Master thesis project

Persistent homology analysis of phase transitions in glassy systems

Super-cooled or quenched liquids often assume amorphous states rather than crystalline states, meaning that many of the structural properties of the liquid are conserved despite the lowered mobility of the constituents; of particular importance is the lack of long-range structural order. Often, minor changes in the pre-cooling set up can swing the outcome of the quench either way. In other words, for many systems it is poorly understood, which physical and chemical properties are key to promoting one type of state over another.

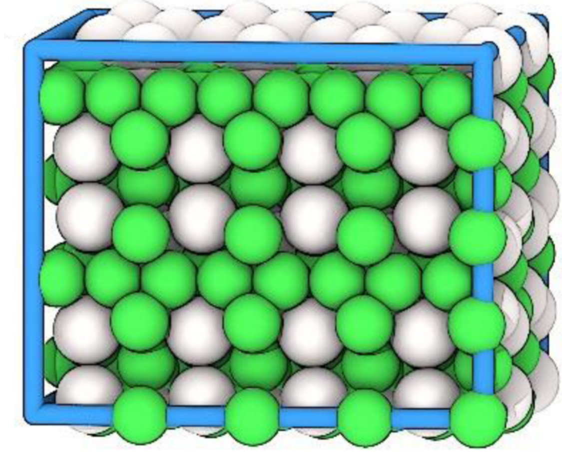


Figure 1: Simulated structure of an $MgZn_2$ crystal.

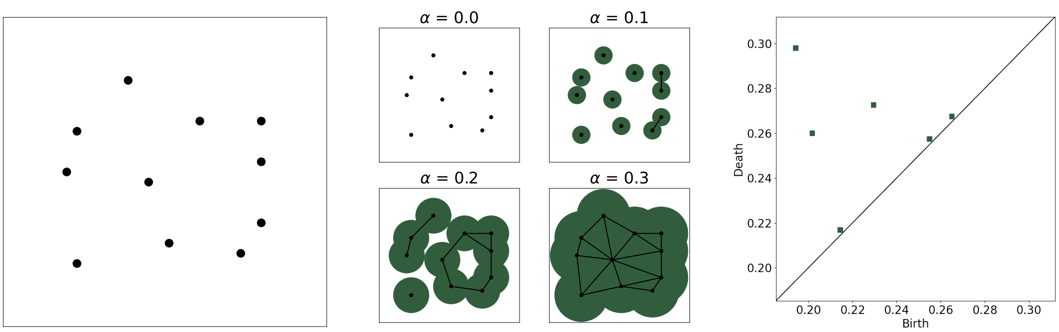
In this project, we aim to apply the ideas behind *topological data analysis* (TDA) to understand this type of transition and structural diversity. In particular, recent developments in applied topology have made the analysis method *persistent homology* attractive for applications in understanding such simulations. The method excels at quantifying key local topological motifs in structures such as the ones discussed here.

This project will focus on setting up appropriate simulations of glassy systems and their crystalline counterparts. After this step, the student will analyze these simulations using the aforementioned methods to understand the assembly and emerging local structure in these systems. In particular, we hope to elucidate which local motifs promote e.g. glassy structures or crystallization.

The student will get hands-on experience with:

- Applied topology and geometry
- Molecular simulations
- Thermodynamics of glassy systems
- Topological data analysis
- Homology groups and their applications
- High-performance computing methods

Martin Cramer Pedersen, Office D304, mcpe@nbi.ku.dk
Jacob Kirkensgaard, jjkk@nbi.ku.dk
Ulf Rørbæk Pedersen, urp@ruc.dk



(a) (b) (c)

Figure 2: In (a), a rendering of a point set of interest, the topology of which we wish to describe mathematically. In (b), we gradually increase the radius of the points and record when topological features emerge and disappear; thereby constructing the *alpha shape filtration* of the point set. For example, we observe that for $\alpha = 0.2$, a loop has appeared in our structure, which has disappeared for $\alpha = 0.3$. In (c), we gather the recorded information into a topological fingerprint of the structure; in this case the first persistence diagram containing information on the "birth" and "death" of loops in our structure. A total of six loops are formed and disappear again; the loop mentioned in the description of (b) gives rise to the point in the top-left part of the plot; as it is "born" at $\alpha \approx 0.195$ and "dies" at $\alpha \approx 0.295$.