TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

MOD-SEM SuSe25

Topic 3 - Phase 1

Hyperuniformity

Generation of hyperuniform structures and their analysis

Contents -Phase 1

- Introduction to hyperuniformity
- Working plan: Generation of hyperuniform structures and their analysis
  - Generating hyperuniform structures
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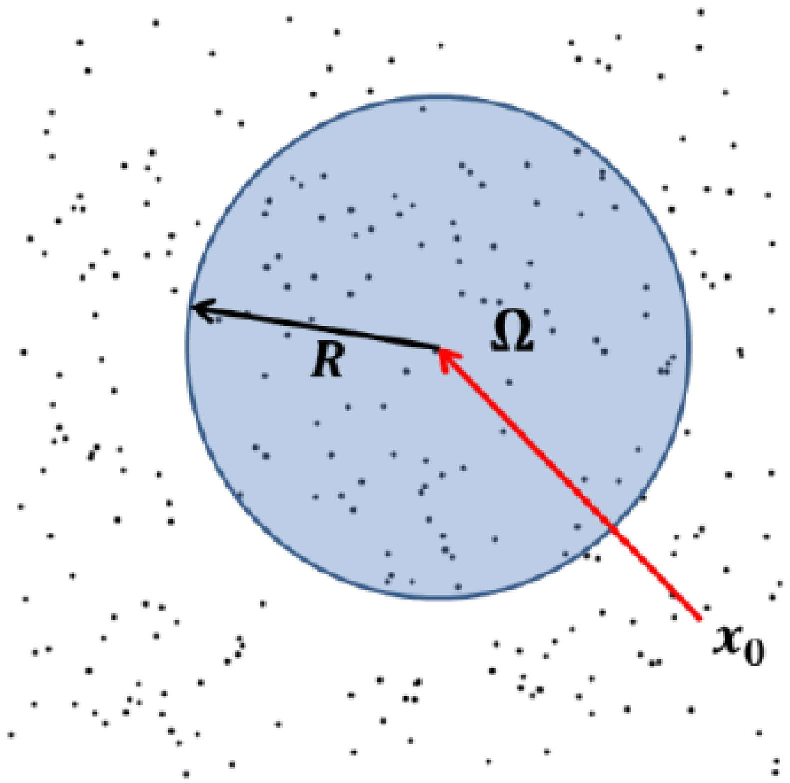
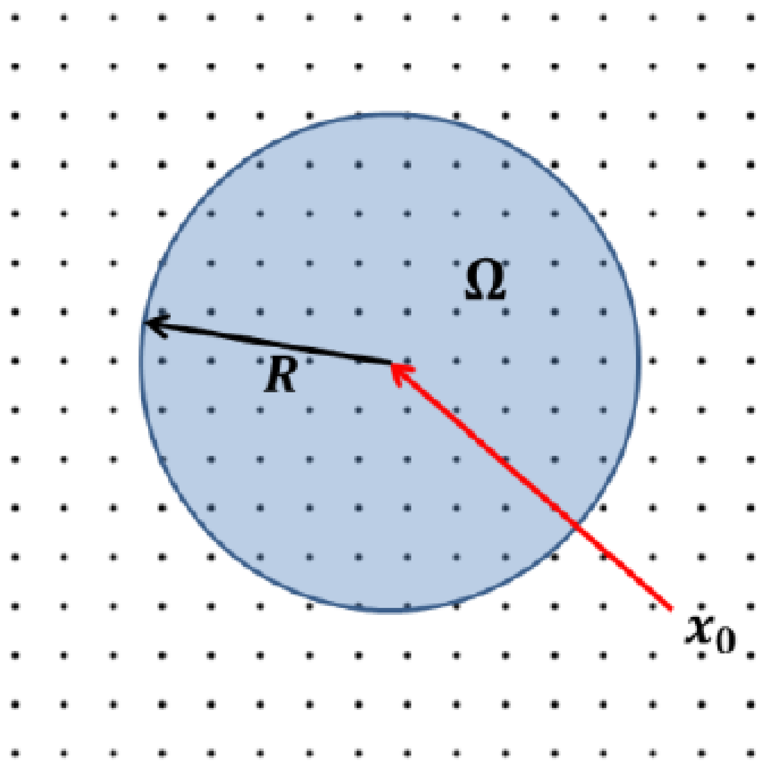
Introduction

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

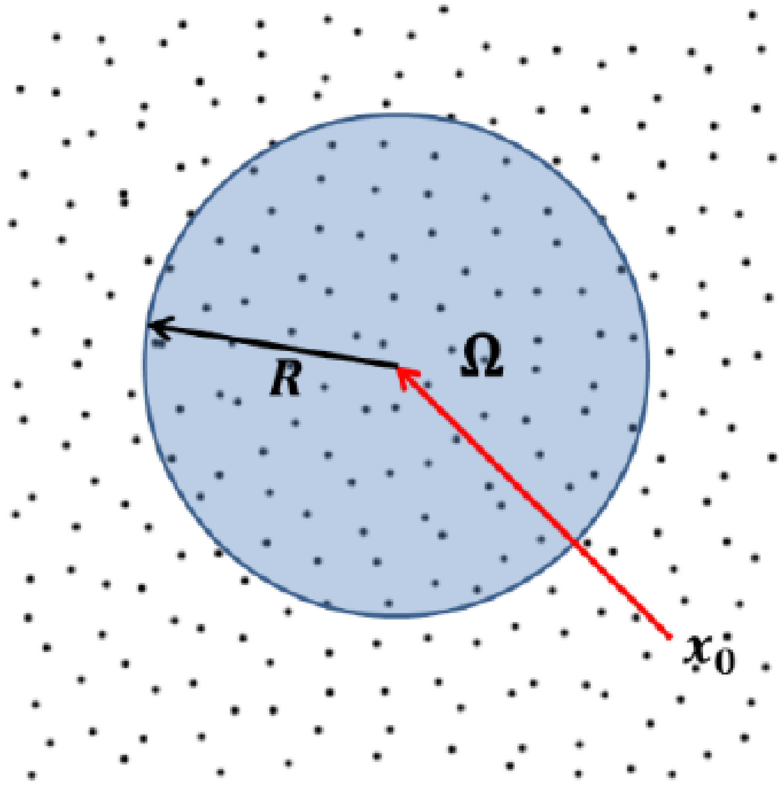
- The number variance inside an observation window grows more slowly than its radius:



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



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



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

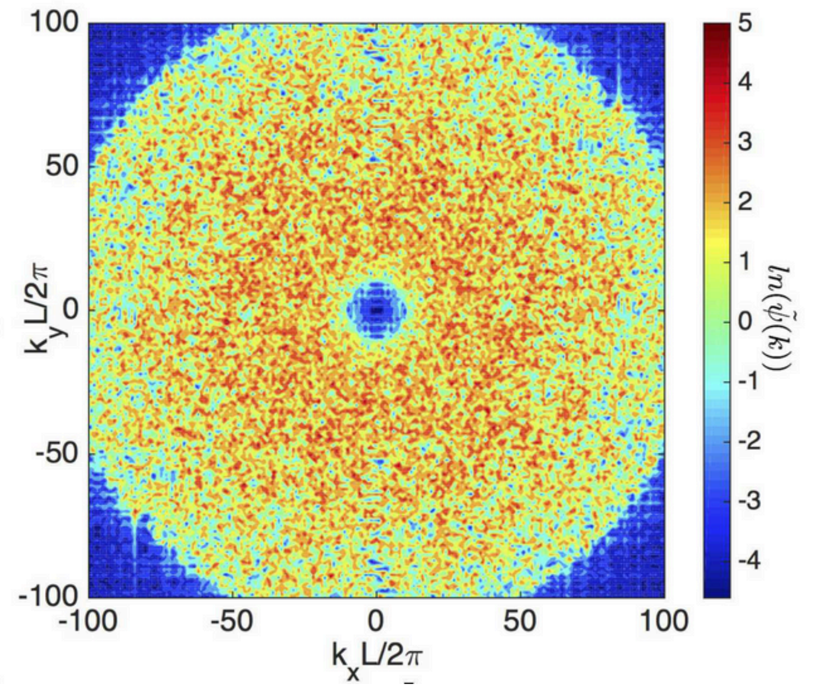
Introduction
The Structure Factor

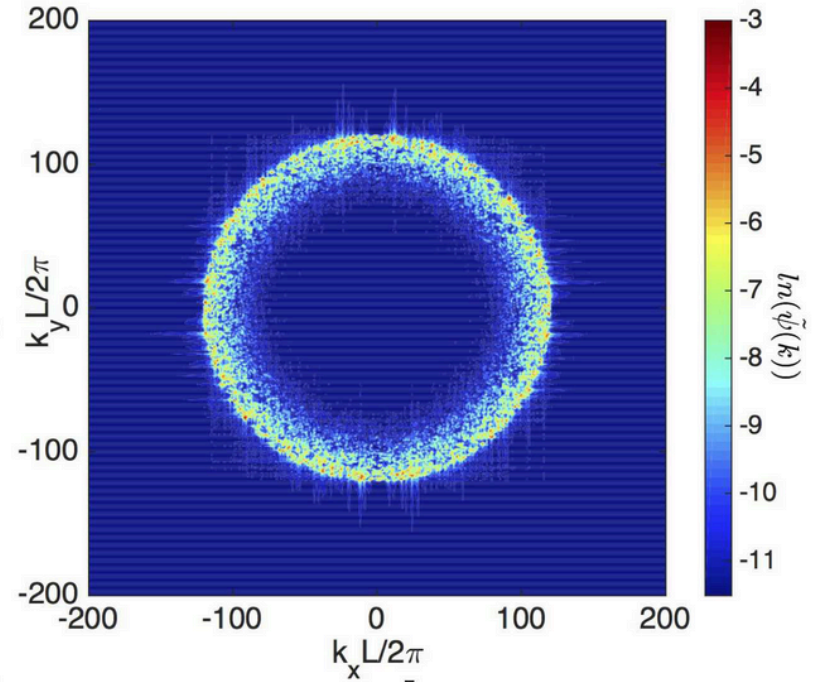
- Equivalently, one can derive from internal correlation and fourier transform [Tor18] that hyperuniformity may be characterized by a vanishing structure factor for small wave vectors

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

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

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





Generating hyperuniform structures

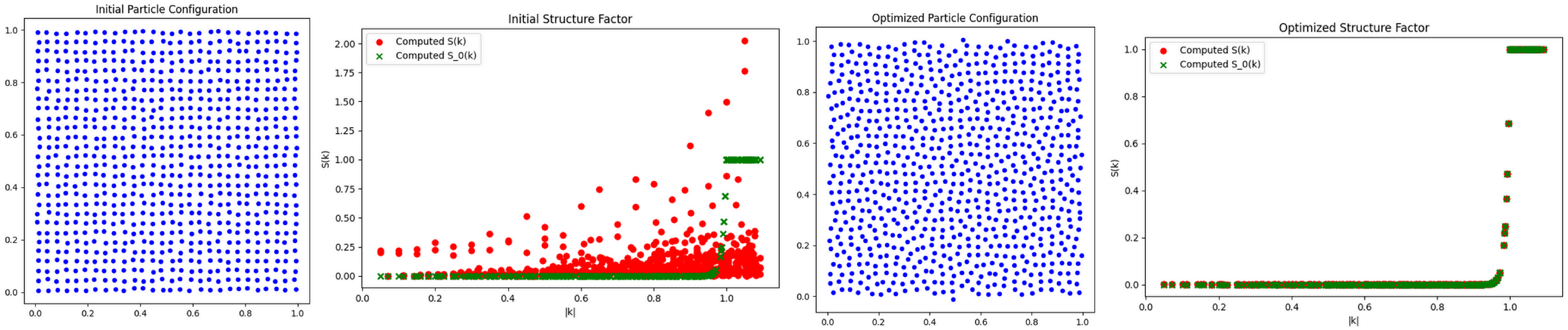
Generating hyperuniform structures
HU point patterns

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

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

<u>Task:</u> 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

<u>Task:</u> generate larger point patterns using nuFFT and compare runtime to previous method

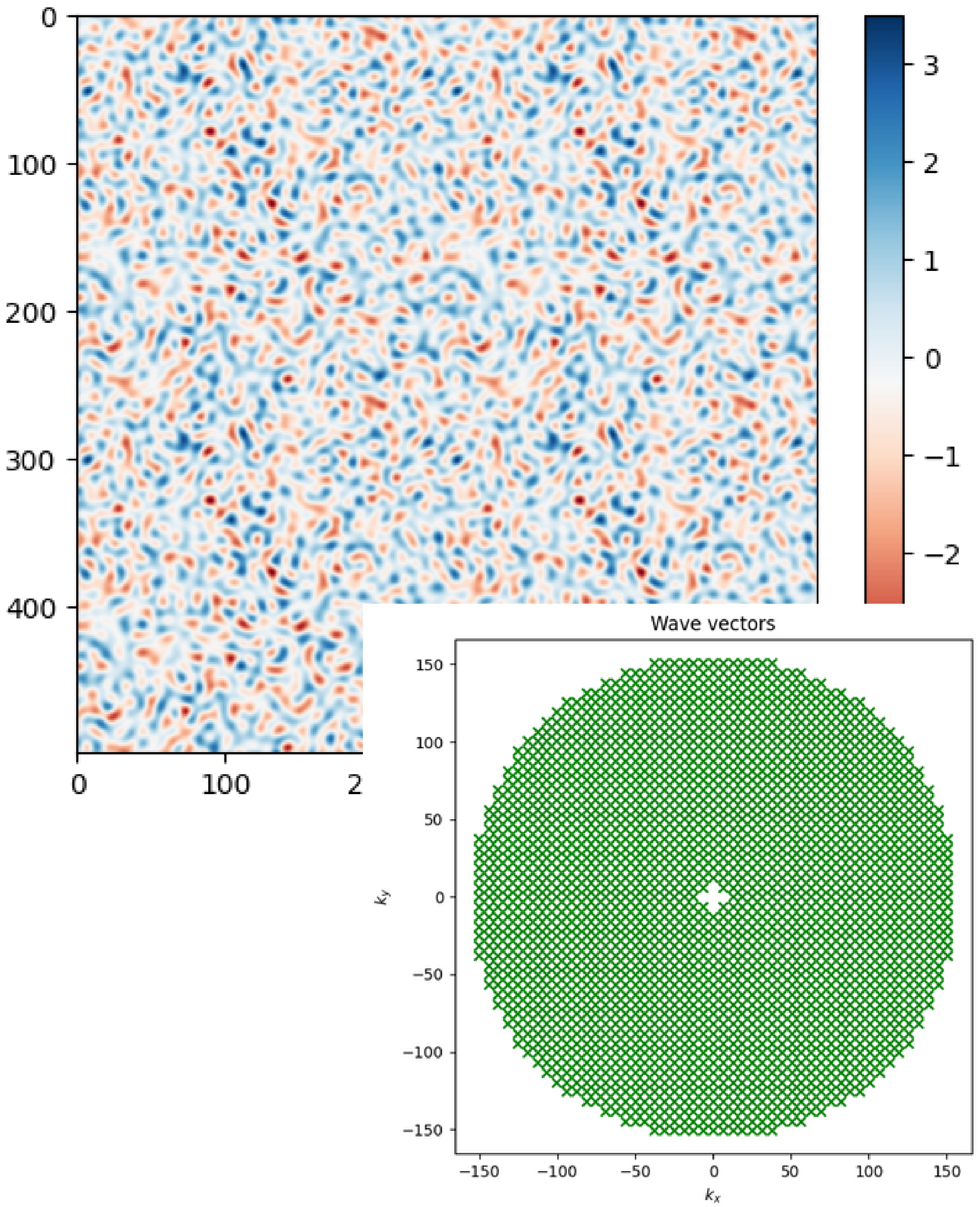
Generating hyperuniform structures
HU scalar fields

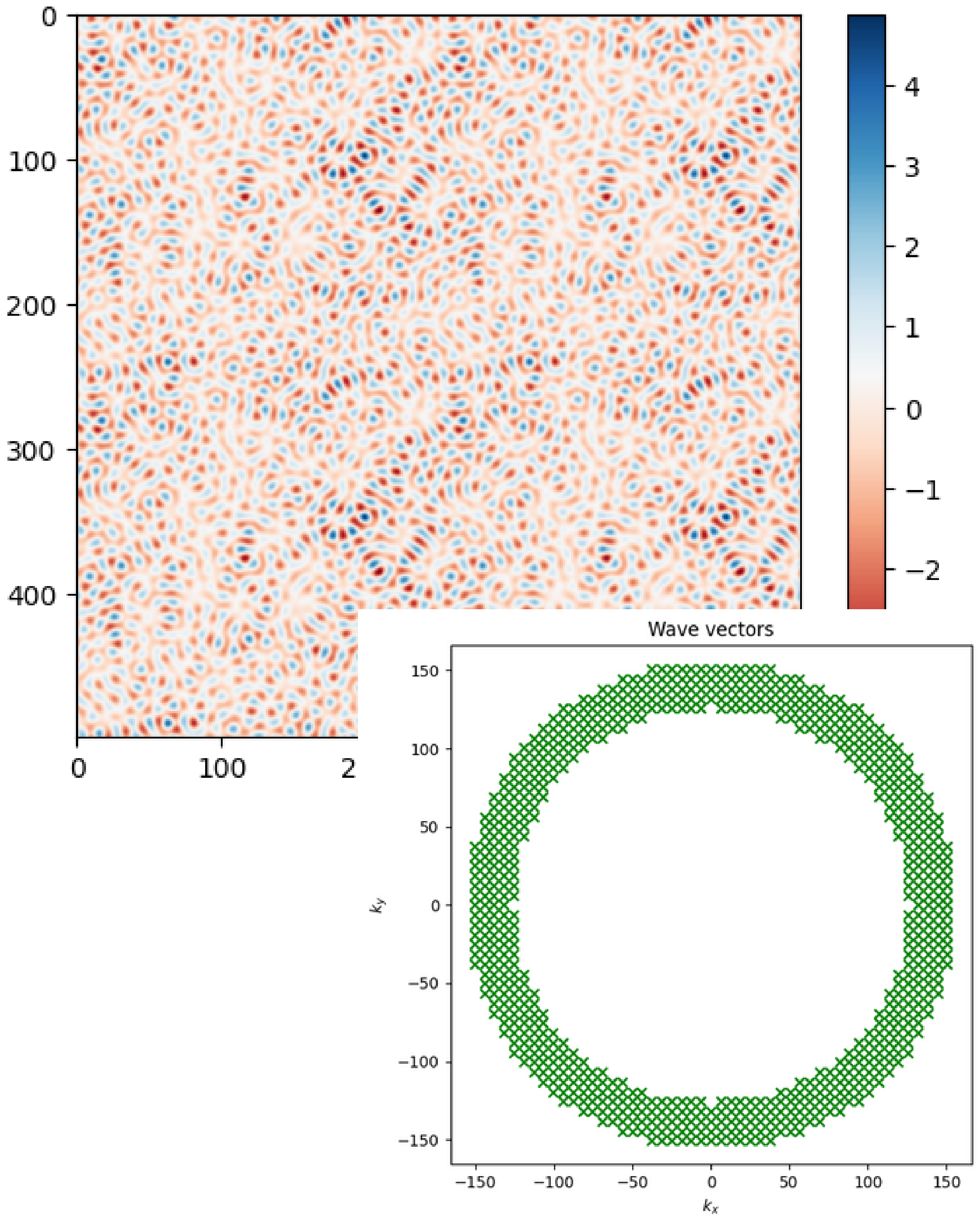
- Hyperuniformity can be extended to scalar fields
- We may be able to extend analysis of HU point patterns to analysis of HU scalar fields

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: *h0* (connected components), *h1* (loops)

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

<u>Task:</u> 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.