On the Geometry and Mathematical Modelling of Snowflakes and Viruses

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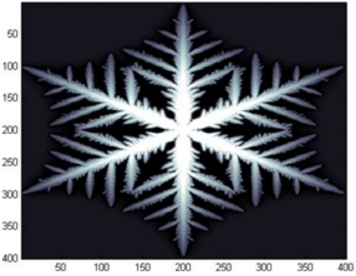
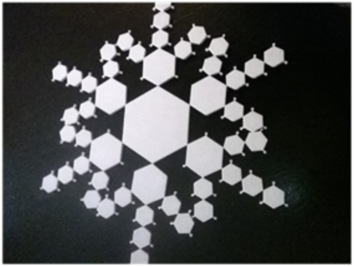
SUMMARY

So far we have studied:

(I) Geometric properties of snowflakes and icosahedral viruses,
(II) Mathematical modeling for visualizing snowflakes,
(III) 3D printed snowflake puzzles.





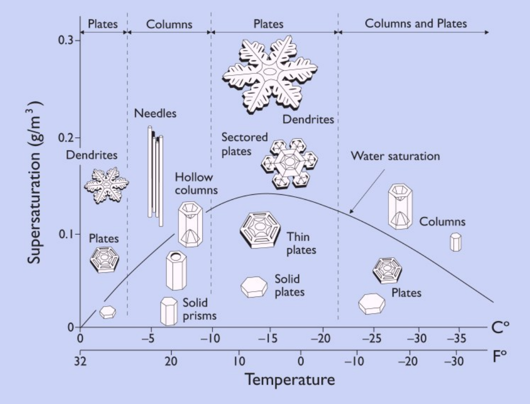
We have begun the study of further questions of model analysis and improvement.

Geometry and Morphology of Snowflakes

Snowflakes - a rich combination of *symmetry* and *complexity*:

- Six-fold symmetry ⇒ hexagonal structure of ice-crystal lattice.
- Complexity ⇒ random motion in the atmosphere.

Different types grow in different morphological environments:



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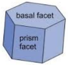
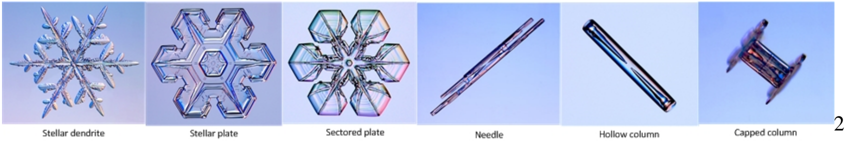
[1] [2] Libbrecht 2005

SNOWFLAKE CLASSIFICATION

- Focus on regular, symmetrical types.
- Most basic shape is a very tiny hexagonal prism.



- More sophisticated crystals grow from prism:
  - Plates and dendrites,
  - Columns and needles,
  - Anomalies and variants.



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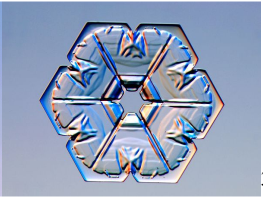
[2] [2] Libbrecht 2005

PLATES AND DENDRITES

- Dendrites: tree-like crystals
  - Main branches grow simultaneously from an initial hexagonal prism and therefore are symmetrical.
  - Seemingly random growth of side branches depends on temperature and humidity.
- Plates: plate-like crystals.
  - Simplest plate is a plain hexogon divided into six equal pieces with thin ridges.
  - More elaborate examples are stellar plates and sectored plates.


[3]

[3] [2] Libbrecht 2005

Objectives of Computer Modeling

Challenges of physics/chemistry modeling: many aspects such as diffusion-limited growth are only understood on a qualitative level. Computer modeling is to

- Capture essential features of snow crystal growth with relatively simple mathematical models,
- Use computer programs to simulate the models to produce snow crystal images,
- Correlate mathematical models/parameters with physical conditions by comparing computer-generated images with actual snow crystals.

BRIEF OVERVIEW OF COMPUTER MODELING

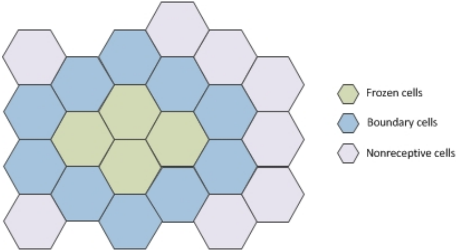
- Wittern and Sandar (1981): diffusion-limited aggregation (DLA) model. A diffusing particle takes random walks on a 2D rectangular integer lattice and freezes if one of its nearest neighbors has been frozen.
- Packard (1984): DLA variant model on hexagonal lattice. Every cell is characterized by a continuous variable - mass, which is updated according to a discrete heat equation rather than random walks to model diffusion.
- Reiter (2005): simplified Packard's model with very few parameters.
- Gravner and Griffeath (2008): refined Reiter's model to incorporate additional physically motivated features.

Reiter's Model

Basic Setup

Tessellate the plane into hexagonal cells. The state of cell x is characterized by *state variable* $s_t(x)$ - the amount of water in the cell at time t. Cells are divided into three types.

- If $s_t(x) \geq 1$, cell x is *frozen*.
- A *boundary* cell is not frozen itself but at least one of the nearest neighbors is frozen.
- The union of frozen and boundary cells are called *receptive* cells.
- A cell that is neither frozen nor boundary is called *nonreceptive*.



Reiter's Model

Initial Conditions

- The growth model starts from a single ice crystal at the origin cell, which represents a thin hexagonal prism.

$$s_0(x) := \begin{cases} 1 & \text{for} \quad x = 0 \\ \beta & \text{for} \quad x \neq 0 \end{cases},$$

  where $\beta =$ constant background vapor density.
- The states of the cells evolve as a function of the states of their nearest neighbors according to *local update rules*.
- Local update rules $=$ the underlying mathematical models.

REITER'S MODEL

LOCAL UPDATE RULES (I): CONSTANT ADDITION

Notation: $^\circ$ and $'$ to denote variables before/after a step is completed.

- At time t, define two intermediate variables $u(x), v(x)$ for cell x.
  - $u(x) := 0, v(x) := s_t(x)$, if cell x is receptive;
  - $u(x) := s_t(x), v(x) := 0$, otherwise.
- For any receptive cell x, let

$$v'(x) := v^\circ(x) + \gamma,$$

  where γ is a positive constant representing water added to the receptive cell from an outside source. The water in a receptive cell is assumed to permanently stay in that cell.

Reiter's Model

Local Update Rules (II): Diffusion

- For any cell x, let

$$u'(x) := \frac{1}{2}u^\circ(x) + \frac{1}{12}\left(u^\circ(y_1) + \ldots + u^\circ(y_6)\right).$$

- More generally,

$$u'(x) := u^\circ(x) + \frac{\alpha}{12}\left(-6u^\circ(x) + \sum_{y\in\mathcal{N}_x, y\neq x} u^\circ(y)\right).$$

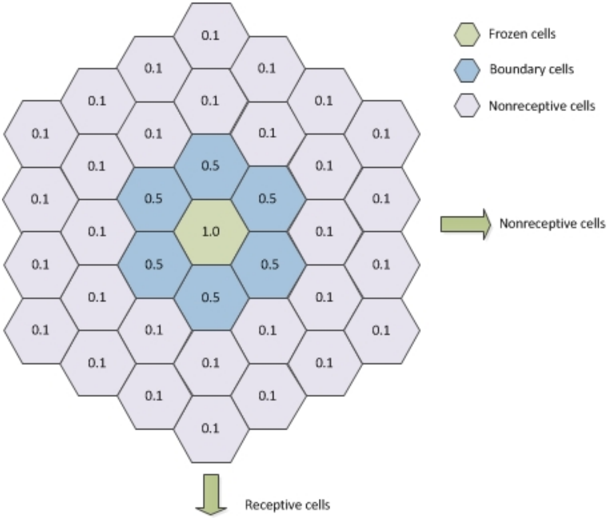
The underlying physical principle is the diffusion equation $\frac{\partial u}{\partial t} = a\nabla^2 u$, where a is a constant and $\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$ is the Laplacian, which can be approximated on the hexagonal lattice as $\nabla^2 u = \frac{2}{3}\left(-6u^\circ(x) + \sum_{y\in\mathcal{N}_x, y\neq x} u^\circ(y)\right)$ Here, $\alpha = 8a$.

Combining the two intermediate variables, the state variable becomes $s_{t+1}(x) = v'(x) + u'(x)$ as time reaches $t+1$.

REITER'S MODEL

LOCAL UPDATE: AN EXAMPLE

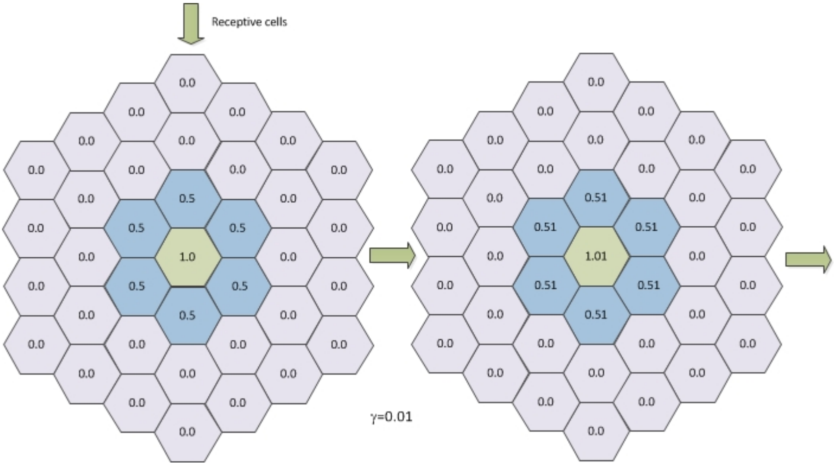
Divide into nonreceptive cells and receptive cells:



REITER'S MODEL

LOCAL UPDATE: AN EXAMPLE

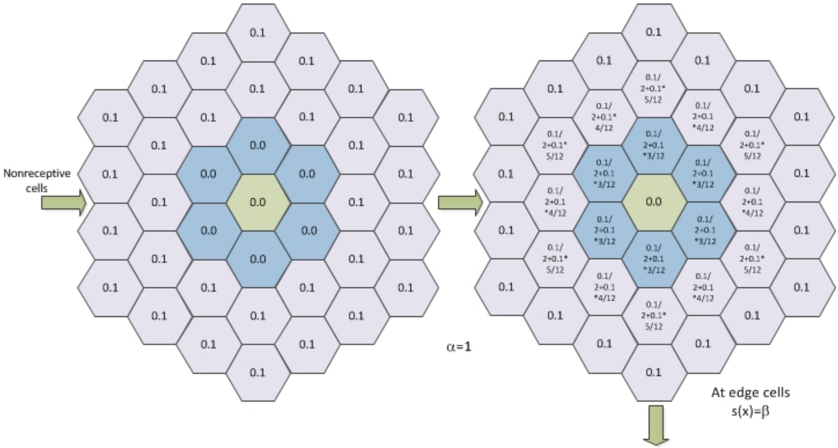
Constant addition for receptive cells:



Reiter's Model

Local Update: an Example

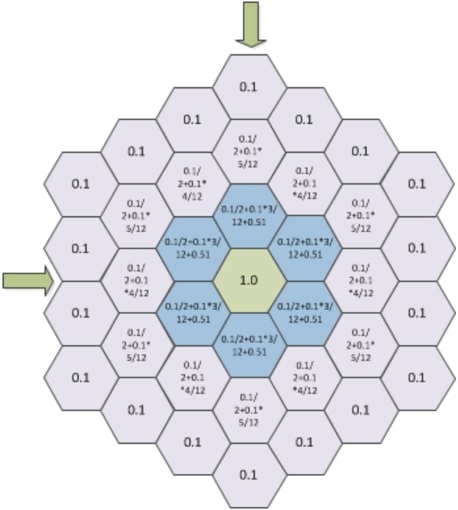
Diffusion for all cells:



REITER'S MODEL

LOCAL UPDATE: AN EXAMPLE

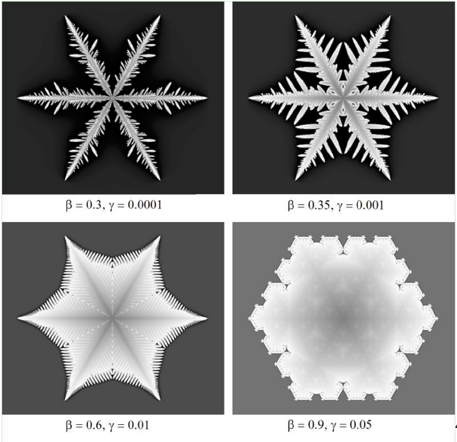
Combine addition and diffusion:



REITER'S MODEL

GENERATED IMAGES

By varying parameters α, β, γ, the Reiter's model generates several geometric forms of snow crystals observed in nature.



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[4] [3] Reiter 2005

Gravner and Griffeath's Model

Basic Setup

Gravner and Griffeath's model is a refinement of Reiter's model that incorporates several physically motivated features.

- State variables: whether cell x is frozen, quasi-liquid (boundary) mass, ice (crystal) mass, and vapor (diffusive) mass.
- Same three types of cells. A frozen cell consists of only ice mass. A boundary cell consists of all three types of mass. A nonreceptive cell consists of only vapor mass.
- Initial conditions very similar to Reiter's model with single frozen cell and constant background vapor density.

Gravner and Griffeath's Model

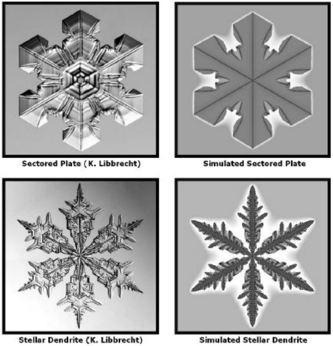
Local Update Rules

- Vapor mass *diffusion*: similar to Reiter's model.
- *Freezing*: in a boundary cell, a proportion of vapor mass converts to ice mass directly and the remaining becomes quasi-liquid mass.
- *Attachment*: a boundary cell may become frozen depending on the states of neighboring cells.
- *Melting*: in a boundary cell, a proportion of quasi-liquid mass and a proportion of ice mass converts to vapor mass.
- *Noise*: in any boundary or nonreceptive cell, add an independent random noise to vapor mass to reflect environment perturbation.

GRAVNER AND GRIFFEATH'S MODEL

GENERATED IMAGES

- Much more sophisticated than the Reiter's model, involving many more control parameters.
- Comparison of natural and simulated crystals generated by the Gravner and Griffeat's model.



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[5] [4] Gravner and Griffeath 2008

Analysis of Computer Generated Images

While computer models generate snowflakes images resembling real ones, there has not been much analysis of the models in the literature. Some questions we may ask are:

- Why main branches grow the fastest? What are the growth rate of main branches? What are the ridges that appear on main branches?
- Why the growth between main branches is the slowest? Why are there permanent holes where cells never become ice?
- What are the growth directions and distributions of side branches? Why do some snow crystals grow leafy side branches while others have hardly any side branches?
- What is the distribution of "time to become ice" as a function of location? What is the asymptotic density?

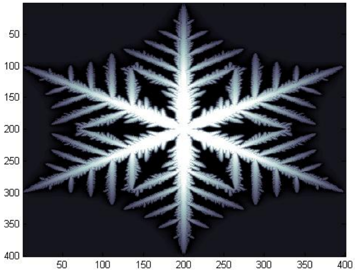
Improvement of Computer Models

- *Observation*: while dendrite images resemble real snow crystals pretty well, plate images are quite different: a plate image is in effect generated as a very leafy dendrite.
- *Conjecture*: Reiter's model takes into account diffusion control but not local geometry.
  - Two basic mechanisms of snow crystal growth: diffusion control (long-range processes) and interface control (local processes)
  - Interface control is based on geometric growth determined by local conditions only such as curvature.
  - Without proper modeling of interface control, computer models are unable to simulate certain features.
- We propose to improve the models by taking into account local conditions, e.g., curvature effect and surface free energy minimization.

Our Implementation of Reiter's model

Comparison of Computer Generated Images

As a first step, we have implemented the Reiter's model in Matlab and have been able to generate images that match what were provided in the literature:



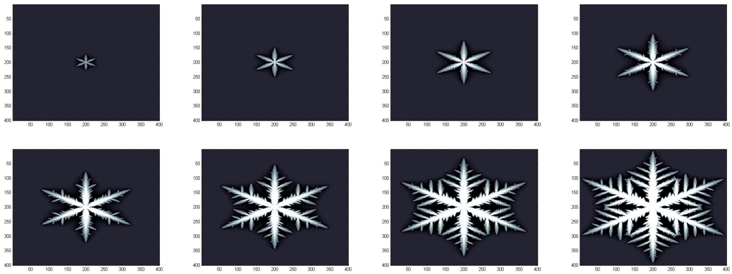

[6]

[6] [3] Reiter 2005

OUR IMPLEMENTATION OF REITER'S MODEL

SIMULATED SNOW CRYSTAL GROWTH PROCESS

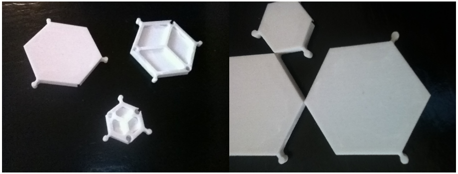
Below are the images of a snow crystal at different simulation times:



We will use the Matlab code to analyze and improve computer modeling.

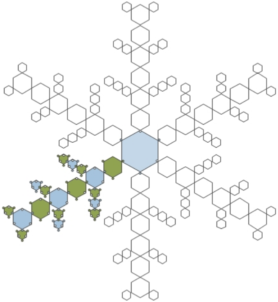
Modular Basic Building Blocks

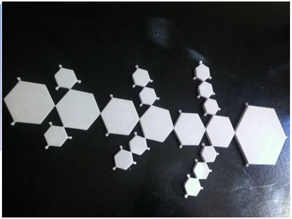
- Basic building blocks: hexagons of different sizes (big, medium, small).
- Special design at the vertices that use the alignment hole pockets to allow the hexagons to interlock with each other.
- A variety of puzzles can be formed with basic building blocks.



Puzzle Design Examples

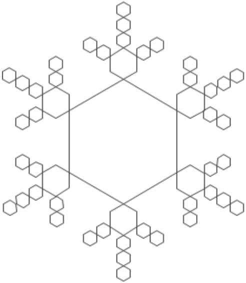
Stellar Dendrite

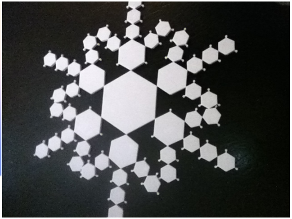




Puzzle Design Examples

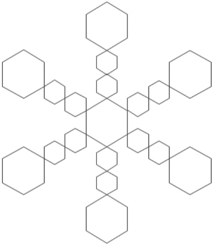
Sectored Dendrite

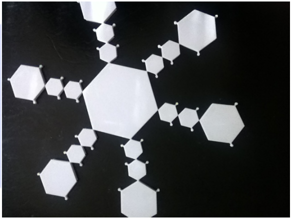




Puzzle Design Examples

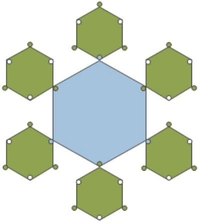
Sectored Plate

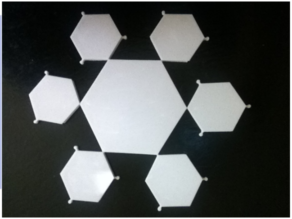




Puzzle Design Examples

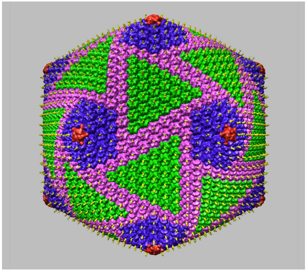
Stellar Plate





ICOSAHEDRAL VIRAL

- An icosahedral viral capsid is constructed from N_{cap} capsomers
  - 20 trisymmetrons (triangular symmetry),
  - 12 pentasymmetrons (pentagonal symmetry).
- An image of color-coded CIV capsid:

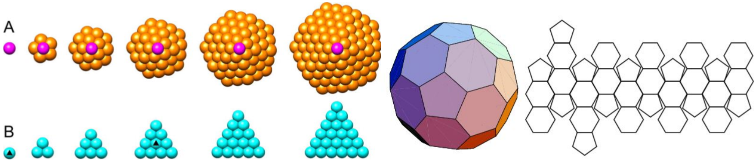


- $N_{cap} = 12 + 10(T-1) = 20N_{TS} + 12N_{PS}$.

GEOMETRIC CONSTRAINTS

We define

- e_{PS} := edge length of pentasymmetrons.
- e_{TS} := edge length of trisymmetrons.
- N_{PS} := size of pentasymmetrons.
- N_{TS} := size of trisymmetrons.
- T := triangulation number, h, k integers.

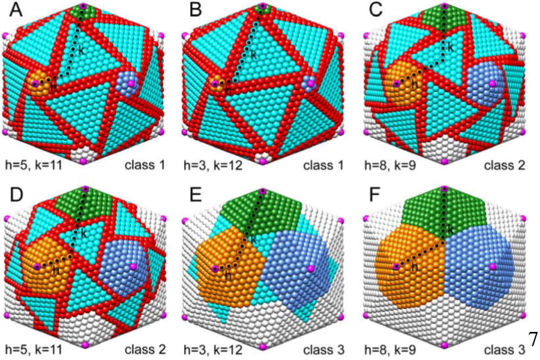


- $N_{PS} = 1 + 5e_{PS}(e_{PS} - 1)/2.$
- $N_{TS} = e_{TS}(e_{TS} + 1)/2.$
- $T = h^2 + k^2 + hk.$
- $e_{TS}(e_{TS} + 1)/2 = (T - 1)/2 - 3e_{PS}(e_{PS} - 1)/2.$

Three Classes of Construction Rules

All possible positive integral solutions categorized into three classes:

	Class 1 (h odd)	Class 2 (k odd)	Class 3 ($h+k$ odd)
e_{PS}	$(h+1)/2$	$(k+1)/2$	$(h+k+1)/2$
N_{PS}	$1+5(h^2-1)/8$	$1+5(k^2-1)/8$	$1+5((h+k)^2-1)/8$
e_{TS}	$(2k+h-1)/2$	$(2h+k-1)/2$	$(k-h-1)/2$
N_{TS}	$((2k+h)^2-1)/8$	$((2h+k)^2-1)/8$	$((k-h)^2-1)/8$



[7]

[7] [6] Sinkovits and Baker 2010

Lattice Properties of Real Viruses

Lattice properties for icosahedral capsids of all large dsDNA viruses with known structures:

Virus	T	h	k	N_{DS} [8]	N_{TS}	N_{PS}
SIV	156	4	10	9	55	16
SIV	129	5	8	0	55	16
SIV	147	7	7	0	55	31
TIV	147	7	7	0	55	31
CIV	147	7	7	0	55	31
FV3	169	7	8	0	66	31
PBCV−1	169	7	8	0	66	31
PpV01	219	7	10	0	91	31

- Three rows labeled as SIV represent different interpretations of SIV images.
- Because of limited quality of the SIV images, some earlier interpretation (the first or second SIV row) might not be accurate $\Rightarrow$ Likely $N_{DS} = 0$ in a modern reconstruction of SIV.

[8] N_{DS} = size of disymmetrons of linear symmetry

ONE OBSERVATION AND FURTHER QUESTION

- While N_{TS} varies for different viruses, $N_{PS} = 31$ in all cases.
- While other solutions are possible mathematically, nature seems to like this particular solution.

Are there additional geometric rules to be discovered regarding icosahedral virus construction?

- Admittedly, the sample size is quite small: $T = 147, 169, 219$.

One Observation and Further Question

Preliminary Thoughts

- For $T = 147$, two possible solutions: $h = 2, k = 11; h = 7, k = 7$. Nature prefers $h = 7, k = 7$, which leads to $N_{PS} = 31$.
- For $T = 169$, two possible solutions: $h = 0, k = 13; h = 7, k = 8$. Nature prefers $h = 7, k = 8$.
  - For $h = 7, k = 8$, two possible solutions: $N_{TS} = 66, N_{PS} = 31; N_{TS} = 0, N_{PS} = 141$. Nature prefers $N_{TS} = 66, N_{PS} = 31$.
- For $T = 219$, only one solution: $h = 7, k = 10$, which has two possible solutions: $N_{TS} = 91, N_{PS} = 31; N_{TS} = 1, N_{PS} = 181$. Nature prefers $N_{TS} = 91, N_{PS} = 31$.

Conjectures

- Nature prefers more “balanced” h, k values.
- Nature prefers more “balanced” N_{TS}, N_{PS} values.

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Thank you for listening.
Questions?