vapor, rocks like felsite, and most non-living substances.

Snow crystals have a rich diversity of forms with striking hexagonal symmetry. The two-dimensional types include dendrite, stellar, sector and plate forms. Physical studies have shown that the particular form of a snow crystal is dependent upon the temperature and saturation in the growth environment. Snow crystals exhibit remarkable, intriguing six fold symmetry while displaying a wide diversity of forms. Kepler suggested in 1611 that the symmetry of snow crystals was related to the hexagonal packing of spheres [1], which is remarkable foresight given the modern understanding of the hexagonal molecular packing of ice crystals[2].

The formation of complex structures during solidification often results from a subtle interplay of nonequilibrium, nonlinear processes, for which seemingly small changes in molecular dynamics at the nano scale can produce profound morphological changes at all scales. One popular example of this phenomenon is the formation of snow crystals, which are ice crystals that grow from water vapor in an inert background gas. Although this is a relatively simple, monomolecular system, snow crystals display a remarkable variety of columnar and plate-like forms, and much of the phenomenology of their growth remains poorly understood, even at a qualitative level [3]. The crystal growth and the cellular Automata have the same features.

2. SNOWFLAKE CRYSTALS

A crystal is a material in which the molecules are all lined up in a specific way called the "crystal lattice". The water molecules in ice form a hexagonal (six-sided) lattice, and all snow crystals have six sides. The crystals form when water vapor condenses directly into ice around tiny bits of dust that have been carried up into the atmosphere. The beautiful patterns form as the crystal grows, dressing up the dirt to look real purrrdy!. Snow is not frozen rain. Sometimes raindrops freeze as they fall, but this is called "sleet". Sleet particles are just frozen water and don't have any of the patterns found in snow crystals.

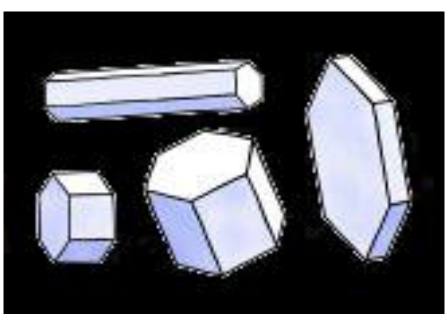

Fig- 1 Basic Shapes of Snowflakes

A snow crystal is a single crystal of ice, but a snowflake can be an individual crystal, or as many as 200 stuck together to form the big "puff-balls" that often fall when the temperature is just below freezing. Snowflakes can be big clusters of snow crystals, or just one individual and unique crystal. No two snow crystals are exactly alike (which is rather surprising given the amount of snow that falls), but their forms usually fall into several basic types and categories. Ice crystal is material in which molecules are arranged as a hexagonal lattice (crystal lattice). Snowflakes patterns arise as snow crystal grow their Growth depends on temperature and humidity

Snow can be further classified into six basic patterns called: Needles, columns, plates, columns capped with plates, dendrites, and stars. Each type is the result of different atmospheric and temperature conditions within the cloud. Snowflake is one of the well-known examples of crystal formation. Snowflakes are collections of snow crystals, loosely bound together into a puff-ball. These can grow to large sizes, up to about 10 cm across in some cases, when the snow is especially wet and sticky. Thus, snow crystals are individual, single ice crystals, often with six-fold symmetrical shapes.

These grow directly from condensing water vapor in the air, usually around a nucleus of dust or some other foreign material. Typical sizes range from microscopic to at most a few millimeters in diameter.

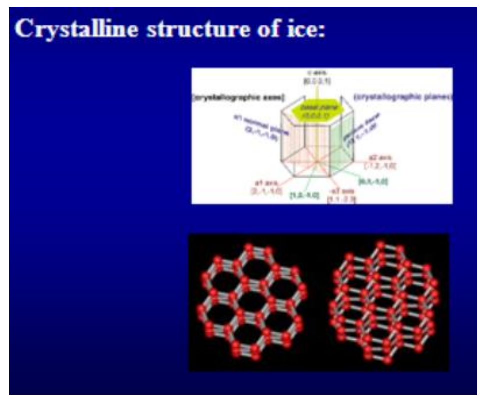

Fig- 2 Crystalline Structure of Ice

The structure of a given snowflake is determined by the temperature and humidity of the environment in which it grows, and the length of the time it spends there. Figure 3 shows some forms of snowflakes that are often seen in nature.

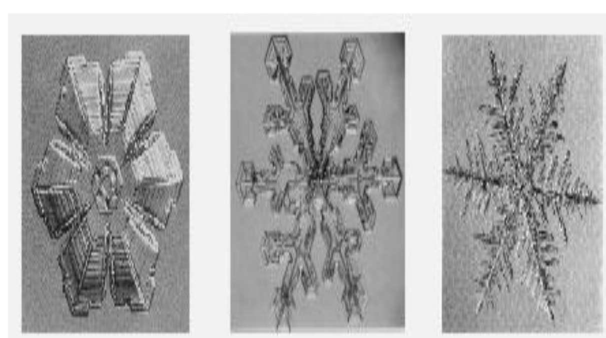

Fig -3 1) Simple sectored plate; 2) Dendritic sectored plate; 3) Fern-like stellar dendrite

2.1 Six-fold symmetry of snow crystals

When water freezes into ice, the water molecules stack together to form a regular crystalline lattice and the ice lattice has six-fold symmetry. It is this hexagonal crystal symmetry that ultimately determines the symmetry of snow crystals.

2.2 Complex symmetrical shapes of snow crystals

The snow crystals form complex shapes because of their simple six-fold symmetry and also because they are both complex and symmetric, and it is this combination that gives them their special beauty The growth usually begins with a dust particle, which absorbs some water molecules that form a nucleus for the ice crystal.

Typically snow crystals need some kind of surface on which to get started. Faceting then causes the newborn crystal to quickly grow into a tiny hexagonal prism. As the crystal grows larger, the corners often sprout tiny arms, since they stick out a bit further into the supersaturated air and thus grow a bit faster. The crystal growth rate strongly depends on the temperature. If there are variations in the temperature, the snow crystal encounters different growth conditions, growing into an intricate shape. Thus, we see such a rich diversity in the shapes of snow crystals in nature. When a snow crystal grows from air supersaturated with water vapor, there are two dominant mechanisms that govern the growth rate. The first is diffusion -- the way water molecules must diffuse through the air to reach the crystal surface. The second involves the surface physics of ice -- the efficiency with which water molecules attach themselves to the ice crystal lattice.

Faceting is the one which operate at the molecular scale to produce the crystal lattice, can control the shape of a snow crystal some ten million times larger. Facets appear on many growing crystals because some surfaces grow much more slowly than others. If we imagine

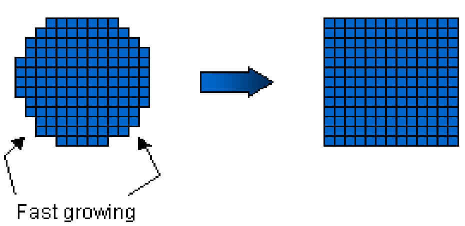

Fig- 4 Crystal faceting

beginning with a small round ice crystal, then mostly we would find that the surface was quite rough on a molecular scale, with lots of dangling chemical bonds. Water molecules from the air can readily attach to these rough surfaces, which thus grow relatively quickly. The facet planes are special, however, in that they tend to be smoother on a molecular scale, with fewer dangling bonds. Water molecules cannot so easily attach to these smooth surfaces, and hence the facet surfaces advance more slowly. After all the rough surfaces have grown out, what remains are the slow-moving facet surfaces.

3. CELLULAR AUTOMATA CONCEPT

A cellular automaton is an array of identically programmed automata, or "cells", which interact with one another. The arrays usually form either a 1-dimensional string of cells, a 2-D grid, or a 3-D solid. Most often the cells are arranged as a simple rectangular grid, but other arrangements, such as a honeycomb, are sometimes used.[4] The essential features of a cellular automaton

("CA" for short) are:

- **Its State** - a variable that takes a separate value for each cell. The state can be either a number or a property.
- **Its Neighborhood** - the set of cells that it interacts with. In a grid these are normally the cells physically closest to the cell in question.
- **Its Program** - the set of rules that defined how its state changes in response to its current state, and that of its neighbors.

Cellular automata are discrete dynamical systems whose behavior depends on local rules. Perhaps the most famous cellular automata is The Game of Life described by John Conway [5,6]. That automaton remains intriguing because its complex behavior is capable of universal computation. However, more serious applications are becoming common because cellular automata allow parallel processing [7]. Real valued cellular automata are also commonly used in applications such as image processing [8]. Such automata were used as a local model for snow crystal growth on a hexagonal lattice [9]. A wide range of growth structures were created, including stellar, dendrite, sector, and 2 plate forms which includes the basic 2-dimensional types seen in physical snowflakes. Of course, the growth exhibited, and was limited to, having 6-fold symmetry as determined by the underlying lattice.

In his cellular automaton (CA) model, each cell (or site) of a planar lattice changes from empty to occupied as that location turns to ice and remains occupied thereafter. A cell “freezes” when it has one frozen neighbor, or when the number of frozen neighbors equals some prescribed higher count. Cells of the original 1984 model had six nearest neighbors, reflecting the hexagonal molecular structure of ice and observed symmetry of actual snow crystals
Cellular Automata models are used to simulate the process of crystal growth and to generate various patterns that the crystals create in nature. Crystals form whenever a solid is formed from fluid. Crystals form from vapors, solutions or

molten materials, and are built from repeating units. Crystals grow from the outside. Crystal formation is called crystallization. Crystallization means "become crystals". At a microscopic level, crystals consist of regular arrays of atoms laid out much like the cells in a cellular automaton. Crystals always start from a seed such as a grain of dust and then progressively adding more atoms to their surface. Some of the examples are: snowflakes formation from water vapor, rocks like felsite, and most non-living substances. There has been a lot of research work done in the field of crystals, which make use of cellular automata models for simulation purposes.

Cellular automata can be applied to emulate snowflakes. the reason is that, it was not the case that every snowflake was identical. However, if every snowflake had a random structure, the information from each snowflake would be meaningless. Therefore, there is a syntax within snowflakes, several main types of structures, which are capable of containing individual ariations.Packard discovered that different weather conditions result in snowflakes taking on different general aspects. One set of conditions yields configurations that look like plates, another determines snowflakes shaped like collections of rods, and another yields dendritic stars. He wrote a cellular automaton simulation in which the “off” cells, those with a value of “0”, represented water vapour, and the “on” cells, those assigned a value of “1”, represented ice, and appeared on the screen in colour. The snowflake would grow outwards from its boundary. A typical set of rules initiated a scan of a cell’s neighbourhood, summed the values of the surrounding cells, and filled the new cells with either ice or water vapour, depending on whether the total was odd or even. The resulting artificial snowflakes lacked the complexity of real snowflakes, particularly those with structures based on patterns of needle-like shapes but they did have plates and dendrites growing from the corners of the plates, from which more dendrites grew; they were easily identifiable as snowflakes.

4. TYPES OF SNOWFLAKE CRYSTAL

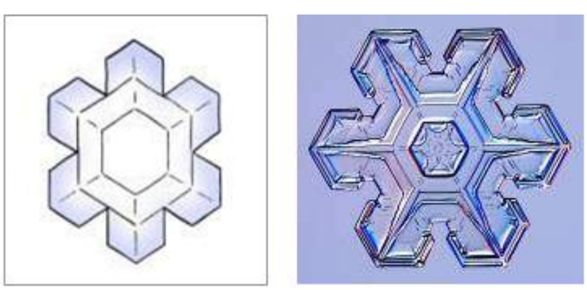

Fig- 5 Stellar Snowflake Crystal

Stellar snowflakes are thin crystals with six broad arms that form a star like shape[10].

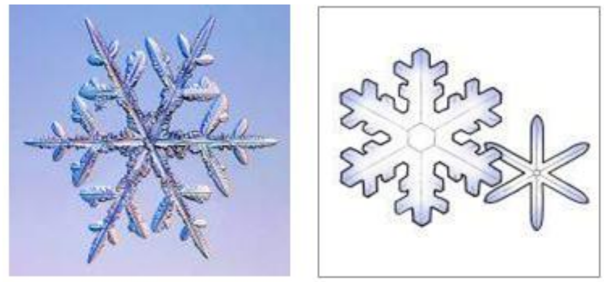

Fig- 6 Stellar Dendrites Snowflake Crystal

Dendritic means “tree like”. These types of snowflakes are fairly large 2-4 mm and an be seen with the naked eye.

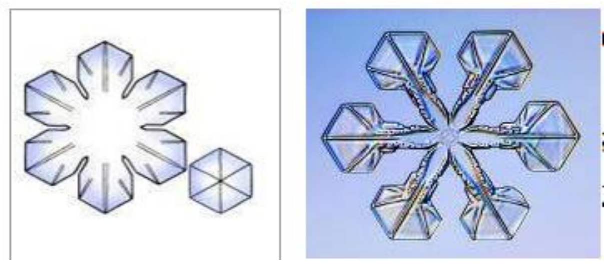

Fig- 7 Sectored plate Snowflake Crystal

Sectored snowflakes are hexagonal crystals divided into six equal pieces.

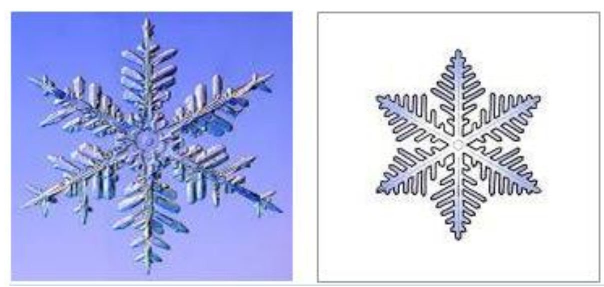

Fig- 8 Fernlike Dendrite Snowflake Crystal

These are the largest crystals up to 5mm, with lots of side fern like side branches

5. CELLULAR AUTOMATA APPLIED TO CRYSTAL GROWTH

CA’s do quite easily reproduce the basic feature of the overall behavior that occurs in real snowflakes. Snowflakes can be modeled with the help of cellular automata to produce simple faceted forms, needle-like forms, tree-like or dendritic forms, as well as rounded forms.

One of the ways to create real snowflake patterns is to use two-dimensional cellular automata displaying 3-state seven sum totalistic rules on a hexagonal grid. Each cell has three states representing growth as a result of different temperature conditions. The state of a cell is updated based on the sum of its six neighbors and its current state.

Crystal growth is an excellent example of a physical process that is microscopically very simple, but that displays a beautiful variety of macroscopic forms. Many local features are predicted from continuum theory, but global features may be analytically inaccessible. For this reason, computer simulation of idealized models for growth processes has become an indispensable tool in studying solidification. Packard presents a new class of models that represent solidification by sites on a lattice changing from zero to one according to a local deterministic rule. The strategy is to begin with very simple models that contain very few elements, and then to add physical elements gradually, with the goal of finding those aspects responsible for particular features of growth.

5.1 Packard's Cellular Automata

The simplest deterministic lattice model for solidification is a 2D CA with two states per site to denote presence or absence of solid, and a nearest neighbor transition rule. Packard considers rules, which have the property that a site value of one remains one (no melting or sublimation)[11]. The rules also depend on neighboring site values only through their sum:

$$a_i^{t+1} = f(\sigma_i^t) \quad \text{With} \quad \sigma_i^t = \sum_{\partial \in Nbrhd} a_{i+\partial}^t$$

The domain of f ranges from zero to number of neighbors; f takes on values of one to zero. These rules display four types of behavior for growth from small seeds:

i. No growth at all. This happens for the rule that maps all values of σ to zero.
ii. Growth into a plate structure with the shape of the plate reflecting the lattice structure
iii. Growth of dendrite structure, with side branches growing along lattice directions; this
iv. type of rule is obtained by adding growth inhibitions to the previous rule. Physically growth inhibition occurs because of the combined effects of surface tension and radiation of heat of solidification.
v. Growth of an amorphous, asymptotically circular form. This form is obtained by adding even more growth inhibition.

The two ingredients missing from the cellular automaton model are:

i)Flow of heat
This may be modeled with the addition of a continuous variable at each lattice site to represent temperature.

ii)Effect of solidification on the temperature field
When solid is added to a growing seed, latent heat of solidification must be radiated away. This is modeled by causing an increment in the temperature field.

An extremely simple prototype for planar growth was proposed by Packard [12]. In his cellular automaton (CA) model, each cell (or site) of a planar lattice changes from empty to occupied as that location turns to ice and remains occupied thereafter. A cell "freezes" when it has one frozen neighbor, or when the number of frozen neighbors equals some prescribed higher count. Cells of the original 1984 model had six nearest neighbors, reflecting the hexagonal molecular structure of ice and observed symmetry of actual snow crystals. Subsequent studies [13,14] include simulations on the two-dimensional integers Z2 with 4 and 8 nearest neighbours, the so-called von Neumann and Moore neighborhoods, respectively. As they grow, hexagonal Packard Snowflakes develop intricate patterns reminscient of real snowflakes .Indeed, Wolfram and others have argued (e.g., in [15,16], and [8]) that the similarity demonstrates the ability of simple local interactions to capture essential features of complex natural processes. Recent advances in our understanding of real snow crystal growth, however, make it clear that the Packard rules evolve in a very different manner than do the sectored plates they resemble at certain stages of development. More realistic lattice algorithms, based on physical principles, are currently being developed by Gravner and Griffeath [17, 18]; Our Packard Snowflakes evolve on the two dimensional integer lattice, so the crystal of frozen sites belongs to the state space

A = {finite subsets A ⊂ Z2}.

Elements of A will generally be denoted by u or v and represented coordinate wise by (x, y).
The state of the crystal at time t is denoted
At = {occupied sites at time t}.
To specify whether or not a site is occupied, we write
At (u) = 1 if u ∈ At ,= 0
otherwise. Our analysis will focus on crystals started from a singleton; i.e., we usually set A0 = {0}. A focus of our analysis will be the final state

$$A_\infty = \lim_{t\to\infty} A_t.$$

Simulations are as follows Temperature is set to a constant high value when new solid is added. Hybrid of discrete and continuum elements. Different parameters used

- diffusion rate
- latent heat added upon solidification
- local temperature threshold

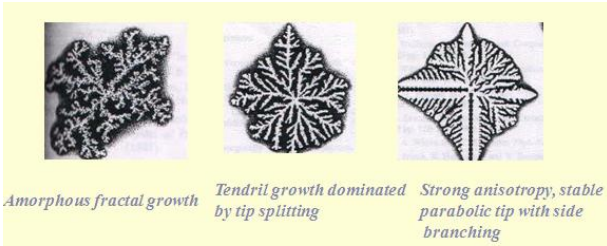

Fig- 10 simulated crystal

6. ADVANTAGES OF CELLULAR AUTOMATA IN CRYSTAL GROWTH

The structure of cellular automata and crystal are one and the same. They have the similar structure. Its very easy to simulate the crystal growth using cellular automata. crystals consist of regular arrays of atoms laid out much like the cells in a cellular automaton. Crystals always start from a seed such as a grain of dust and then progressively adding more atoms to their surface. The crystal growth and the cellular Automata have the same features.

CONCLUSIONS

Cellular automata (CA) modeling is one of the recent advances in spatial–temporal modeling techniques in the field of various growth dynamics.These models provide novel tools that support for better understanding of the modeling process. CA models have been successfully used to simulate different growth behavior of crystals. It is very fascinating to see the different intricate and complex forms that one sees during crystal growth. In this paper, I have described the different types of crystals, their formation and how to model using cellular automata This paper shows some of the snowflake patterns generated using packards CA model.

REFERENCES

[1]. J. Kepler ,The six sided snowflake (1611): translation,Oxford University Press, Oxford (1966)
[2]. Libbrecth k,Rasmussen P,The Snowflake:winters Beauty.stillwater: voyageur press 2003. http:/www.snowcrystals.
[3] Physically Derived Rules for Simulating Faceted Crystal Growth using Cellular Automata," K. G. Libbrecht, arXiv:0807.2616 (2008).
[4]. Wolfram,A new kind of science,2002
[5]. E. Berlekamp, J. Conway, and R. Guy. Winning ways for your mathematical plays.Academic Press, New York, 1982.
[6] Callahan P. Paul's page of Conway's life miscellany. http://www.radicaleye.com/lifepage/lifepage.html..
[7]. Callahan P. Paul's page of Conway's life miscellany.http://www.radicaleye.com/lifepage/lifepage.html.
[8] Wolfram S. A new kind of science. Champaign: Wolfram Media; 2002.
[9] Reiter CA. A local cellular model for snow crystal growth, Chaos, Solutions and Fractals, to appear
[10]www.snowcrystals.com
[11]. Packard Snowflakes on the von Neumann Neighborhood. Journal of Cellular Automata (2008). [pdf] C. D. Brummitt, H. Delventhal, M. Retzlaff
[12]Packard N. Lattice models for solidification and aggregation. Institute for Advanced Study Preprint. Reprinted (1986). Theory and Application of Cellular Automata, Wolfram S. (ed.).World Scientific, 305–310, 1984.
[13]. Wolfram S. A New Kind of Science. Champaign:Wolfram Media. 2002.
[14] Packard N. and Wolfram S. Two dimensional cellular automata. Journal of Statistical Physics 38 (1985), 901–946.
[15] Wolfram S. Computer software in science and mathematics. Scientific American 251 (1984),188–203.
[16]Levy S. Artificial Life: The Quest for a New Creation. New York City: Pantheon Books,1992.
[17] Gravner J. and Griffeath D. Modeling Snow Crystal Growth II. To appear, 2007.
[18] Gravner J. and Griffeath D. Modeling Snow Crystal Growth III. In preparation, 2007.