Quantifying patterns in the Vicsek Model with topological tools

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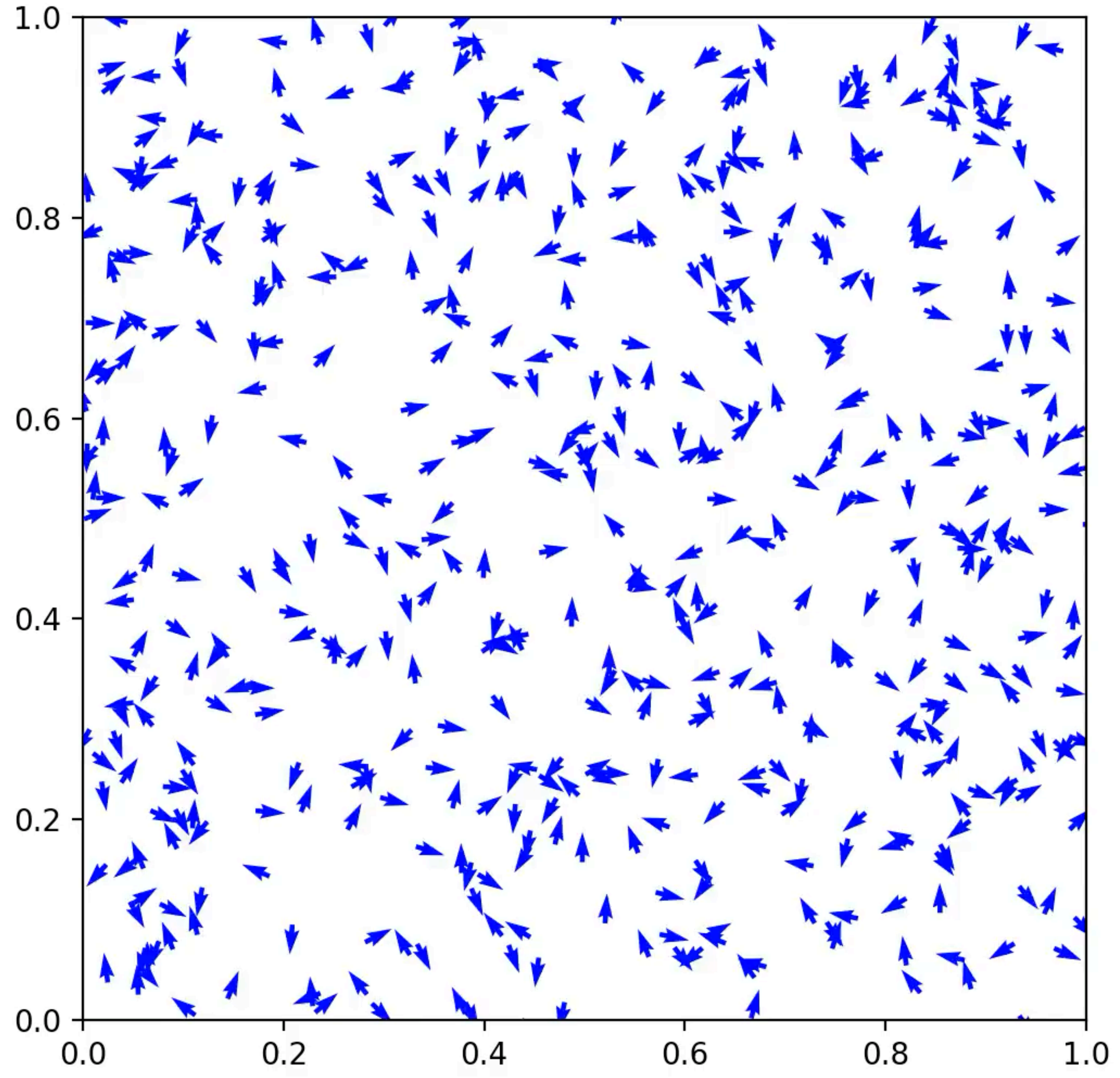
Dynamical Systems and Topology

The signature of the mechanics of the dynamical system is hidden in its topology.

Poincaré in 1892 had instigated the question of whether it is possible to identify dynamical systems and their evolution in terms of topology through his work *" Les Méthodes Nouvelles de la Mécanique Céleste"*



Vicsek Model

$$x_i(t+1) = x_i(t) + v_i(t+\nabla t)\nabla t$$

$$\theta_i(t+\nabla t) = \frac{1}{N}\sum_{|x_i-x_j|\leq R}\theta_j(t) + U(\frac{-\eta}{2},\frac{\eta}{2})$$

The standard Vicsek model describes the collective motion of living matter represented by points whose positions $\{x_i\}$ are tracked over discrete timesteps. Where v_i has constant magnitude but direction Θ_i is influenced by the neighbouring particles within radius R and noise perturbation η.

Some Topological studies :

- ***Topaz, Chad M., Lori Ziegelmeier, and Tom Halverson. "Topological data analysis of biological aggregation models." PloS one 10.5 (2015): e0126383.***
- ***Bonilla, Luis L., Ana Carpio, and Carolina Trenado. "Tracking collective cell motion by topological data analysis." PLOS Computational Biology 16.12 (2020): e1008407***
- ***Bhaskar, Dhananjay, et al. "Topological data analysis of spatial patterning in heterogeneous cell populations: clustering and sorting with varying cell-cell adhesion." npj Systems Biology and Applications 9.1 (2023): 43.***

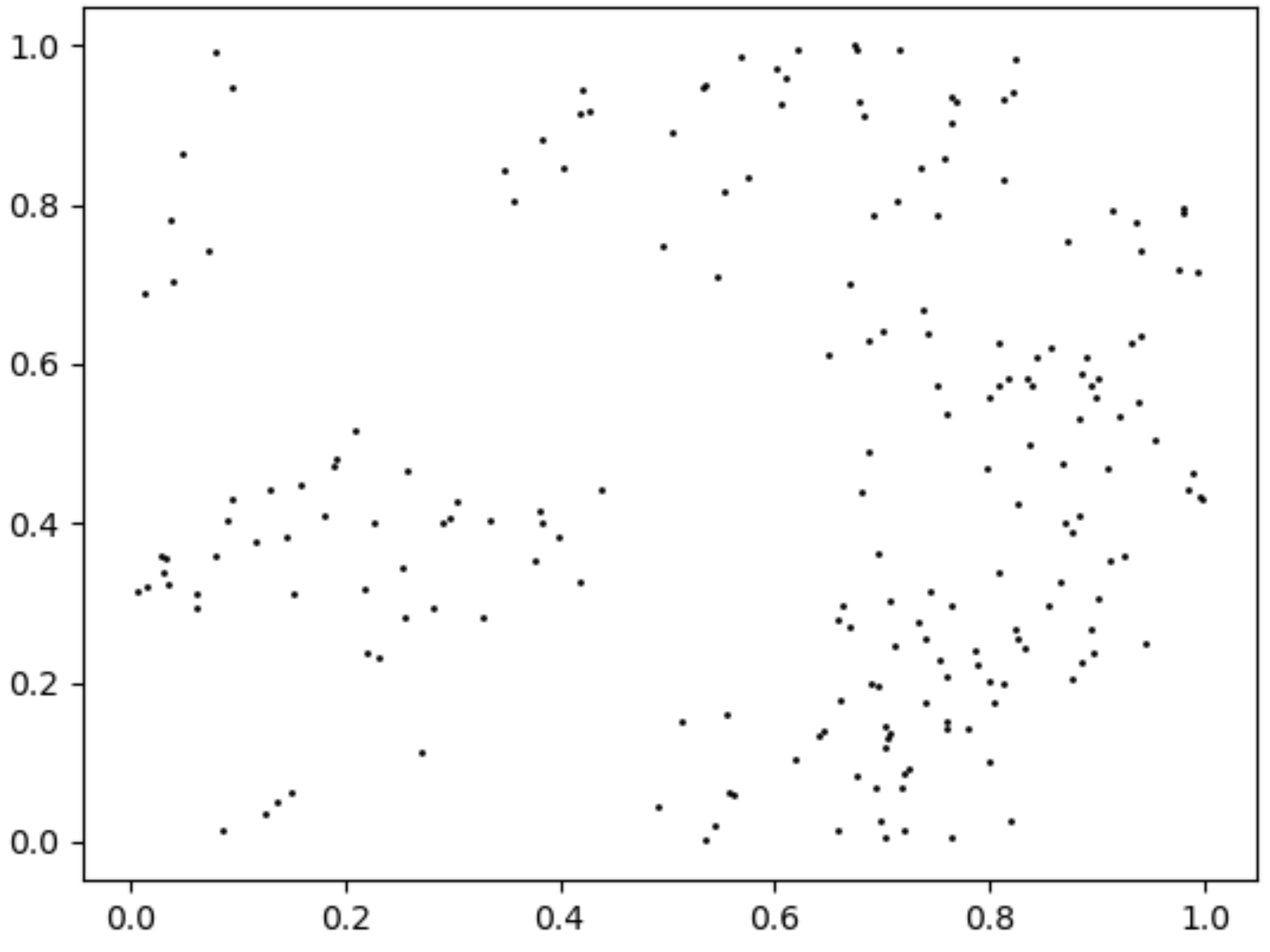
Topological Data Analysis and Pattern Study :

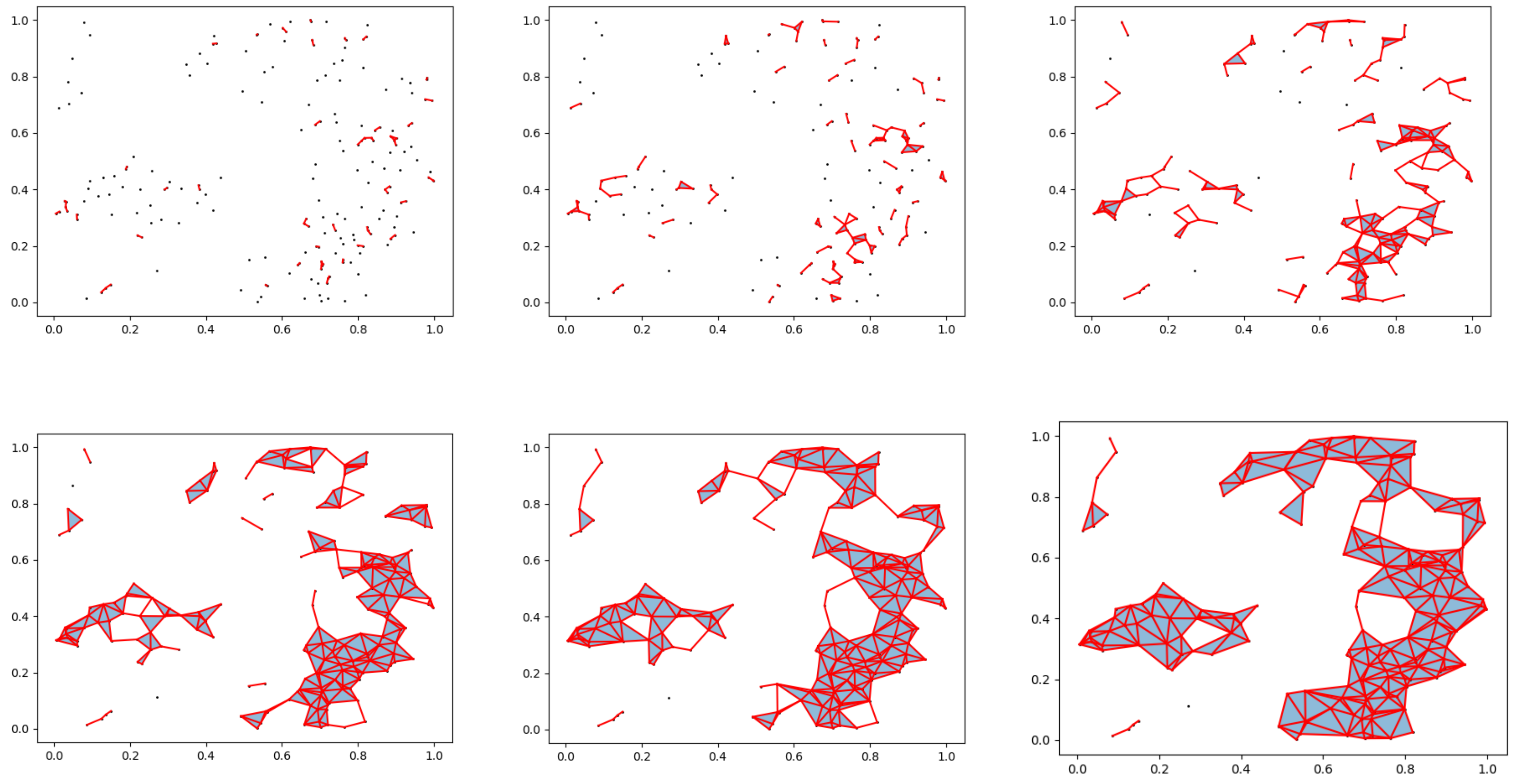
Point cloud

Cell complex / Simplicial complex

Multi scale

topological study



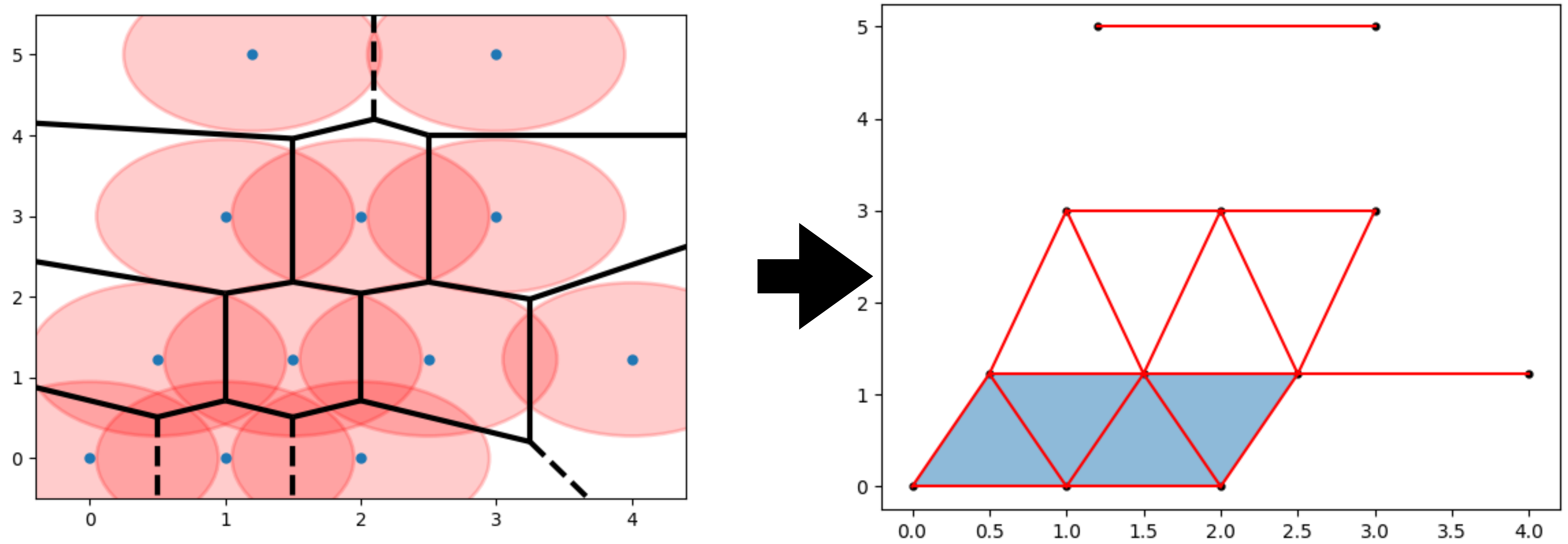


Questions :

- How efficiently can we extract the pattern from a point cloud
- For a temporally evolving point cloud, how do these patterns evolve?
- What do we understand about aggregation dynamics from studying these patterns?
- Can we find any correlation between the aggregation dynamics and the oder-disoder transition ?

The tools : Simplicial Complex

To analyse the topology inherent in a point cloud, TDA involves constructing a "continuous" shape on top of the discrete data. This is done through a filtration, making a nested family of simplicial complexes that reflects the data's structure across a range of scales.



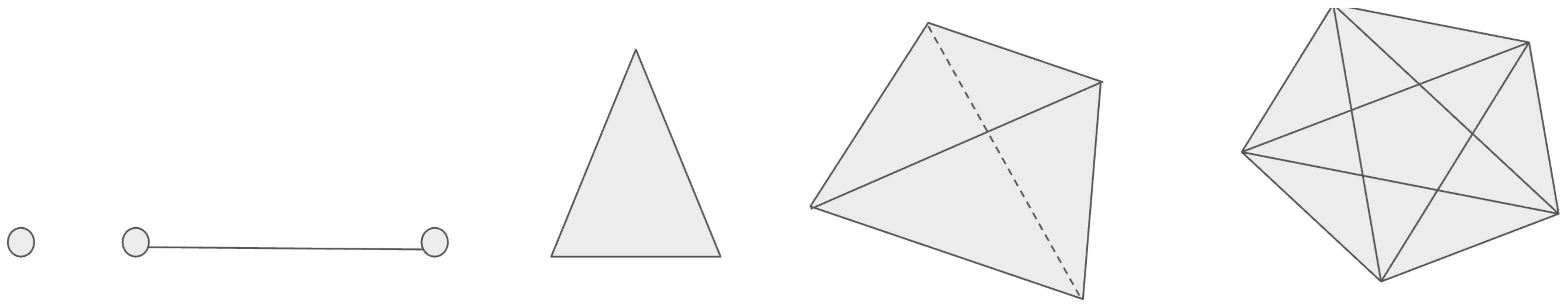
Simplicial complex is higher dimensional analogue of planar triangulation.

It is collection of higher dimensional simplices(generalization of triangle) . We break down complex shapes into simplices and study the relationships between these simplices.

$$\mathcal{N}(\{V_s \cap B(s,r)\}_{s\in S}$$

Alpha complex: Nerve complex for fusion of Čech complexes and Delaunay triangulations.

A geometric k-simplex σ in R^d is a convex hull of affinely independent family $\{v^o, v^1, \ldots, v^k\}$, $k<d$



0-simplex 1-simplex 2-simplex The 3-simplex The 4-simplex

Z. Virk, Introduction to Persistent Homology, 2022. doi:10.51939/0002.

The tools: Betti Number & Euler Characteristic

In general, n-th Betti number (β_n) corresponds to the nth dimensional hole.

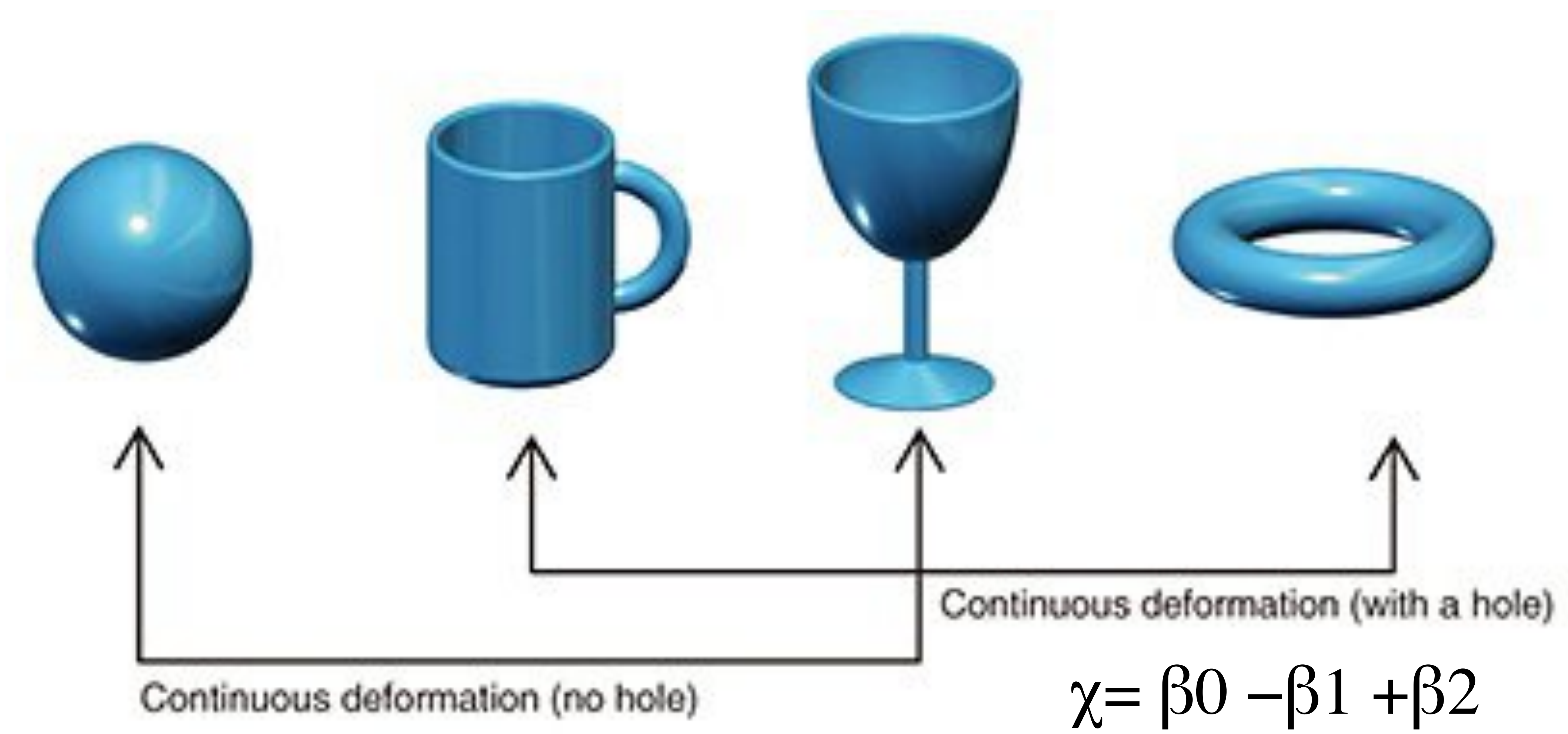
It is given by the dimension of the nth homology group of a simplicial complex. For each dimension *n*, the *n*-th Betti number (β_n) is defined as the rank of the *n*-th homology group, and it essentially counts the number of independent *n*-cycles that do not form the boundary of any collection of (*n*+1)-dimensional simplices.

β_0= no. of connected components

β_1= no. of loops(1-d holes)

β_2= no. of caves (2-d holes)

The Euler characteristics (χ) = $\beta_0 - \beta_1 + \beta_2 - \ldots\ldots + (-1)_n \beta_n$

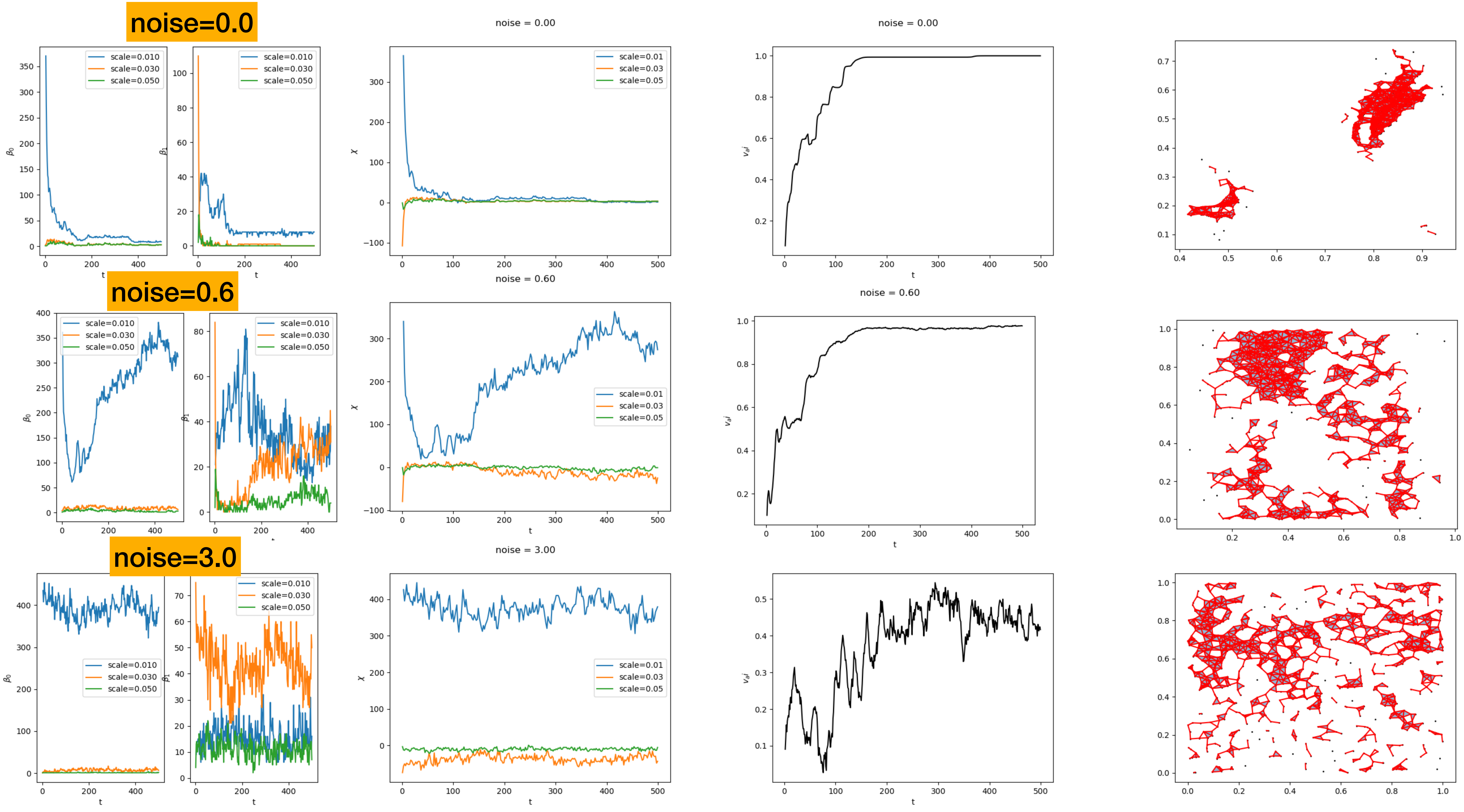


$\chi = \beta 0 - \beta 1 + \beta 2$
$= 1 - 0 + 0 = 1$

$\chi = \beta 0 - \beta 1 + \beta 2$
$= 1 - 2 + 1 = 0$

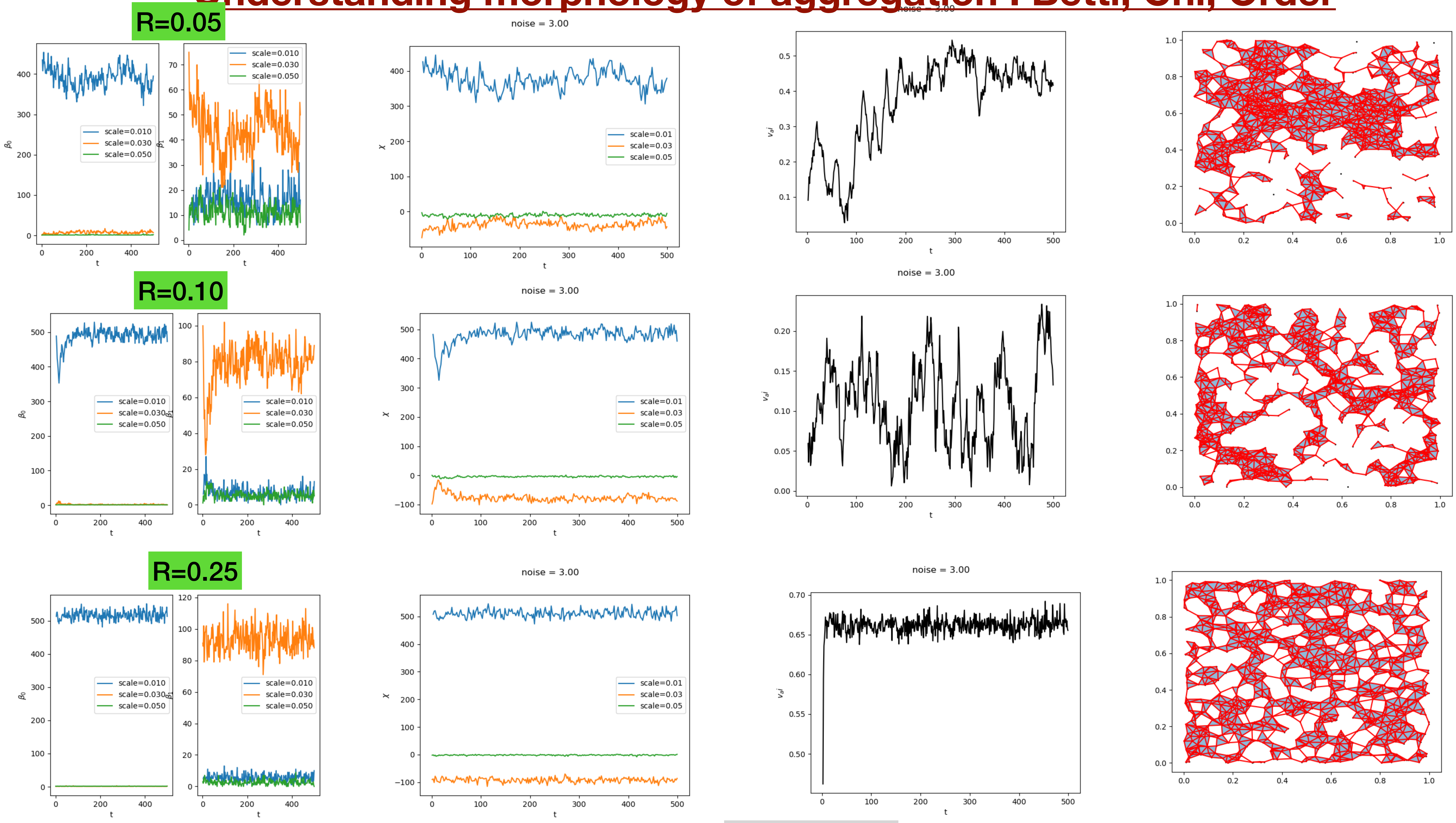
Euler Characteristic is a topological invariant: it remains the same if the system has a continuous deformation (stretching, bending and not tearing/glueing.)

Understanding morphology of aggregation : Betti, Chi, Order



Different noise, R=0.05, N=1000

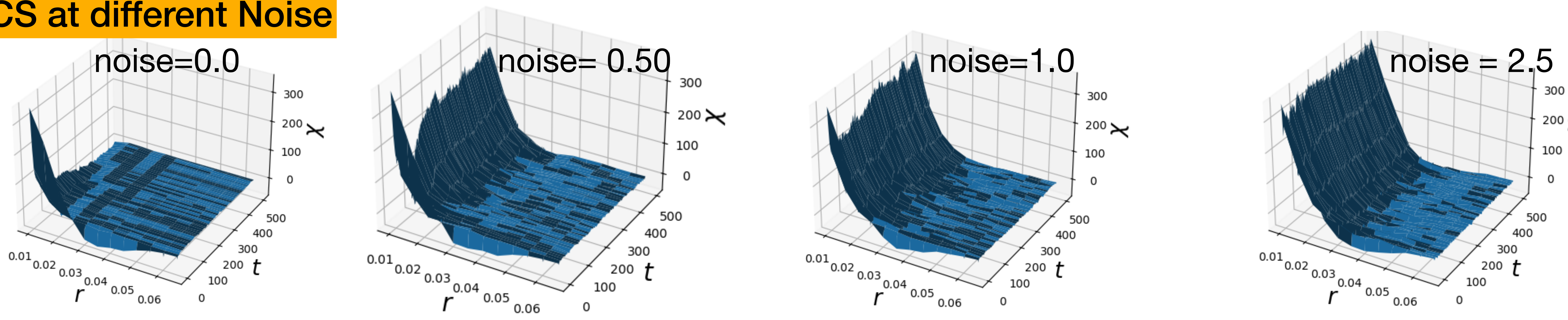
Understanding morphology of aggregation : Betti, Chi, Order



Different R, noise=3.0, N=1000

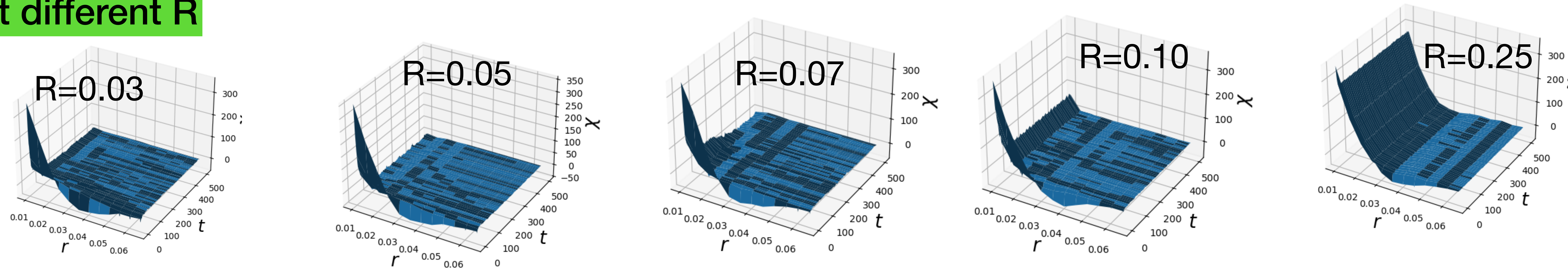
Euler Characteristic Surface(ECS): Topological Summaries

ECS at different Noise



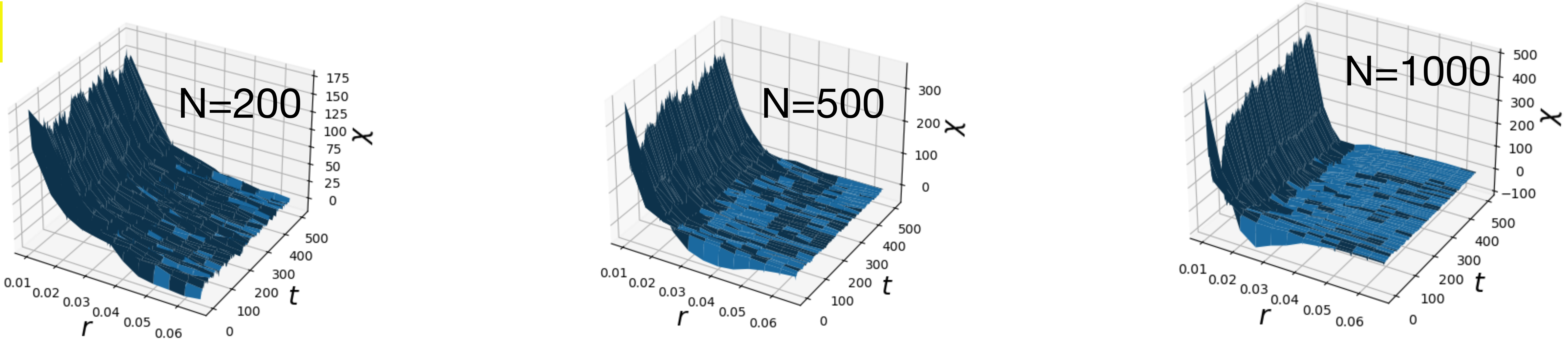
N=500,
R=0.05

ECS at different R



N=500,
noise=0

ECS at different N

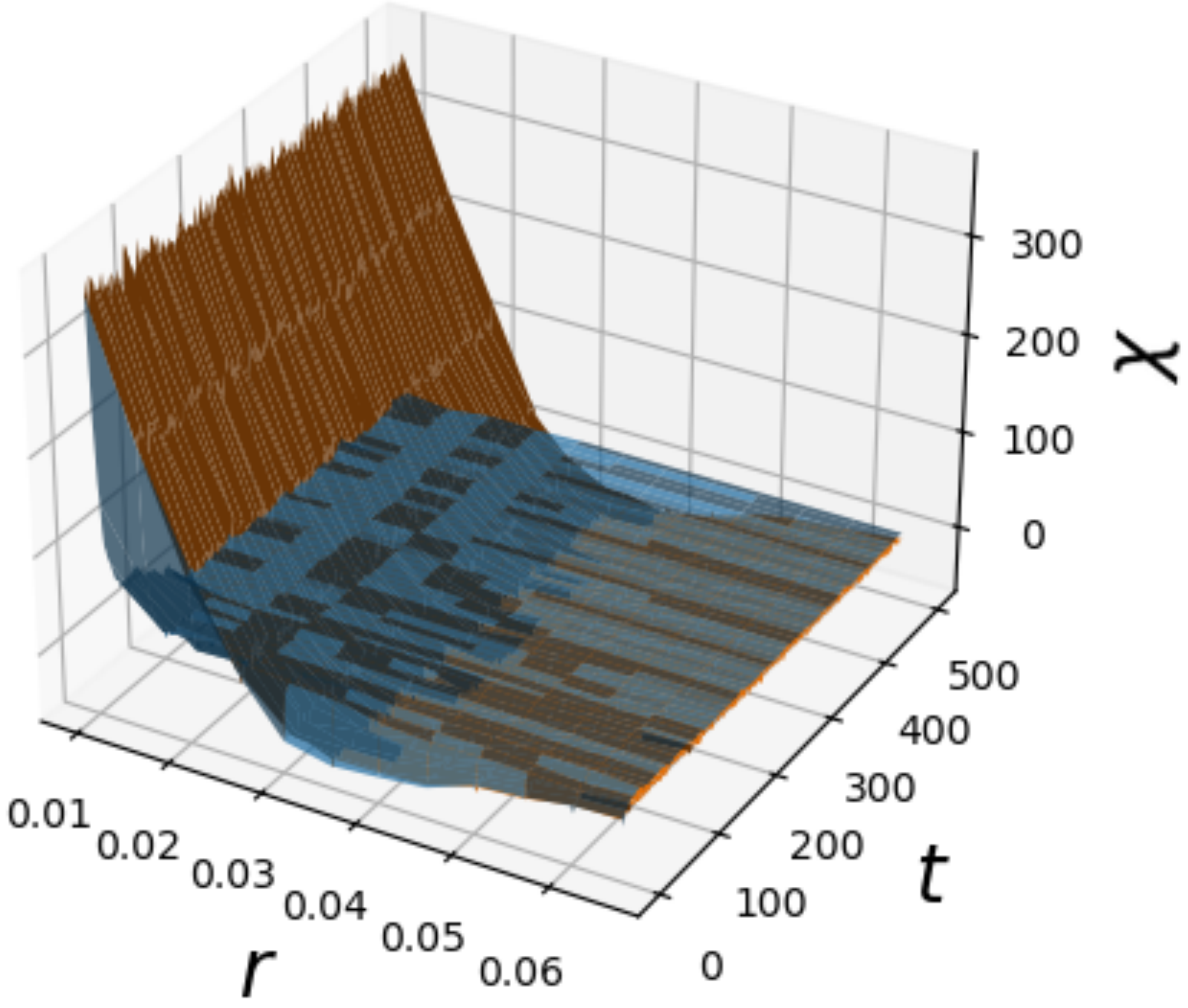


R=0.05,
noise
=1.0

Euler Metric (EM):

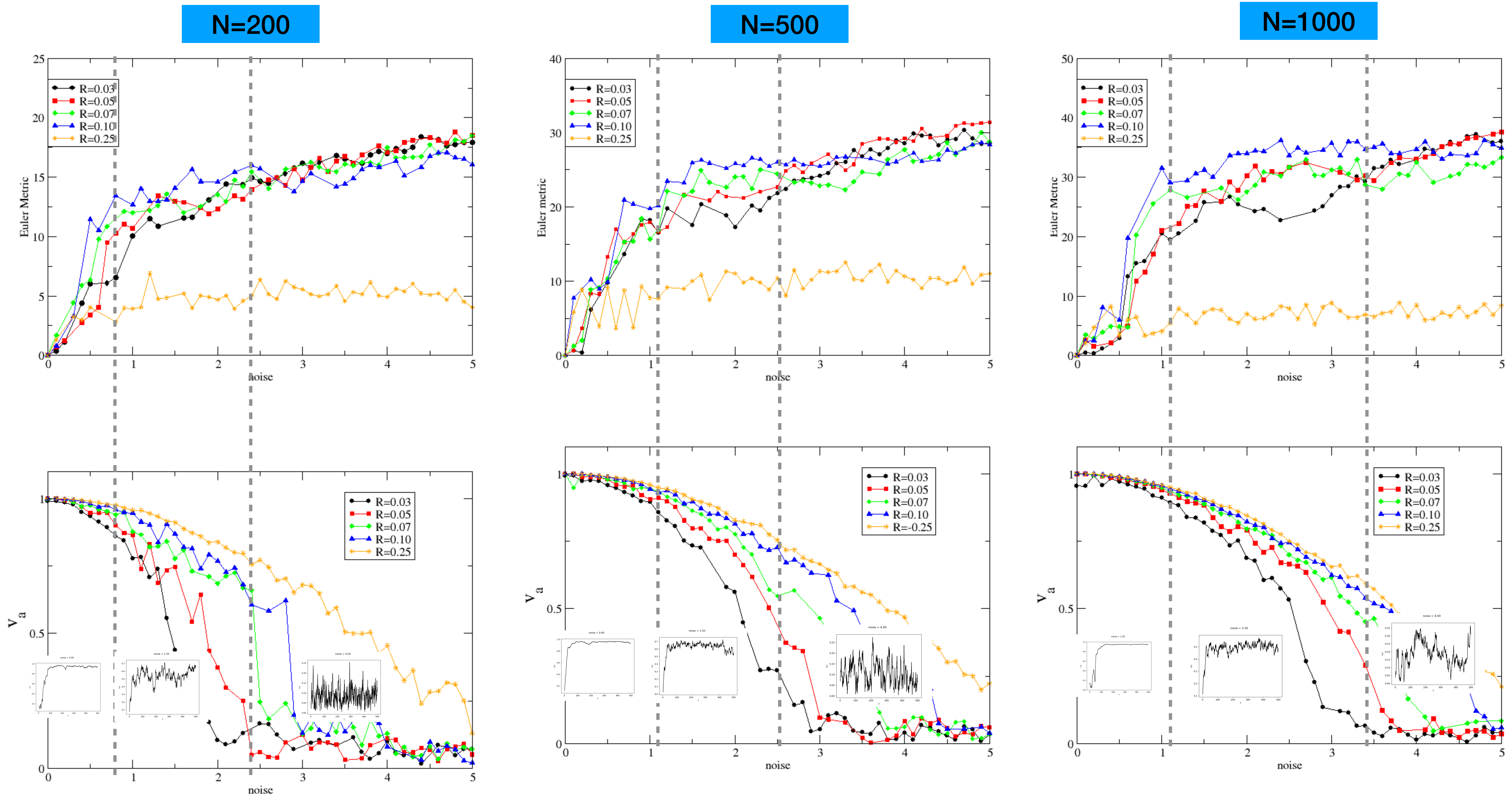
Given two temporally evolving point sets F1 and F2 for a dynamical system of the same size, we quantify the dissimilarity between the corresponding Euler characteristic surfaces χ_{F1} and χ_{F2} by calculating the L2 -norm distance between these surfaces as,

$$d(\chi_{F_1}, \chi_{F_2}) = \|\chi_{F_1} - \chi_{F_2}\|_2 = (\int_{[0,R]\times[0,T]} (\chi_{F_1} - \chi_{F_2})^2)^{\frac{1}{2}}$$



Here, I took the Euler Characteristic Surface with zero noise as the reference and estimated the Euler Metric between ECSs of different noises and ECS of zero noise. Along with that, the traditional order parameter has been estimated. $v_a = \frac{1}{Nv} \mid \sum_{i=1}^{N} v_i \mid$

Euler Metric & Order parameter: Finding cues



Where it stands now !

- The Betti curves can help us to understand aggregation morphology at different scale of resolution.

Which gives us an insight into how the parameters can be tuned to form dense/ porous aggregates.

- It is memory-wise expensive to store snapshots at every time step at multiple scales. But the study of Betti curves, along with order parameter, can give us a rough idea about the flocking dynamics.
- Studying the topological invariant Euler Characteristic give us the domain where the system is more topologically stable.
- The Euler Characteristic Surface (ECS) works like a topological fingerprint for a temporally evolving point set , further the Euler Metric (EM) quantifies the similarity/dissimilarity between these ECSs and the dynamical patterns
- Studying the variation of the Euler Metric(EM) with respect to noise shows a cue with the order-disorder transition !
- How effective can be designing of parameter recovery using the Euler Metric with ML algorithms .

Roy, A., et al. "Characterizing fluid dynamical systems using Euler characteristic surface and Euler metric." ***Physics of Fluids*** **35.8 (2023).**

Roy, Anamika, Atish J. Mitra, and Tapati Dutta. "Euler Characteristic Surfaces: A Stable Multiscale Topological Summary of Time Series Data." ***arXiv preprint arXiv:2408.09400*** **(2024).**

Thank you !