# Collaborators

**Joint Work With:**
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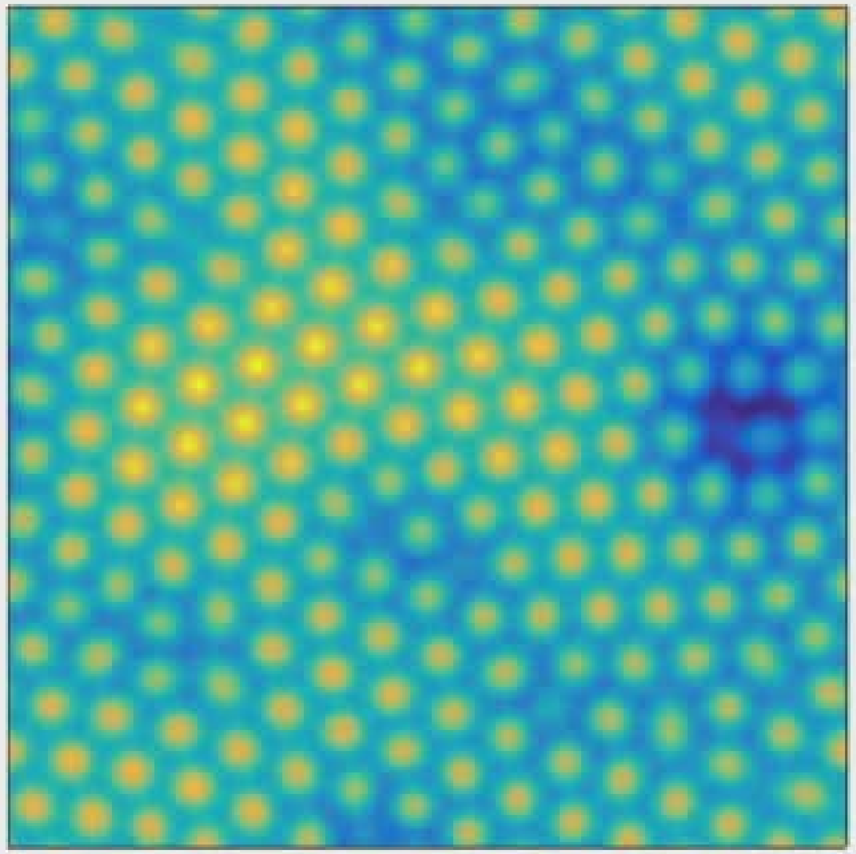
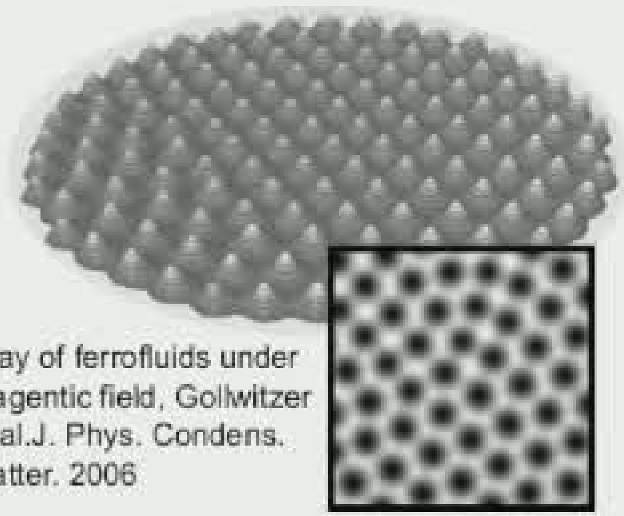
Daniel Pearson (Colorado State University)

*Measures of Order in Nearly Hexagonal Lattices.* Physica D: Nonlinear Phenomena, 380-381 (2018) 17-30.



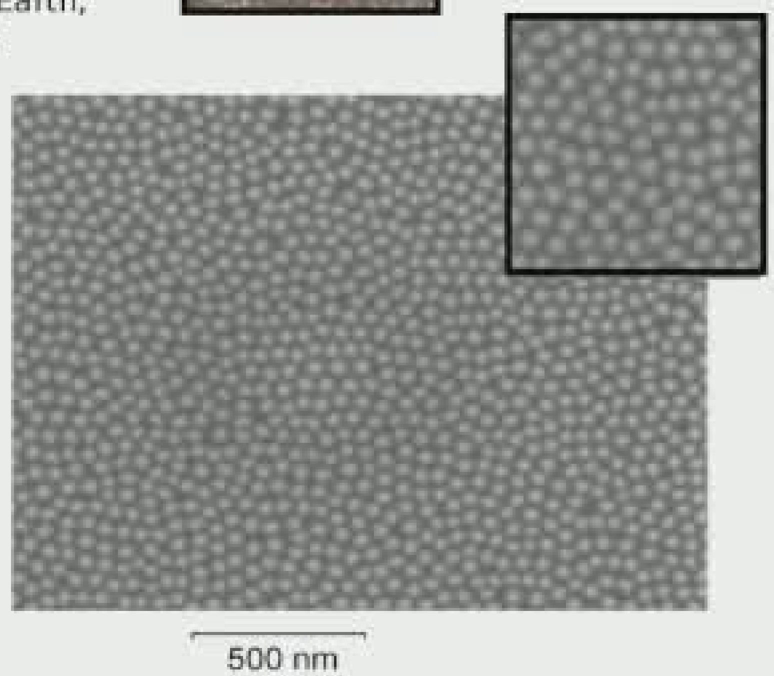
# Motivation

Mineral pattern, Google Earth, Somalia

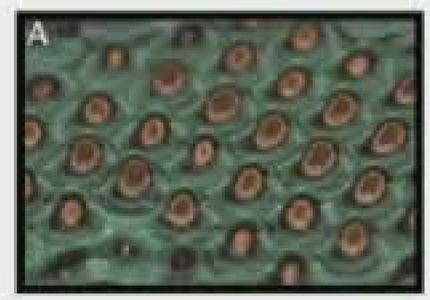


X-ray of ferrofluids under magentic field, Gollwitzer et al.J. Phys. Condens. Matter. 2006

Vegetation pattern in drylanc Google Earth, Ethiopia




Nanodots on ion bombarded GaSb surface. Facsko et al., Science, 1999.

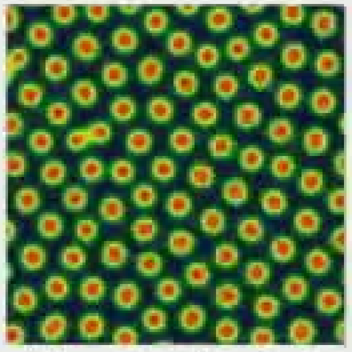


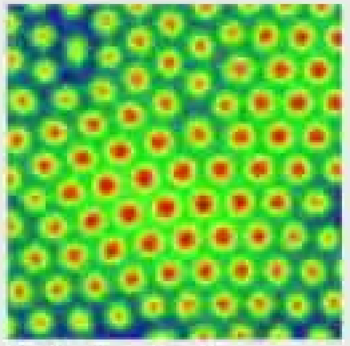

Faraday waves, silicone oil in water. Bush, PNAS, 2010.

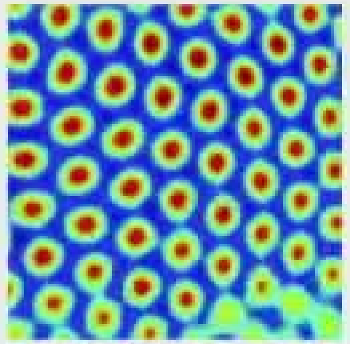
spotted trunkfish, diverosa.com

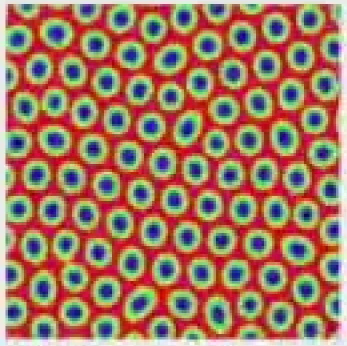
Visually similar patterns result from a variety of mathematical models that describe a number of different physical mechanisms.

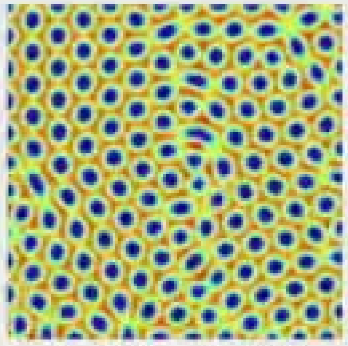
# Motivation

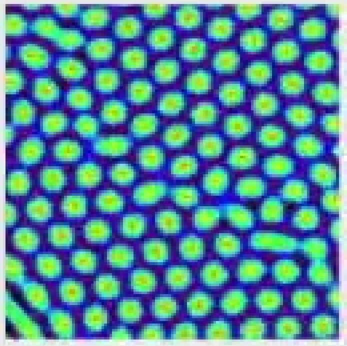

github.com/allove-lab/Allove-GrayScott


Bradley-Shipman Equations


Bénard-Marangoni Convection, Wu et al., CPL, 2017


Institut für Theoretische Physik, 2D Swift-Hohenberg


Brusselator Model, http://basilisk.fr

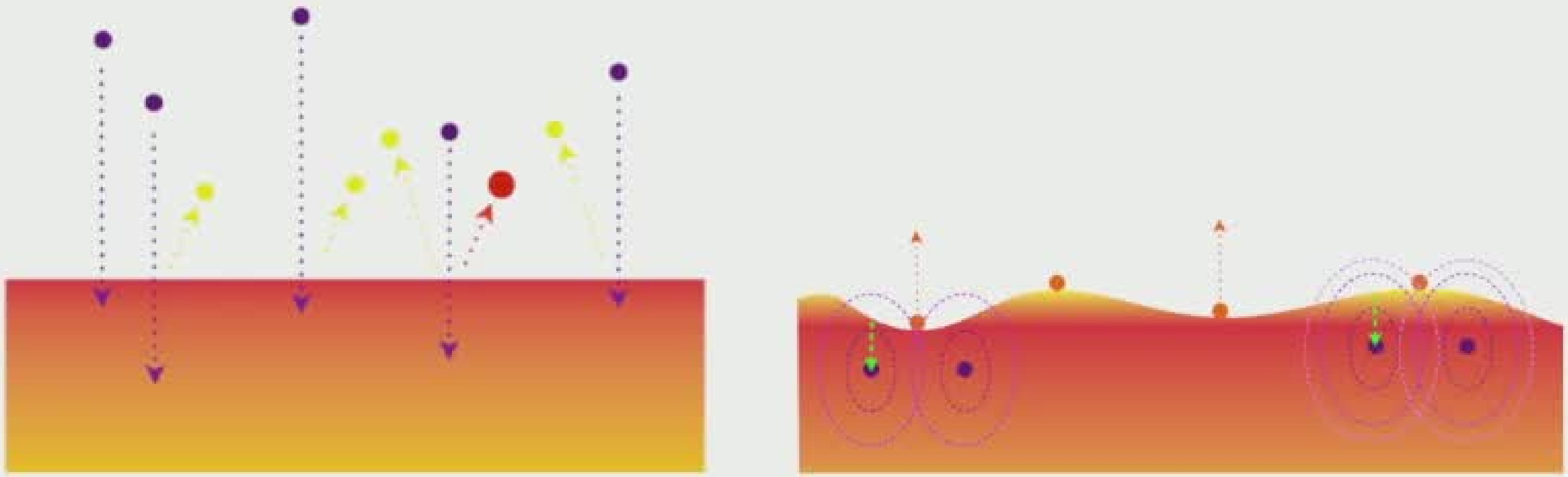

Young and Riecke, PRL 2003

Visually similar patterns result from a variety of mathematical models that describe a number of different physical mechanisms.

- ▷ How can one characterize, quantify and compare spatio-temporally complex patterns?
- ▷ How can defects in pattern-forming systems be detected and tracked?
- ▷ How can changes in geometric and topological structure tell us something about the mechanisms driving the dynamics in the system or the partial differential equation (PDE) model?
- ▷ How can models and data be qualitatively compared?

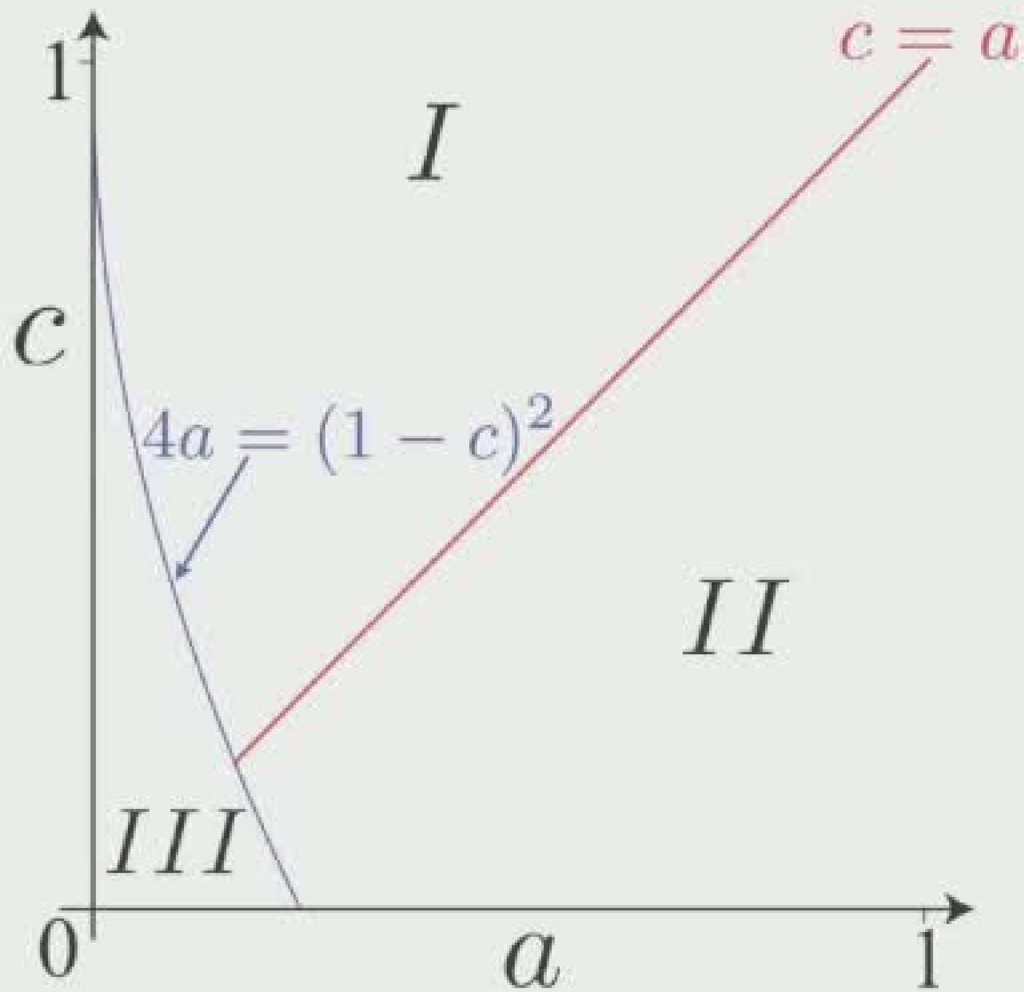
# Ion Bombardment of a Binary Compound

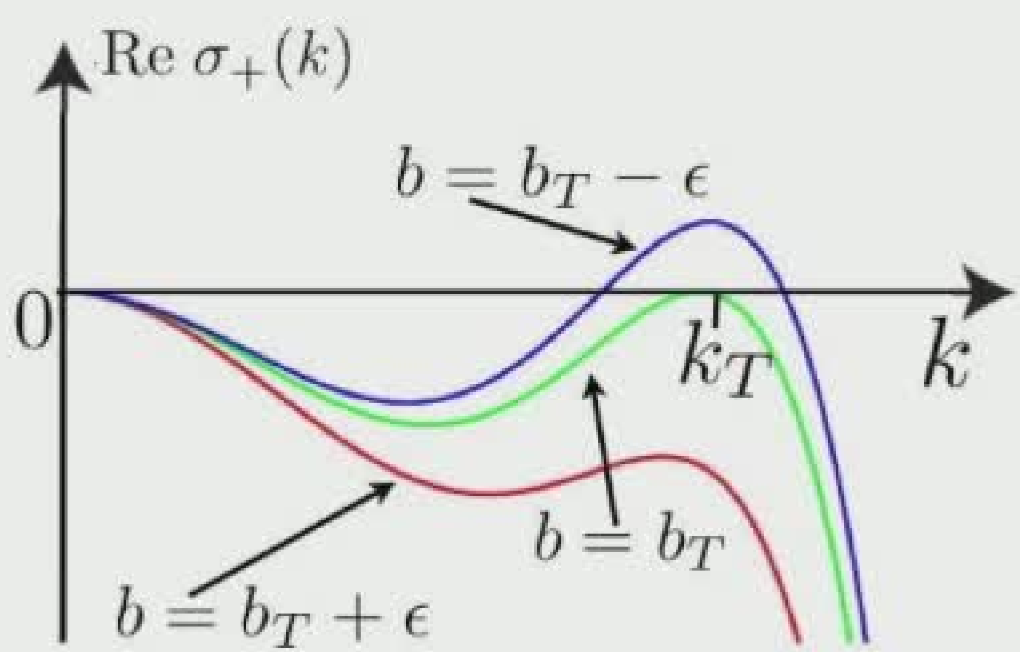
- A nominally flat binary solid composed of two species, A and B is subjected to normal incidence ion bombardment
- B is preferentially sputtered



- Coupling between topography and surface composition leads to the formation of near-hexagonal arrays of nanodots
- Curvature dependent sputter yield causes peaks to grow and troughs to deepen

# Bradley-Shipman Equations - Linear Stability Analysis




- The linearized system has solutions of the form

$$\begin{pmatrix} u \\ \phi \end{pmatrix} = \begin{pmatrix} u_* \\ \phi_* \end{pmatrix} e^{i\mathbf{k}\mathbf{x}+\sigma(\mathbf{k})\mathbf{t}}$$

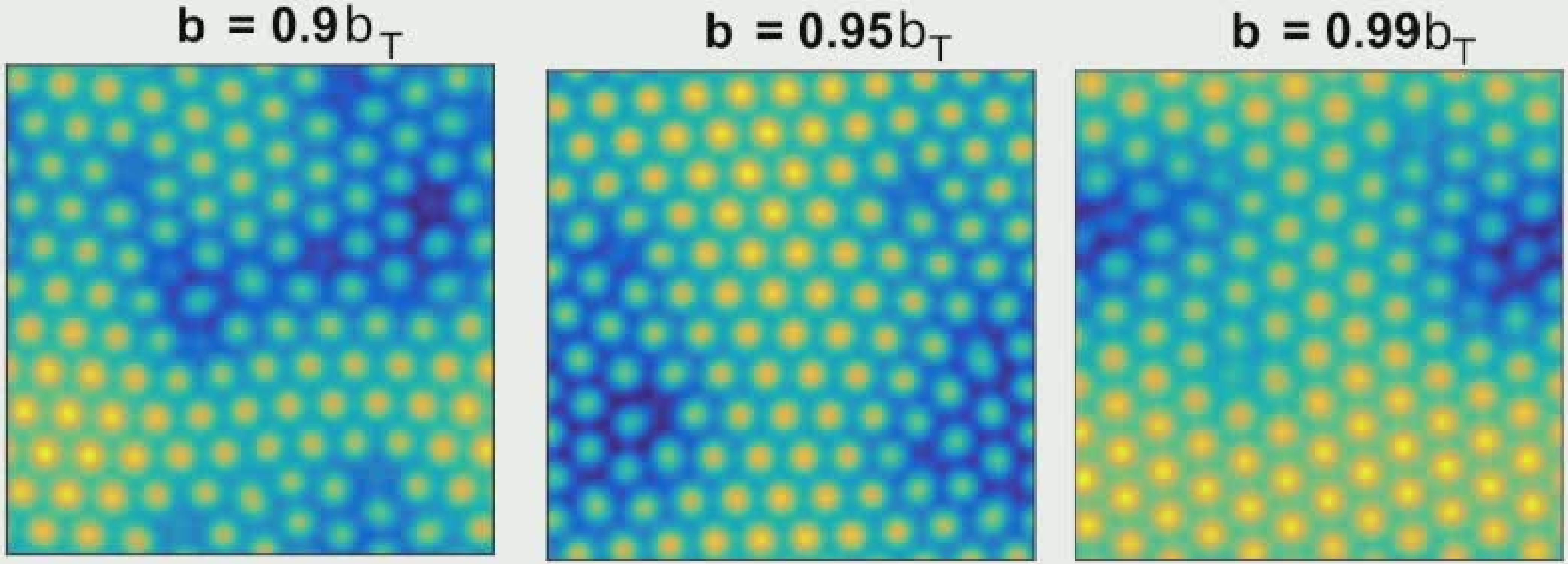
- In parameter region *I* the spatially uniform solution is stable for $b > b_T$

$$b_T = \frac{(a+c)^2}{4c}$$

- In *I*, for $b$ slightly less than $b_T$, $Re(\sigma_+(k)) > 0$ in a narrow band of wave numbers centered on the critical wave number $k_T$

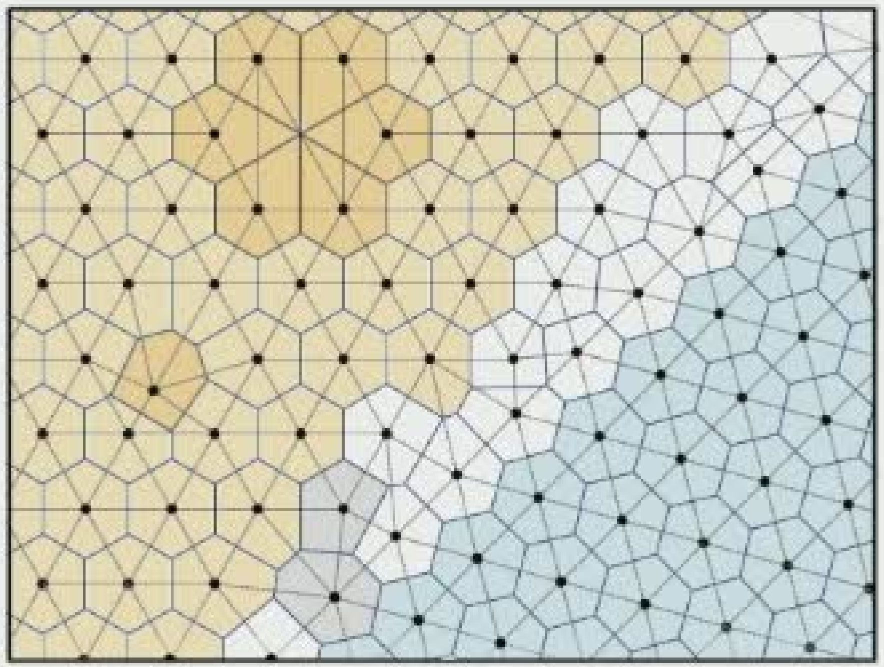
$$k_T^2 = \frac{(c-a)}{2c}$$

# Varying Linear Parameter $b$




- If $b - b_T$ is small, a well-ordered hexagonal array of nanodots form
- As $b < b_T$ is decreased, the rate at which the amplitude of the Fourier mode attenuates and the width of the annulus of linearly unstable wave numbers grows
- It is reasonable to expect hexagonal order will diminish as $b$ is decreased and the band of active modes broadens

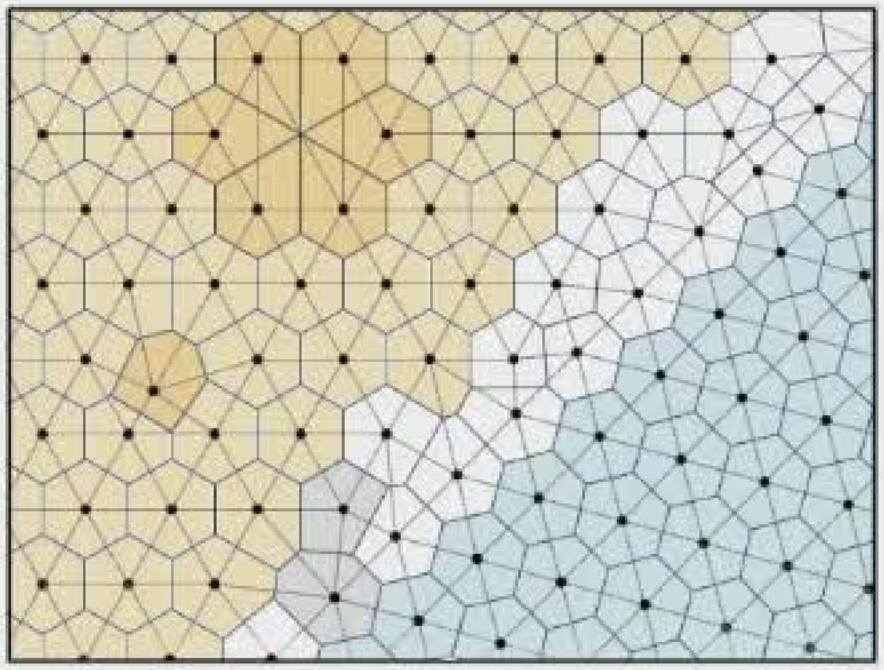
# Defects



Lattice Defects:

- Grain boundaries
- Penta-hepta defects
- Perturbed or missing peaks

# Defects



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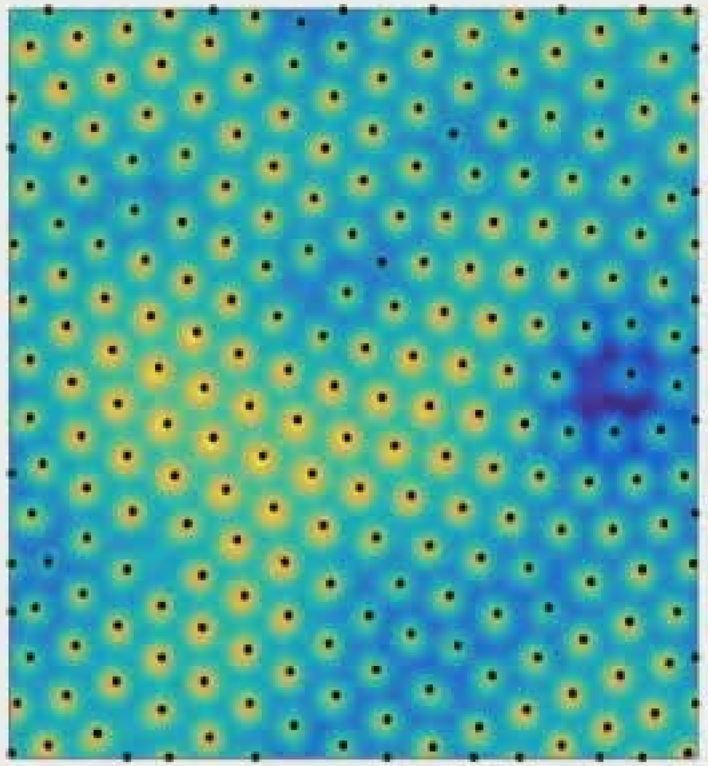
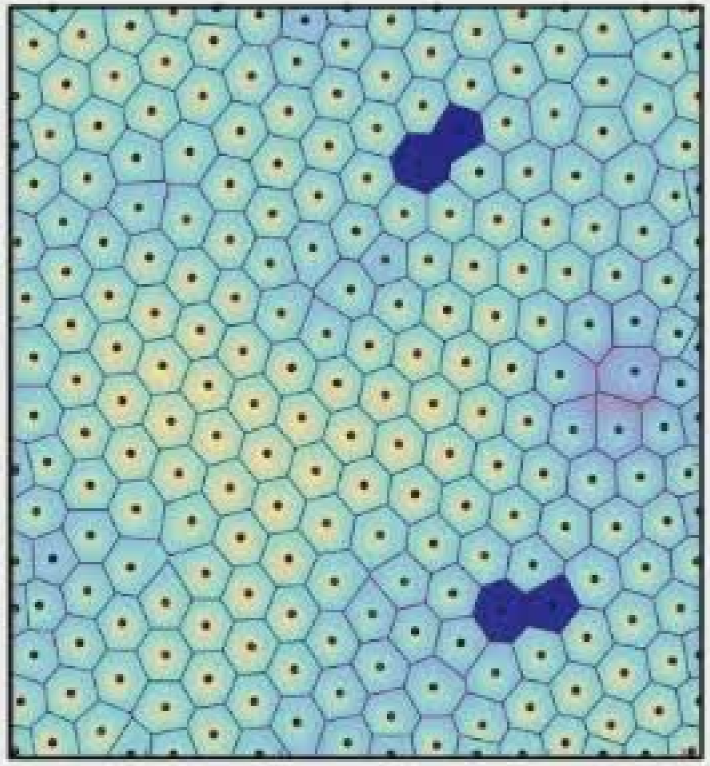
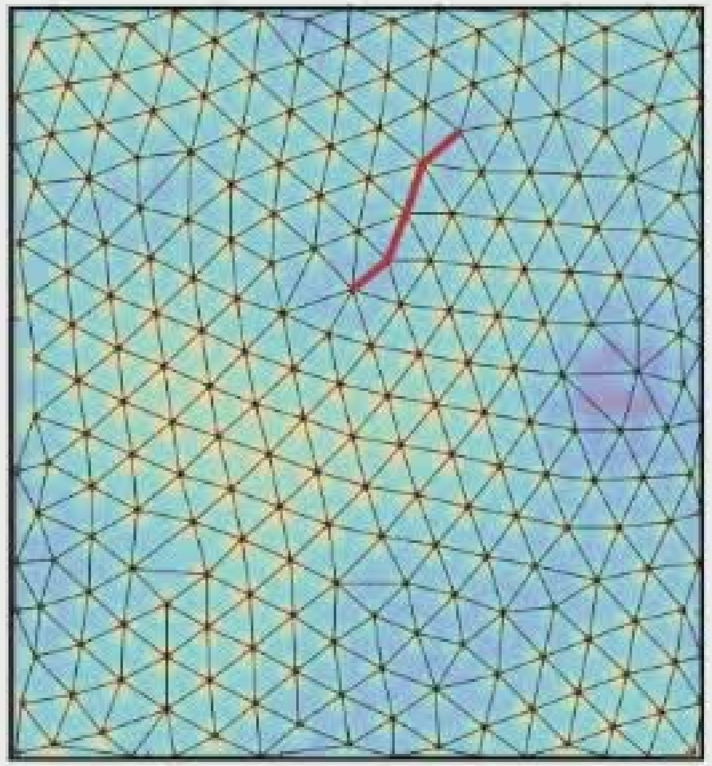
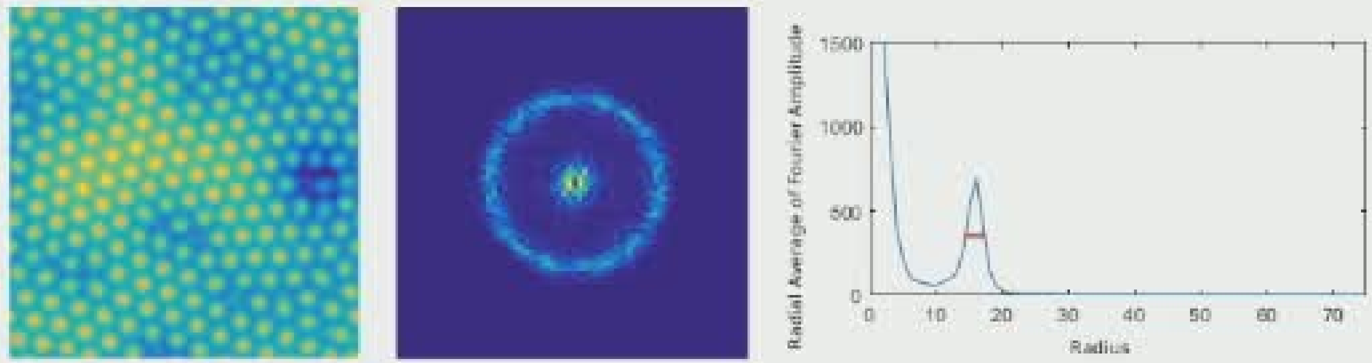






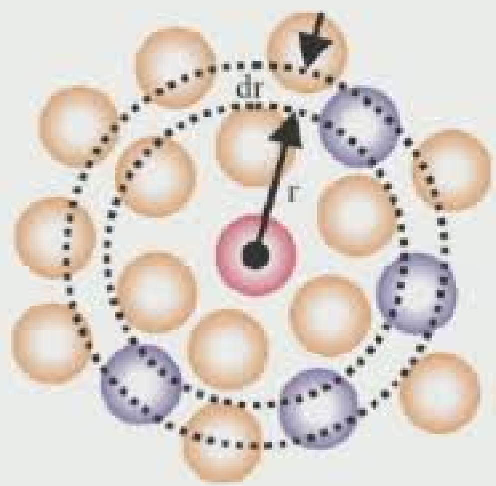
# Some Measurements of Order

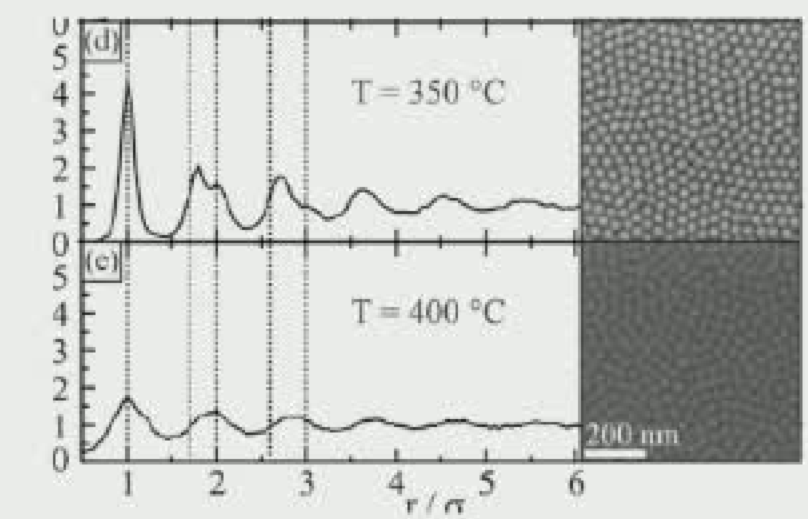
- **Spectral:** Full-width-at-half-max (FWHM) of the first-order Fourier peak




may not be able to distinguish types of defects

- **Geometric:** Correlation Length : the region of exponential decay in the autocorrelation function

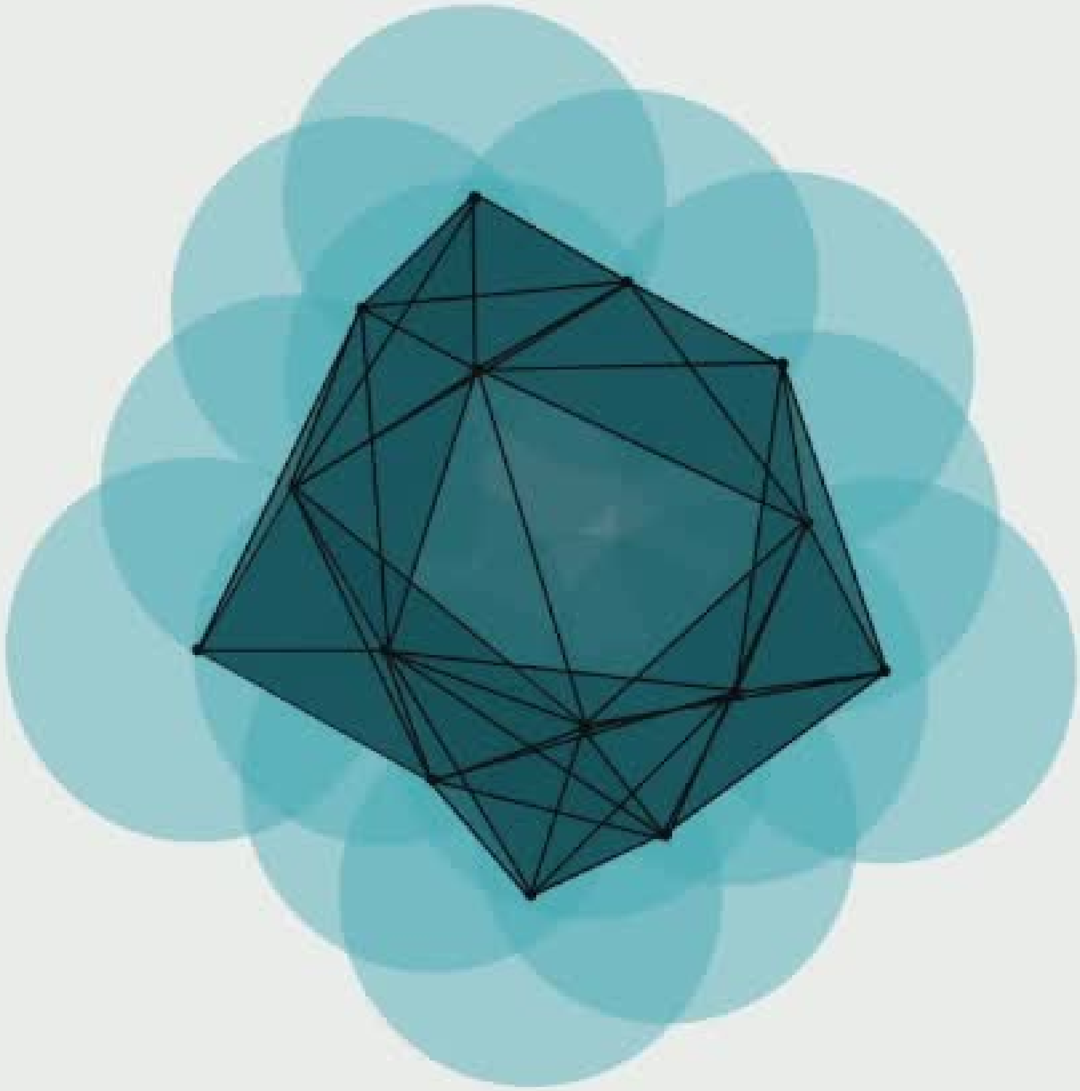


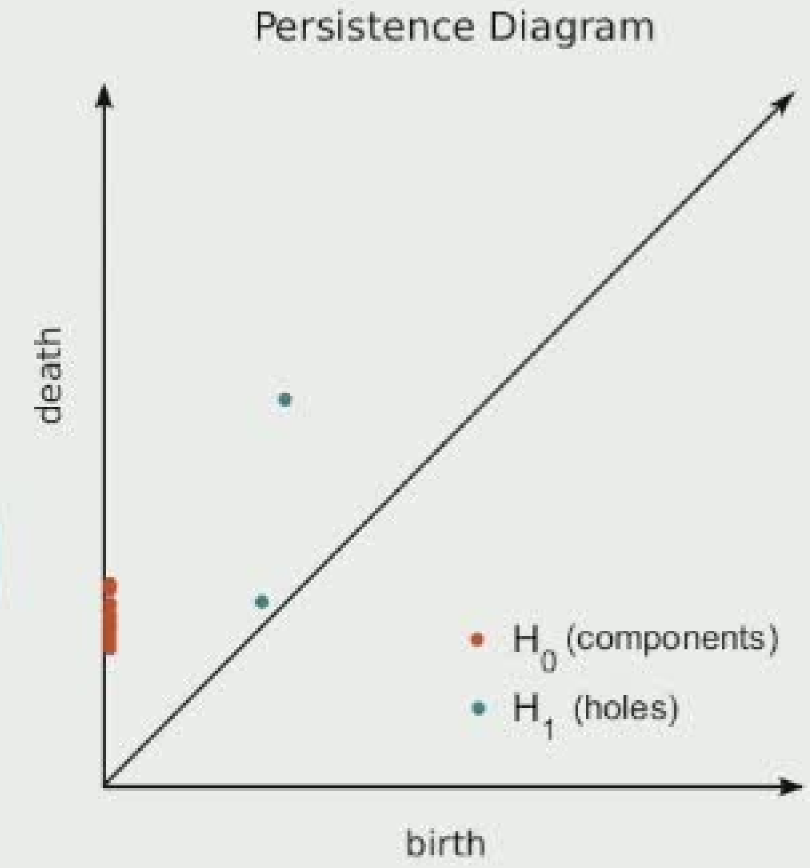



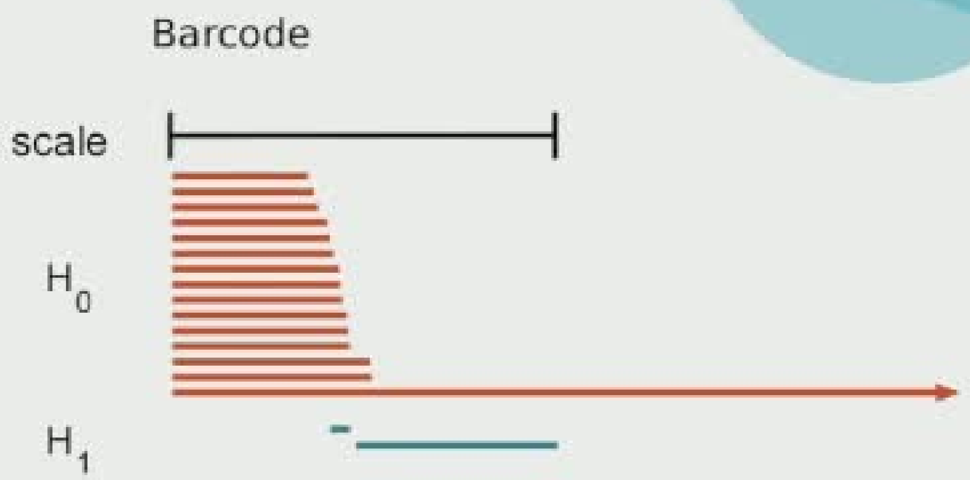

measure has been shown to be stable as order increases

R. Böttger, L. Bischoff, S. Facsko, and B. Schmidt. *Quantitative analysis of the order of bi ion induced dot patterns on ge.* (2012)

# Persistent Homology





For a near hexagonal lattice, the persistence diagram detects defects in the lattice structure and can be summarized as

- Variance of $H_0$ bars:

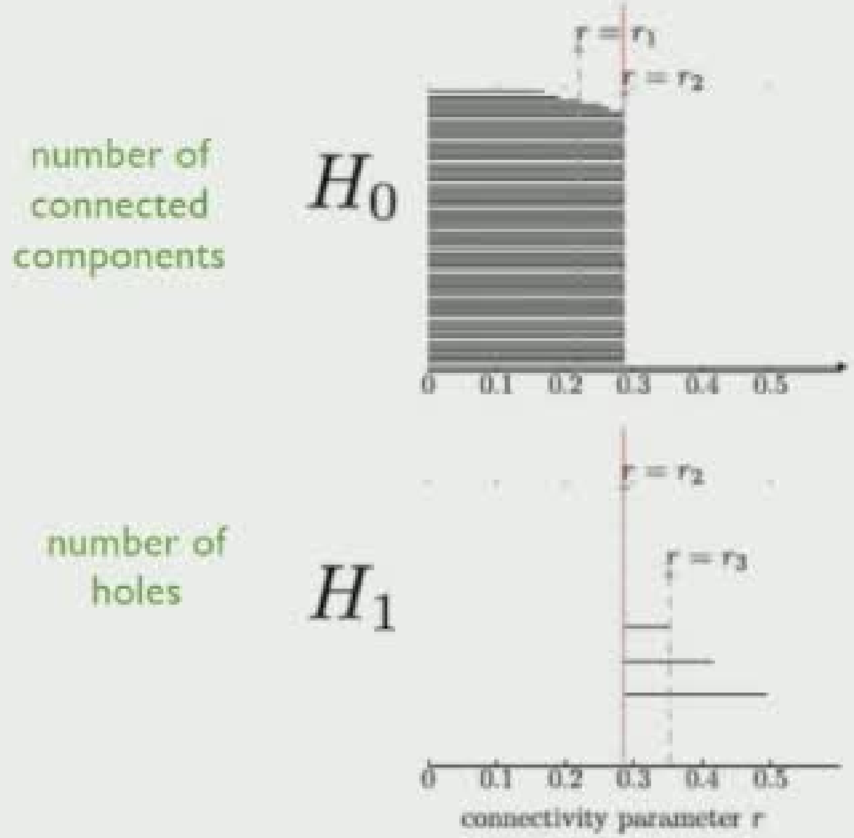
$$Var(H_0) = \sum_i (d_i - \mu)^2$$

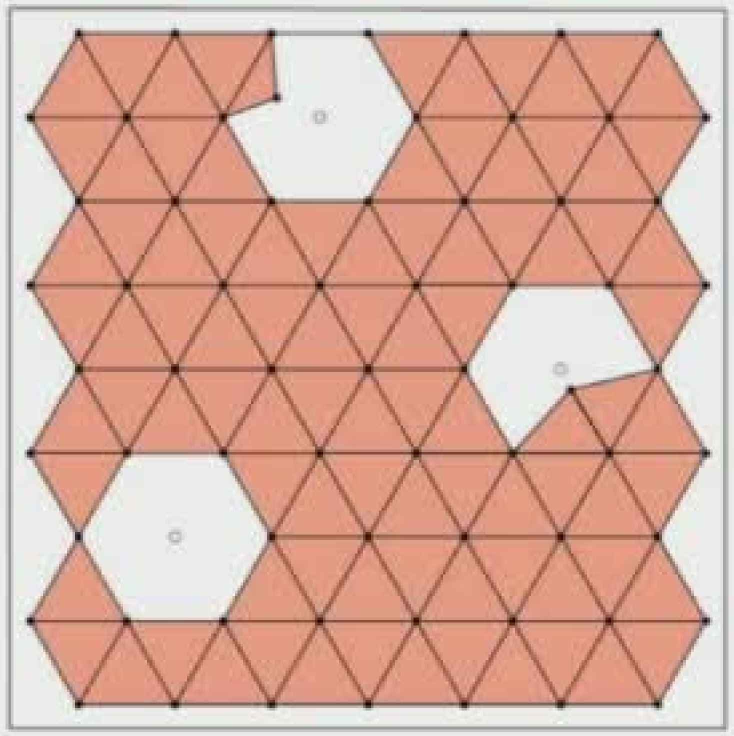
- Sum of $H_1$ bars:

$$\Sigma H_1 = \sum_i (d_i - b_i)$$

- Linear Combination:

$$CPH = 2Var(H_0) + \frac{1}{2-\sqrt{2}}\Sigma H_1$$



# A Note on Boundaries and Normalization

**Challenge**:

The most linearly unstable wave number $k_T$ does not depend $b$, however as the surface evolves nonlinear effects influence the characteristic wavelength of the observed pattern (and therefore the spacing of neighboring nanodots)

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**Challenge:**

The most linearly unstable wave number $k_T$ does not depend $b$, however as the surface evolves nonlinear effects influence the characteristic wavelength of the observed pattern (and therefore the spacing of neighboring nanodots)

**Strategy:**

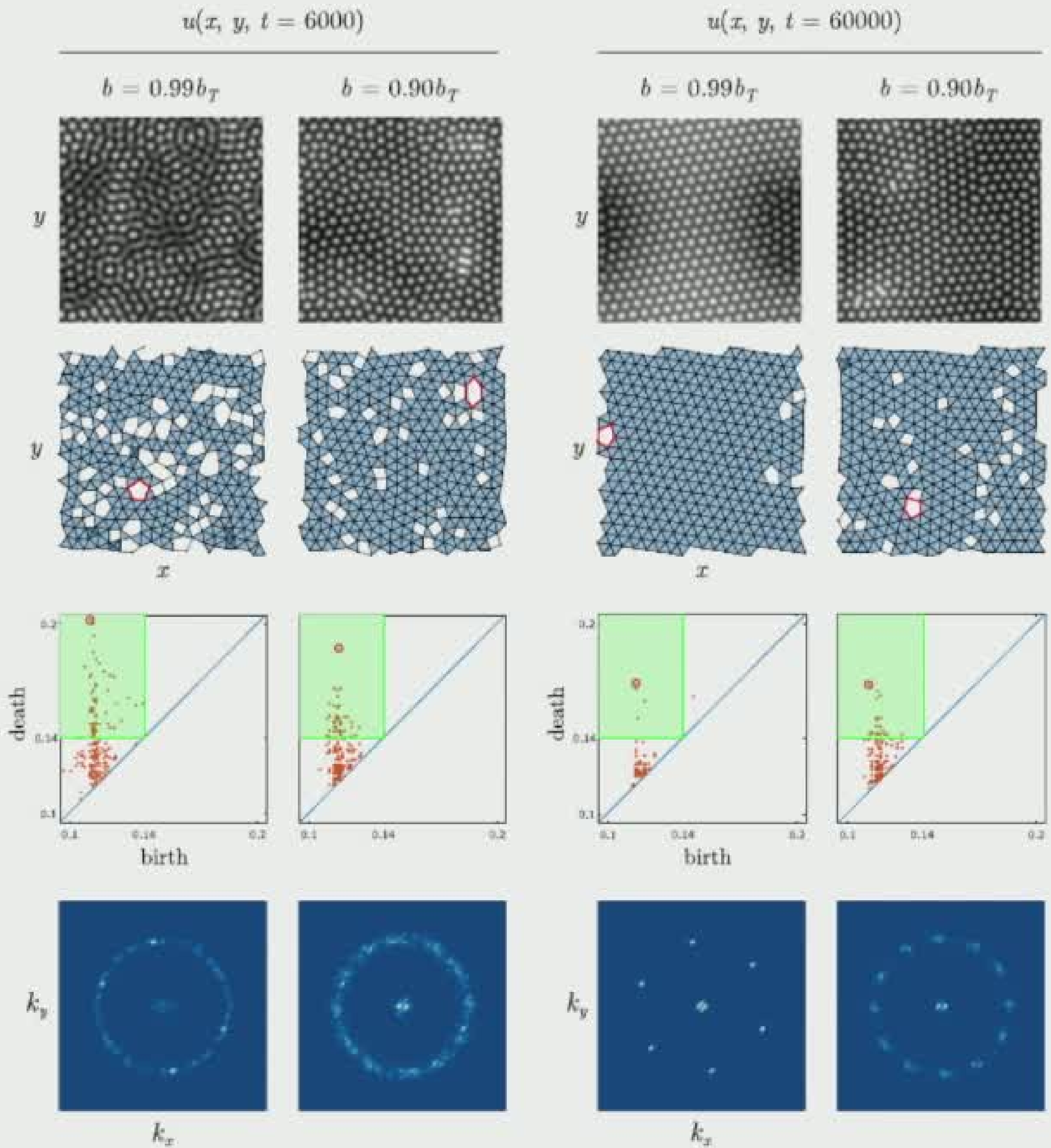
Retain a fixed number of nanodots in a square and rescale to fit the square $[-1, 1] \times [-1, 1]$

This is an essential step for

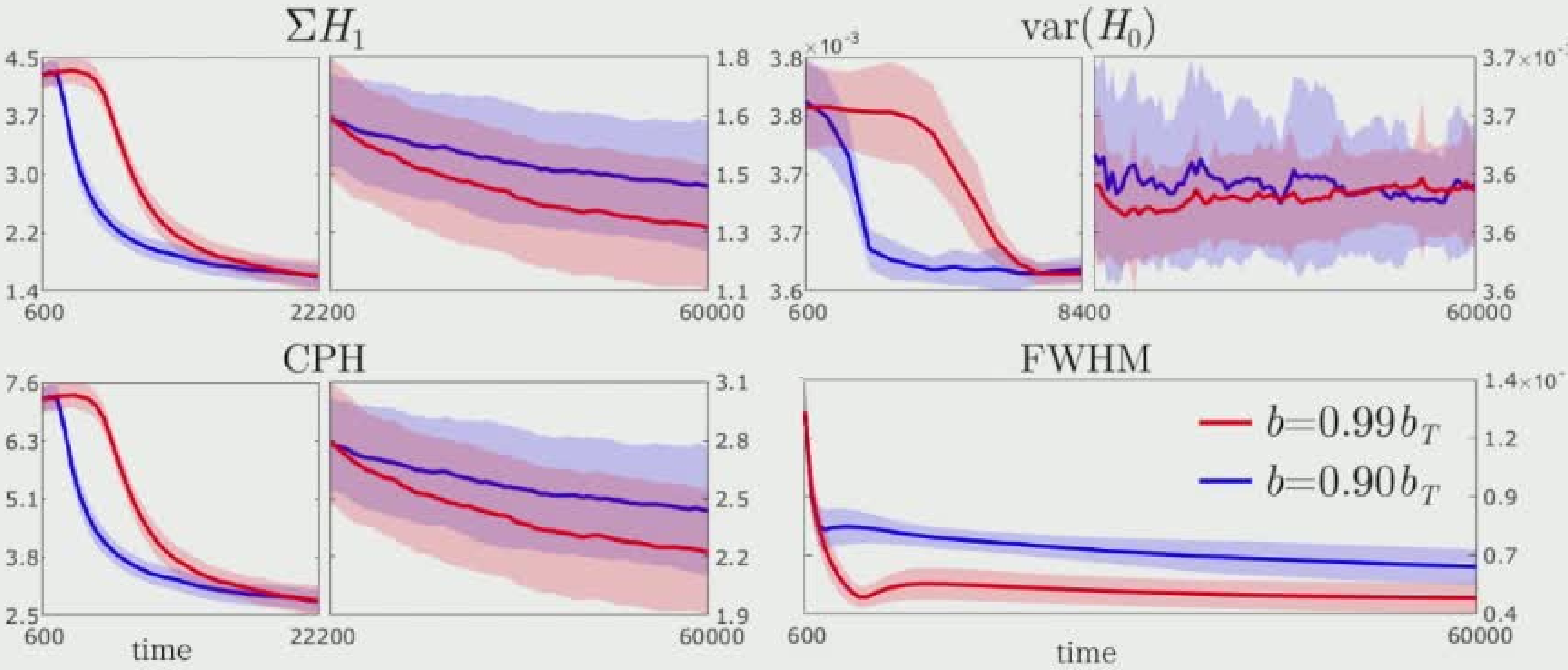
- tracking order statistics over time
- comparing simulated and experimental data

Experiment:

- fix parameters $a, c, \nu, \lambda$ and $\eta$ (where the systems undergoes a Turing bifurcation at $b_T$)
- generate 50 white noise initial conditions, perform 50 simulations with $b = 0.99b_T$ and $b = 0.90b_T$
- expect at long simulation time, the hexagonal order is improved for $b$ closer to $b_T$



# Comparison of Measures over Time




- Surprisingly, hexagonal order during the initial transient dynamics is much better for $b = 0.90b_T$ than $b = 0.99b_T$
- FWHM does not capture the observation that rapid commitment to a pattern may hinder long term order

# Dependence of Order on Bifurcation Parameter

Experiment:

- fix parameters $a, c, \nu, \lambda$ and $\eta$ (where the systems undergoes a Turing bifurcation at $b_T$)
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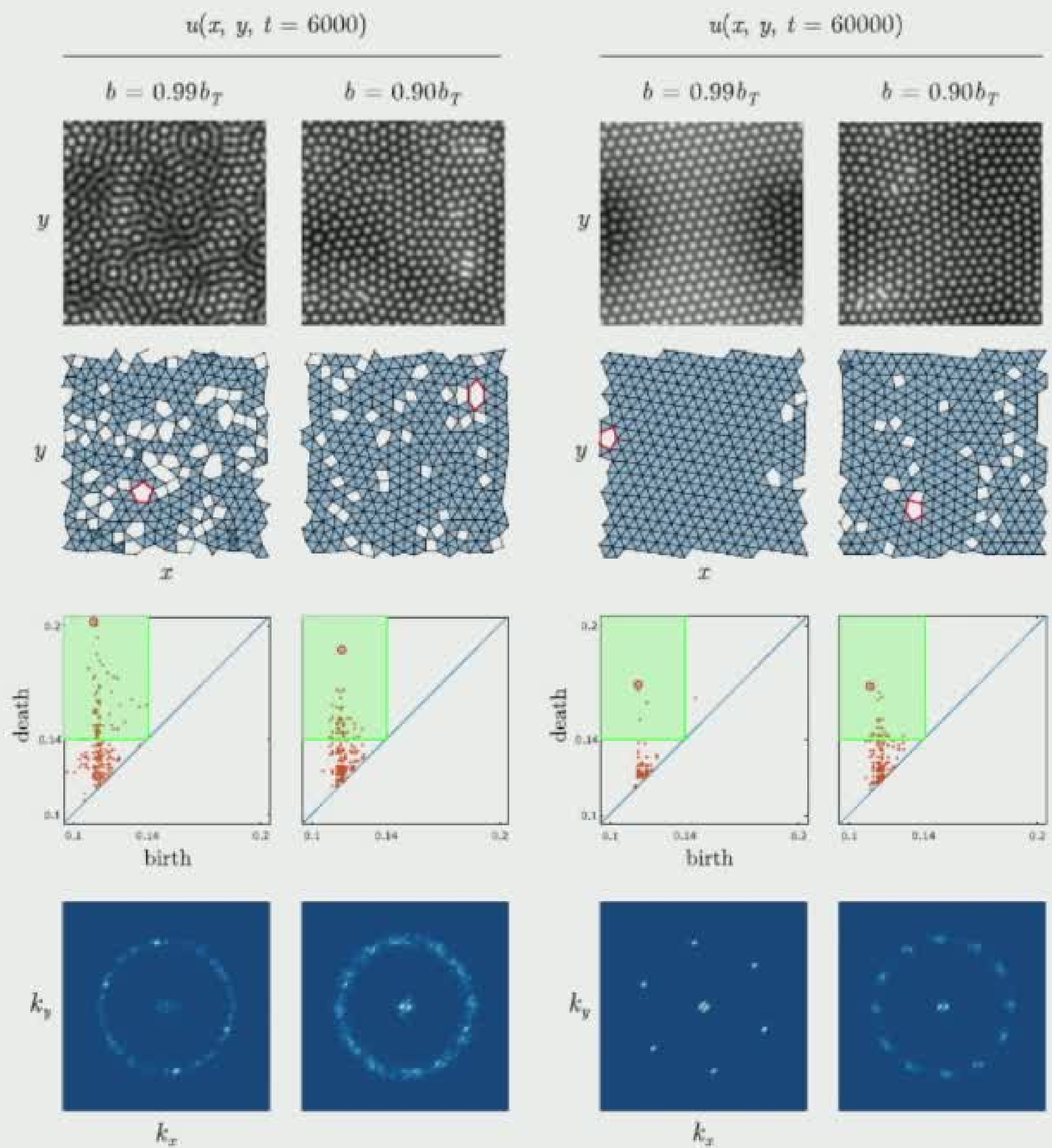


## Soft Mode

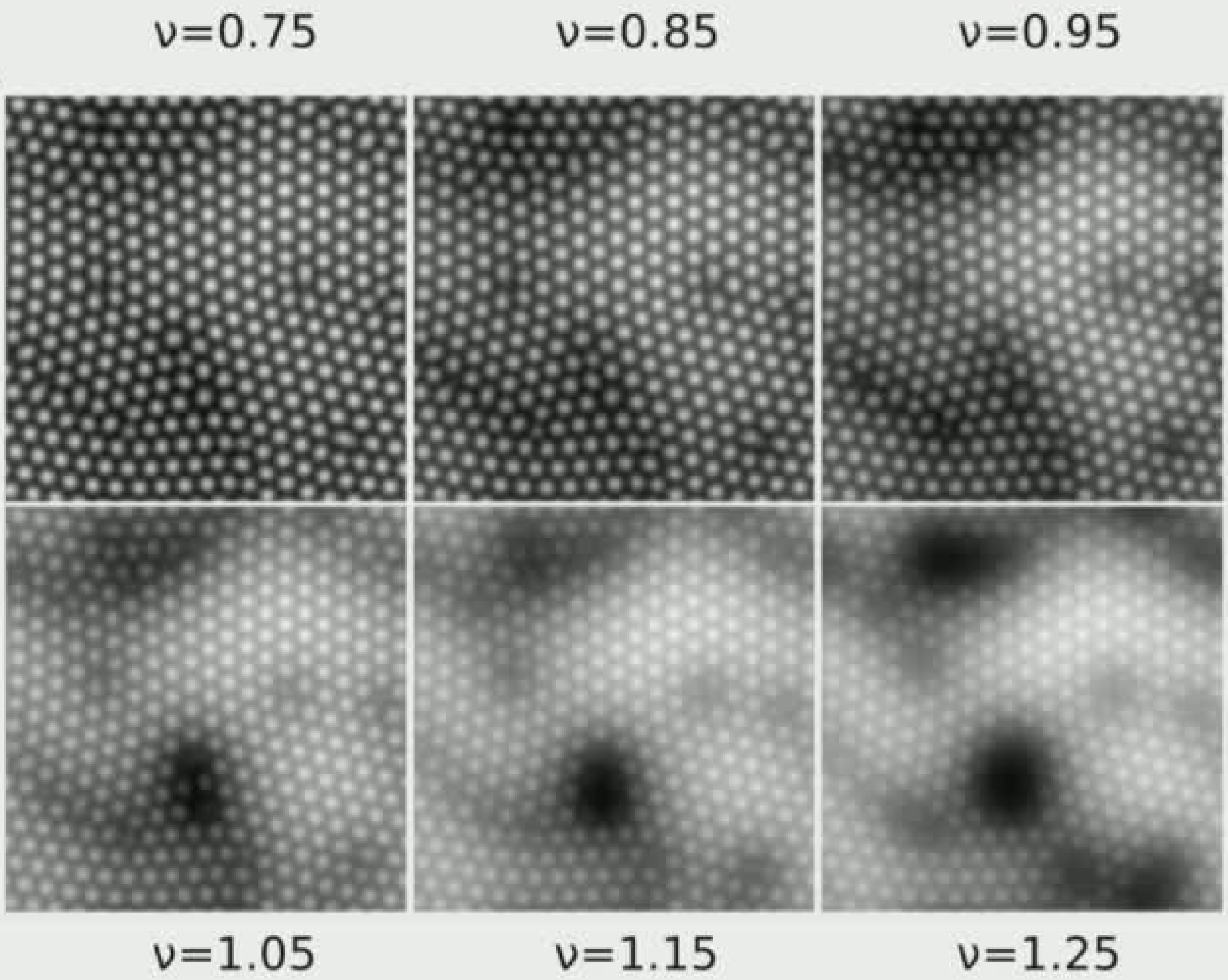
Approximate solution to the nonlinear BS-equations (for $b - b_T < \epsilon$)

$$u(x,t) = \sum_{k_k \in C} \left( A_j(t) e^{i k_j \cdot x} + c.c. \right) + G(t)$$

$$\frac{dG}{dt} = \left[ \lambda(1 - \frac{a}{c}) + \frac{2\nu}{a} \left( \frac{a^2 - c^2}{4c^2} \right)^2 \right] \sum_{j=1}^{3} A_j A_j^* + \frac{2\eta}{a} \left( \frac{a^2 - c^2}{4c^2} \right)^3 \mathrm{Re}(A_1 A_2 A_3)$$

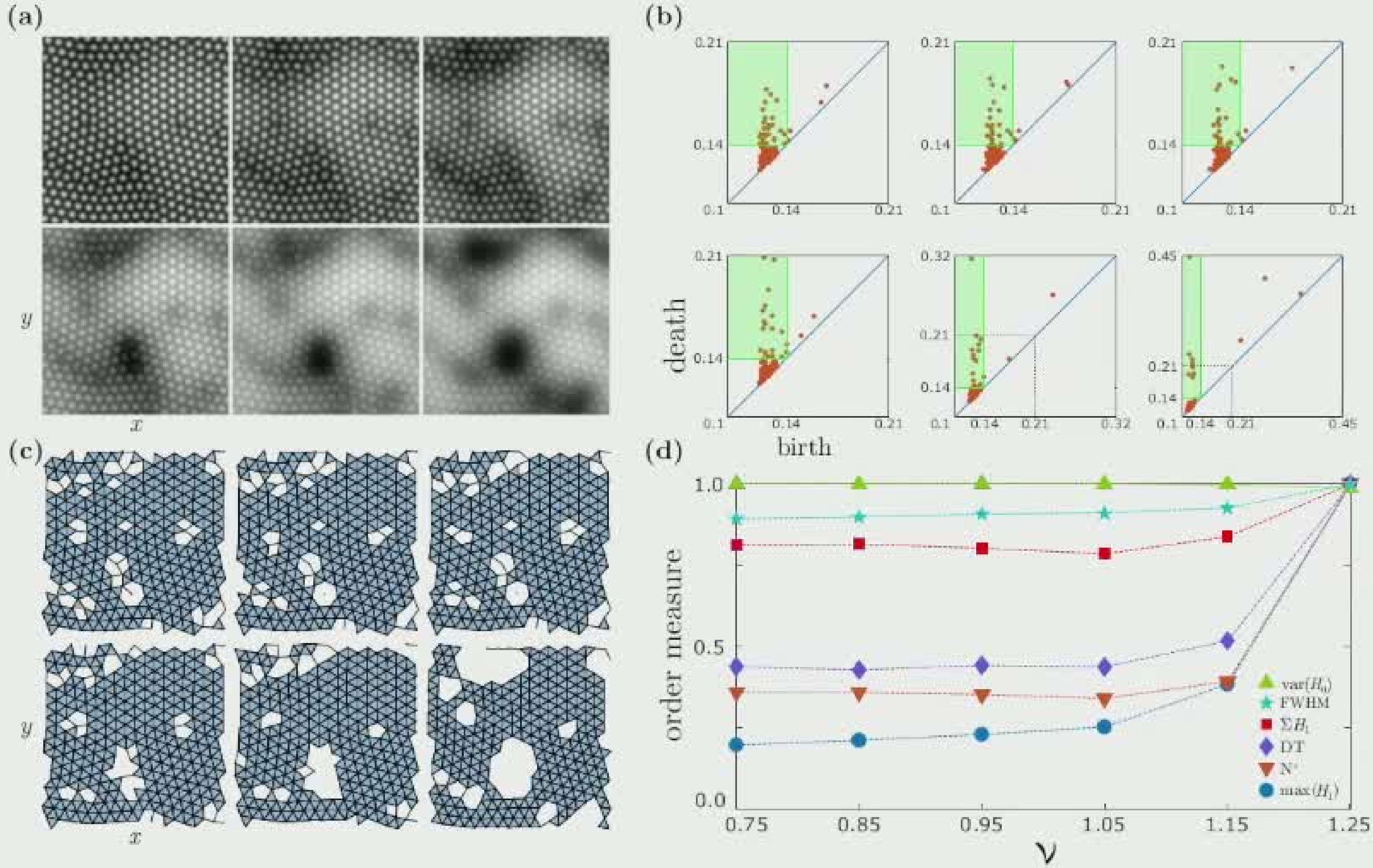
- $A_1$, $A_2$, and $A_3$ are amplitudes of wave vectors that resonate with **0** (the zero mode) through nonlinearities
- These low frequency modes are called Soft modes (Goldstone modes) and effect long range order
- Soft modes change net sputter yield, impact defect formation, and play a role in whether defects resolve over time

# Dependence of Order on Zero Mode




- Increasing $\nu$ increases the effect of the zero mode
- at long time, this leads to an increase in the average height disparity between defects and defect-free regions
- $\nu$ has very little influence on the configuration of nanodots until a critical value is reached

# Dependence of Order on Zero Mode



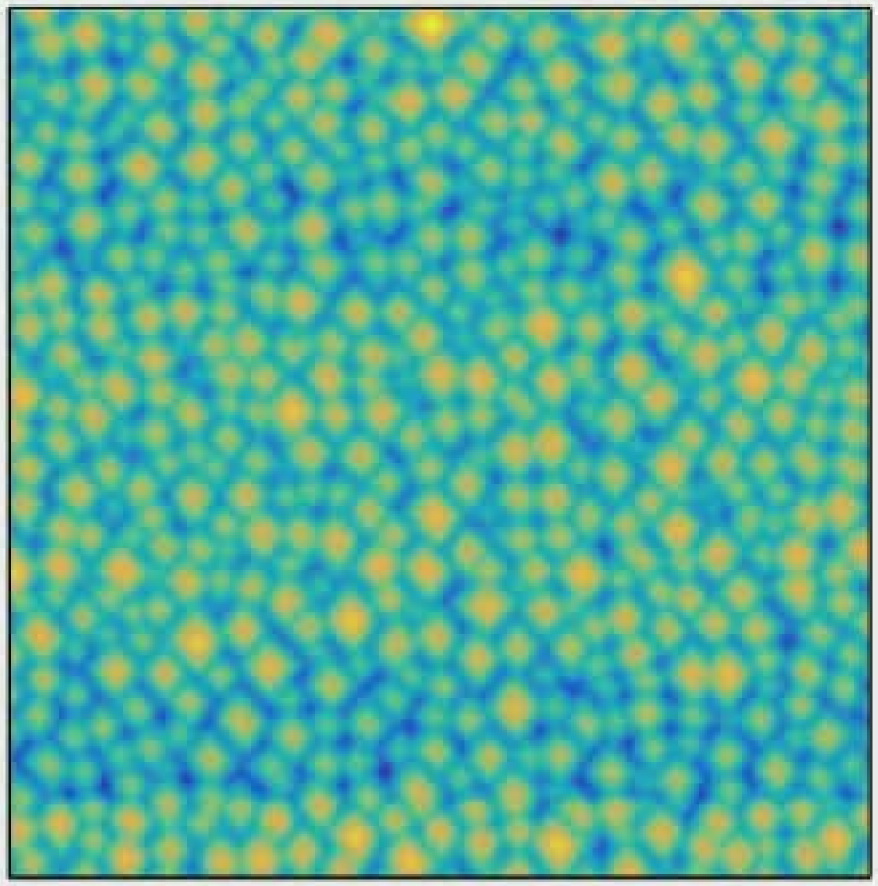
# A Few Conclusions

**Big Picture:**

- Summaries of persistence diagrams characterize order in the evolution of a pattern
- This technique is a practical way of quantifying order and detecting defects
- Studying dynamics through this lens can lead to novel observations
- Summaries for persistence diagrams contained discriminating information regarding parameter values

# Switching Gears– Checkerboard Patterns

- Elemental Ge is bombarded with noble gas ions above the recrystalization temperature
- The surface is amorphized by ion bombardment
- Surface diffusion and mass distribution cause smoothing
- Ehrlich-Schwoebel (ES) barrier creates uphill atomic currents and induces an instability
- Checkerboard pattern emerges, and coarsens in time



# Pyramidal Structures

$$\frac{\partial u}{\partial t} = -\nabla^2 u + \overbrace{\kappa\nabla^2\nabla^2 u}^{\text{surface diffusion}} - \underbrace{\sigma\nabla^2(\nabla^2 u)^2}_{\text{nonlinear current}} + \overbrace{\delta(\partial_x u_x^3 + \partial_y u_y^3)}^{\text{ES surface current}}$$

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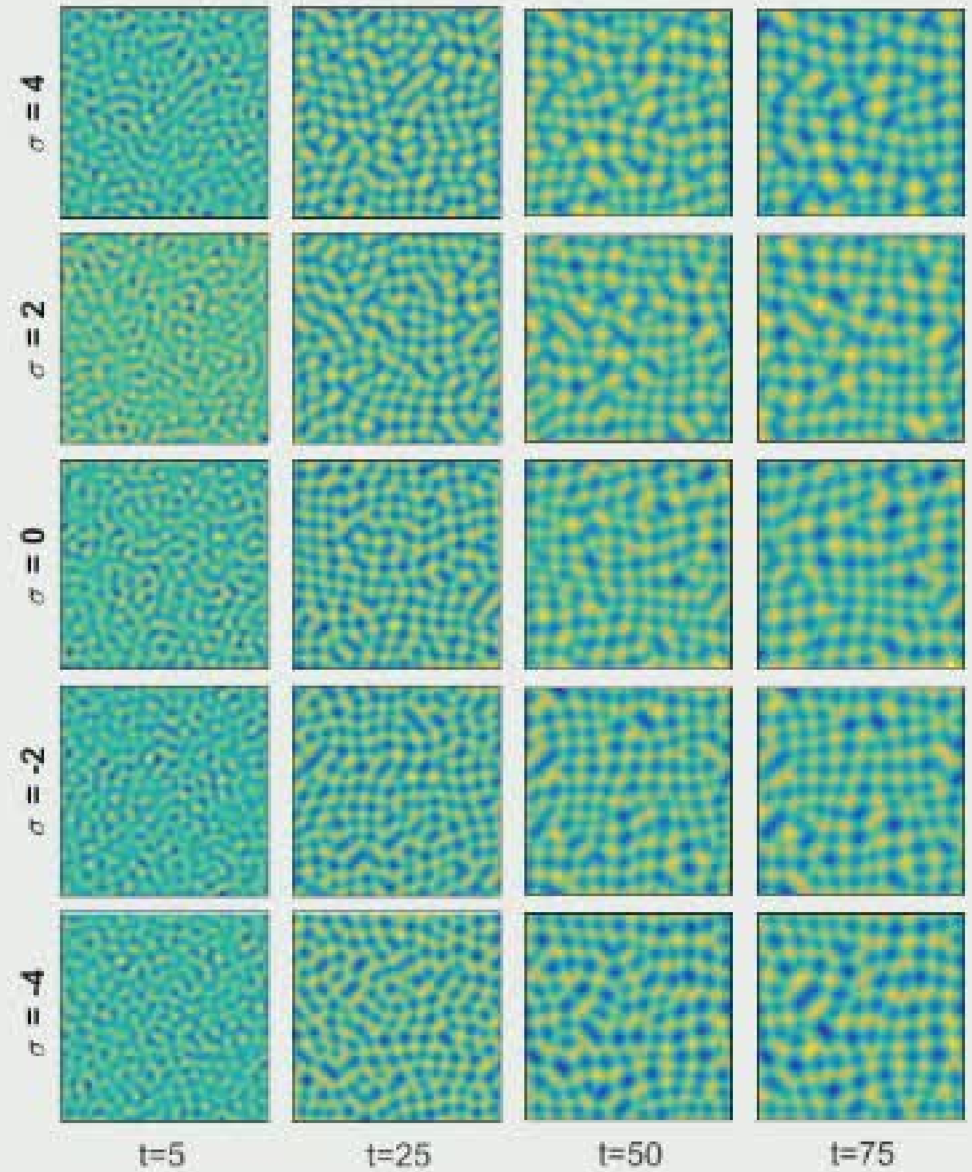
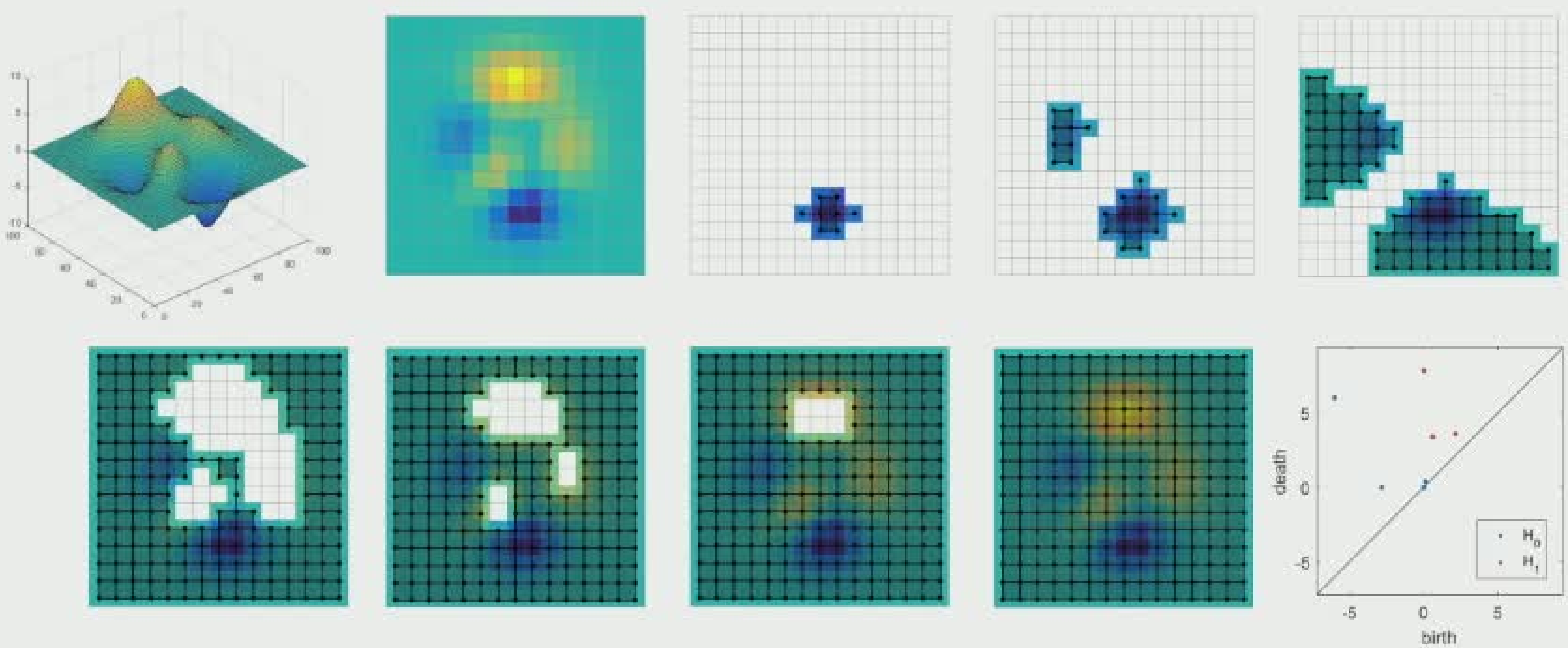


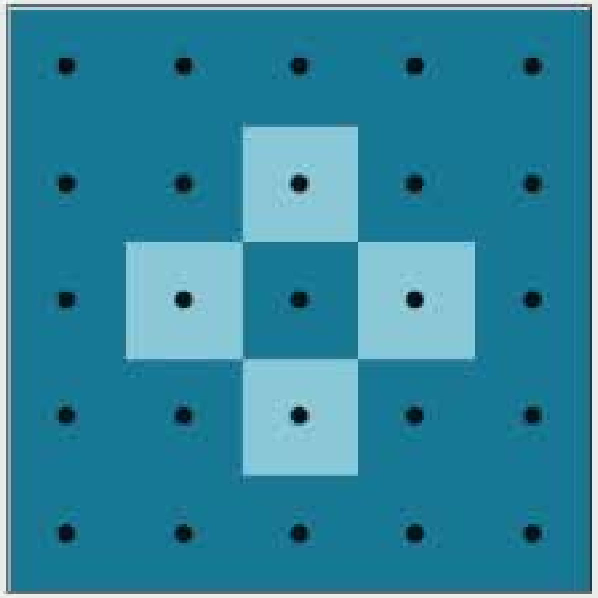

Ou et al., Phys. Rev. Lett. 2013

# Persistent Homology: Sublevel Set Filtration

- Construct a cubical complex on the sublevel set of the data at each threshold
- Track the connected components and holes present of sublevel sets as the height threshold increases



# A Few Notes on Cubical Complexes



- $H_0$ ($u$) measures the prominence of valleys or pits
- $H_1$ ($u$) measures the prominence of peaks

**Careful!**

- When computing homology, we are concerned with connectedness – should we think of 4-neighbor or 8-neighbor connectedness?
- (Both) we need a discrete version of the Jordan Curve Theorem, so build the cubical complex on 4-neighbor connections.
- Look to 8 neighbors for considering whether islands are connected components
- so $H_0$ and $H_1$ are summarizing structures in slightly different ways –
- exploit a duality between $H_0$ of sublevel sets and $H_1$ of superlevel sets and use $H_0$ of the surface and of the inverted surface to build a statistic