

MOD-SEM SuSe25

# Topic 3 - Phase 1

## Hyperuniformity

Generation of hyperuniform structures and their analysis

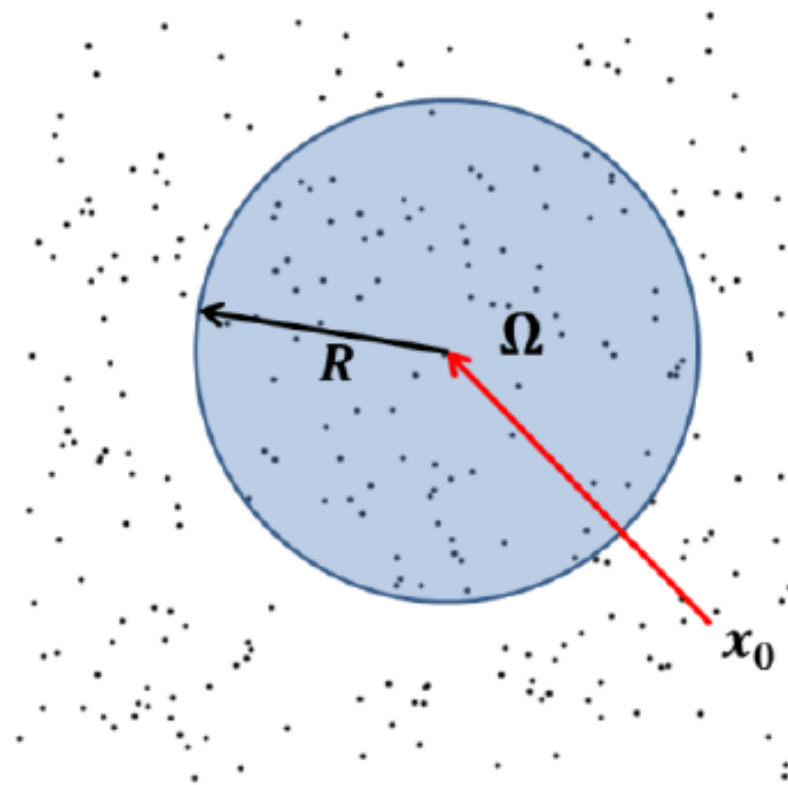
# Contents -Phase 1

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- Literature

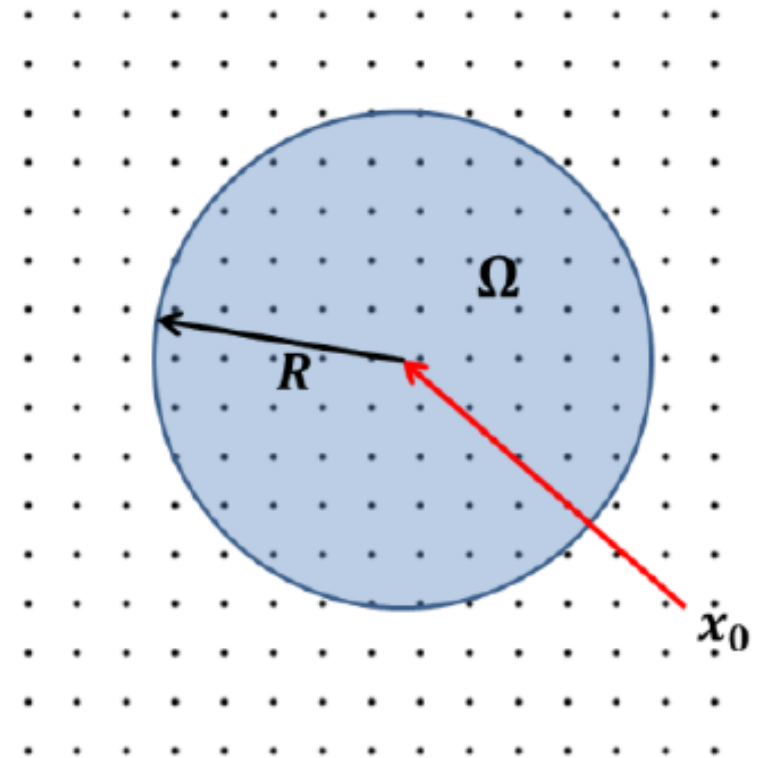
# Introduction

*Hyperuniform systems are defined by the suppression of density fluctuations over large spatial scales.*

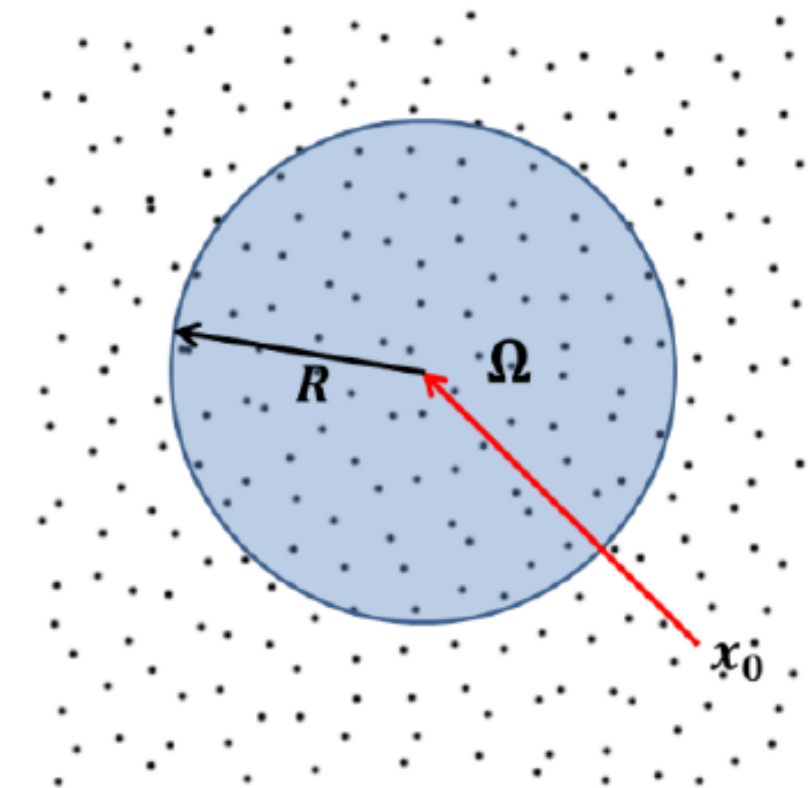
- The number variance inside an observation window grows more slowly than its radius:



$$\lim_{r \rightarrow \infty} \frac{\sigma_N(r)}{r^d} = \text{const.}$$



$$\lim_{r \rightarrow \infty} \frac{\sigma_N(r)}{r^d} = 0$$



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# Introduction

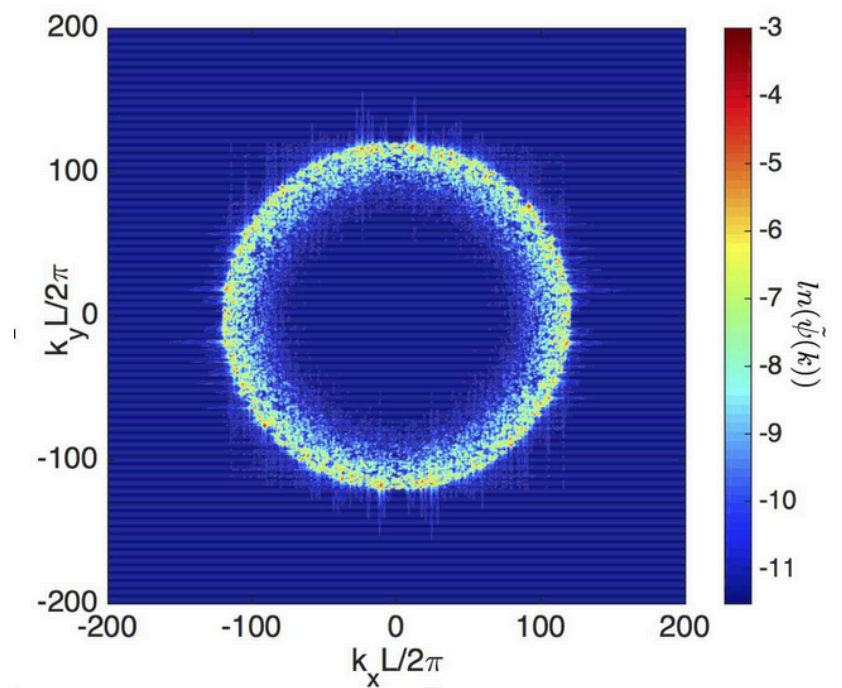
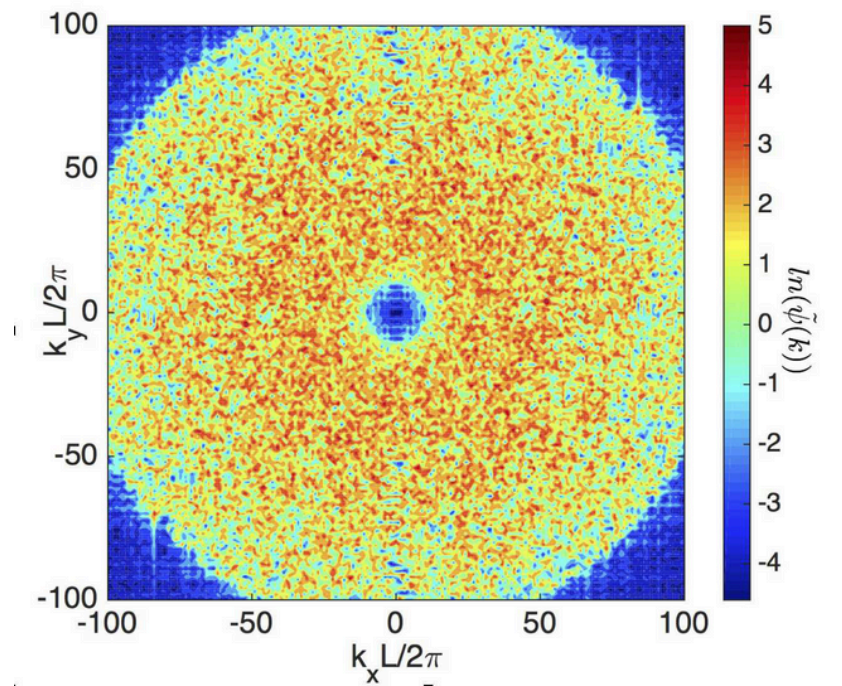
## The Structure Factor

- Equivalently, one can derive from internal correlation and fourier transform [Tor18] that hyperuniformity may be characterized by a vanishing structure factor for small wave vectors

$$\lim_{|k| \rightarrow 0} S(k) = 0$$

For a single periodic configuration with a finite number of  $N$  points, the structure factor is identical to [Tor18]:

$$S(k) = \frac{1}{N} \left| \mathcal{F} \left( \sum_{j=1}^N \delta(r - r_j) \right) \right|^2 = \frac{1}{N} \left| \sum_{j=1}^N \exp(ik \cdot r_j) \right|^2, k \neq 0$$



# Generating hyperuniform structures



# Generating hyperuniform structures

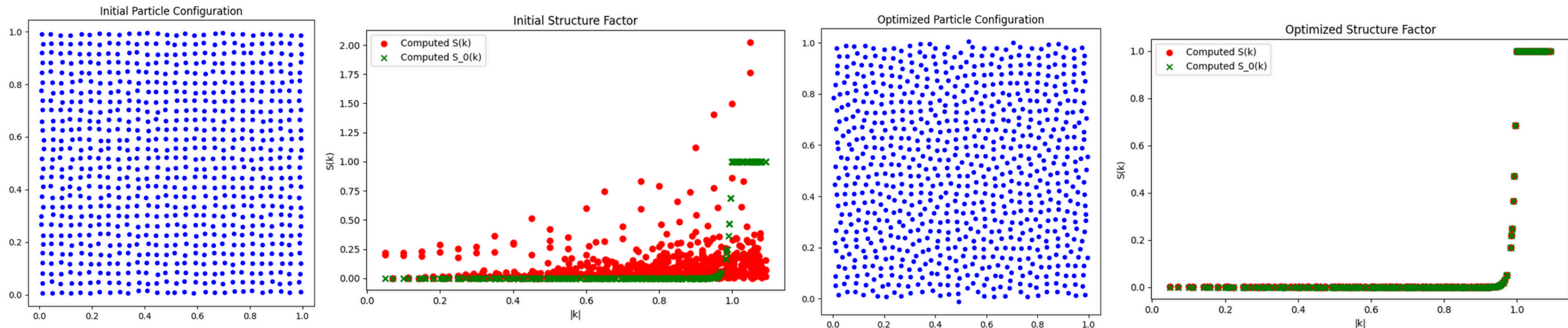
## HU point patterns

- We may use a method based on optimization [SSDV24] towards a given structure factor

$$\min_{r_1, \dots, r_N} \sum_k |S(k) - S_0(k)|^2$$

**Task:** generate different kinds of hyperuniform point patterns as in [SSDV24], Section II

- Current progress:
  - Some more testing needed for different  $S_0$  parametrizations



# Generating hyperuniform structures

## Scalable HU point patterns

- We want to generate large point patterns for later analysis
- In [SCM24] an scalable fft-based approach to generating HU point patterns is proposed

**Task:** generate larger point patterns using nuFFT and compare runtime to previous method

# Generating hyperuniform structures

## HU scalar fields

- Hyperuniformity can be extended to scalar fields
- We may be able to extend analysis of HU point patterns to analysis of HU scalar fields

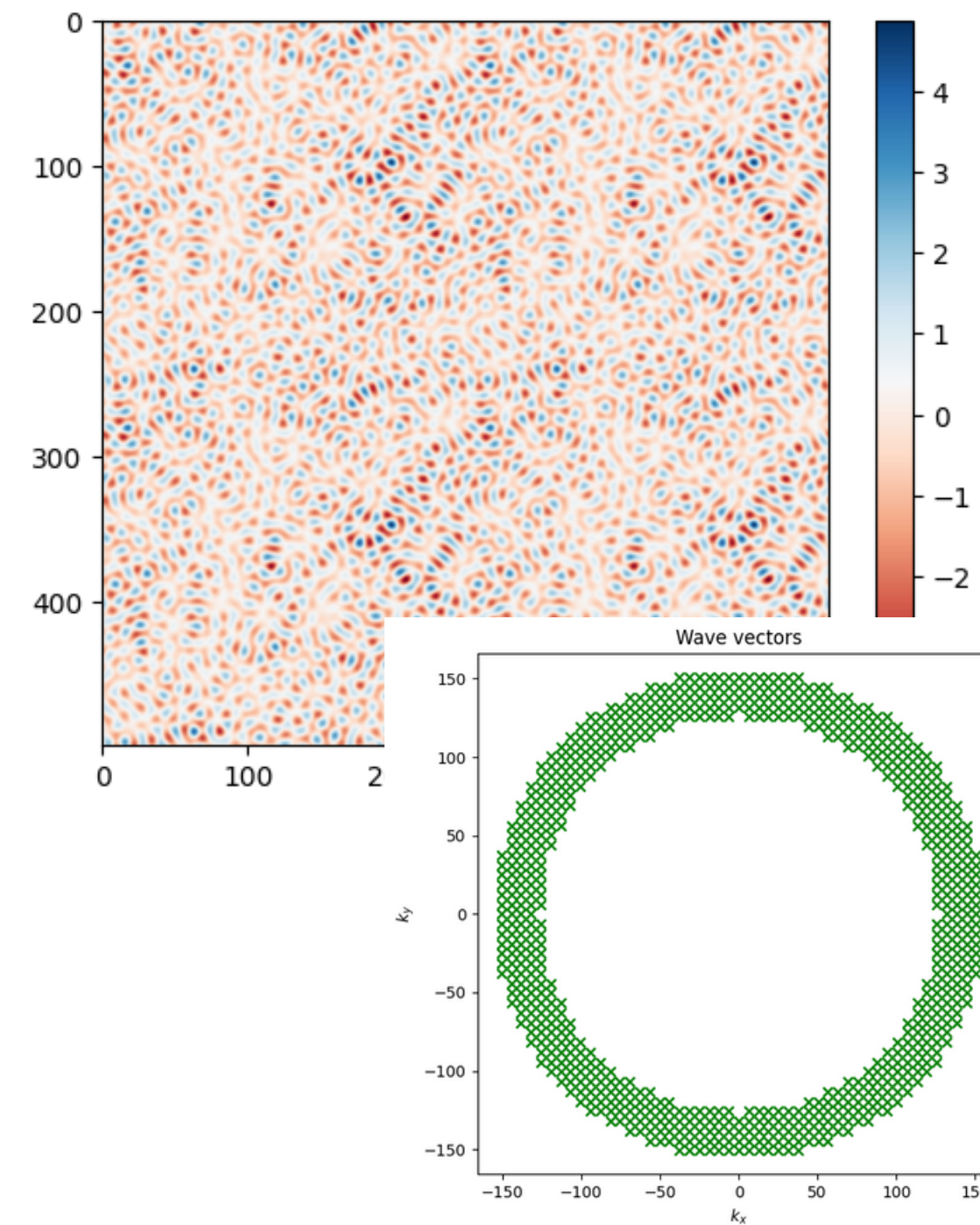
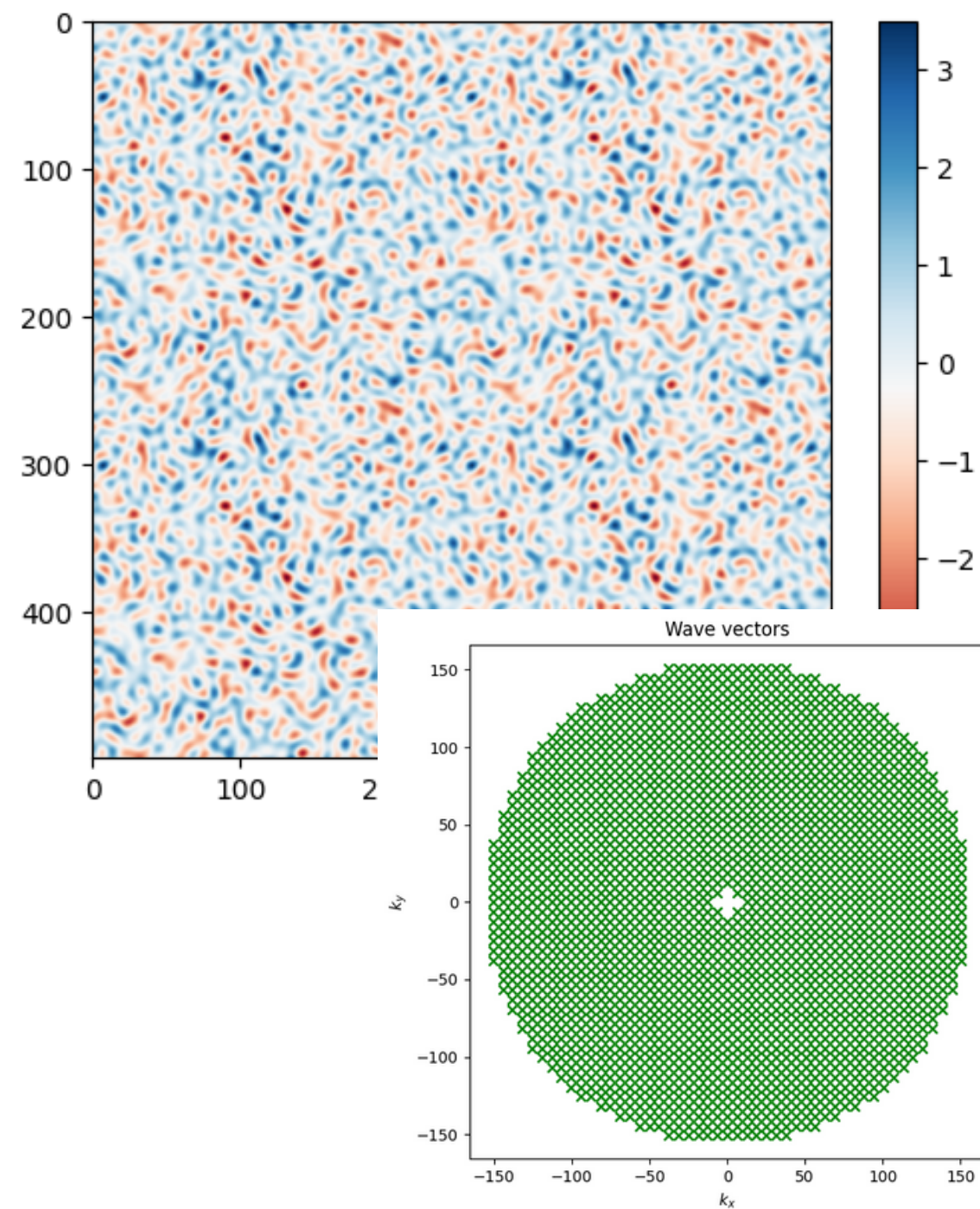
**Task:** Generate hyperuniform scalar field from a gaussian random field [MT17], Section III & IV

- Current progress:
  - Prototype: Able to generate gaussian random fields with a certain spectrum
  - We still use constant amplitude instead of an dynamic amplitude based on the wave vector  $k$



# Generating hyperuniform structures

## HU scalar fields



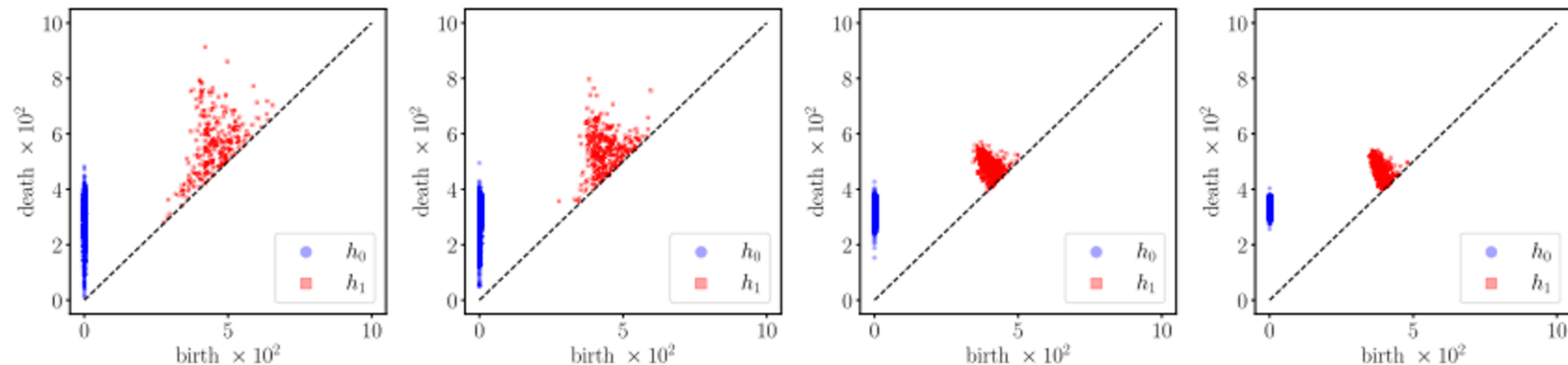
# Persistent homology and topological statistics of hyperuniform point clouds [SSDV24]

# Persistent homology [SSDV24]

## Persistent Homology and Topological Analysis

- A Vietoris–Rips complex is built by growing balls of radius  $r$  around each point
- Homological features are computed:  $h_0$  (connected components),  $h_1$  (loops)
- Persistence diagrams and histograms of death times are analyzed to capture topological features.

**Task:** Use *ripser* or *GUDHI* to compute persistent homology and analyze the resulting diagrams





# Persistent homology [SSDV24]

## Topological Comparison and Robustness to Finite Sampling

- Wasserstein distances  $W1, W2$  are used to compare persistence diagrams:
  1. Across different pattern parameters
  2. Between full systems and cropped subsets

$$W_p(A, B) = \inf_{\gamma} \left( \sum_{\mathbf{x} \in A} (\|\mathbf{x} - \gamma(\mathbf{x})\|_q)^p \right)^{1/p},$$

- The study shows that HU properties are preserved in subsets above a certain size

**Task:** Compare diagrams using Wasserstein distance, identify HU regions in parameter space, and analyze robustness to partial data

# Literature

- [Tor18] Salvatore Torquato. Hyperuniform states of matter. *Physics Reports*, 745:1–95, 2018. Hyperuniform States of Matter.
- [SSDV24] Marco Salvalaglio, Dominic J. Skinner, Jörn Dunkel, and Axel Voigt. Persistent homology and topological statistics of hyperuniform point clouds. *Phys. Rev. Res.*, 6:023107, May 2024.
- [MT17] Zheng Ma and Salvatore Torquato. Random scalar fields and hyperuniformity. *Journal of Applied Physics*, 121(24):244904, 2017.
- [SCM24] Aaron Shih, Mathias Casiulis, and Stefano Martiniani. Fast generation of spectrally shaped disorder. *Phys. Rev. E*, 110:034122, Sep 2024.