Materials TDA and random/statistical topology

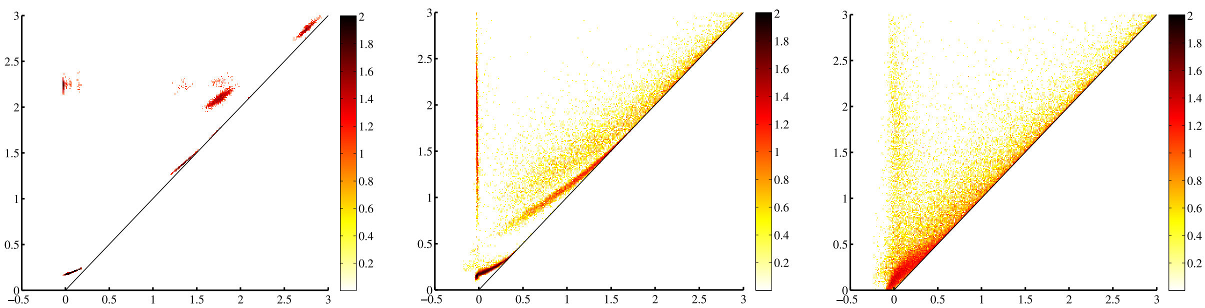
Yasu Hiraoka[1]

[1]*AIMR, Tohoku* University
hiraoka@tohoku.ac.jp

In this talk, I will briefly explain our recent activity of topological data analysis on materials science (e.g. [1,2]). Our main tool is the persistent homology, which is an emerging mathematical concept for characterizing shapes of data. In particular, it provides a tool called the persistence diagram that extracts multiscale topological features such as rings and cavities in atomic configurations and digital high dimensional images. I present a unified method using persistence diagrams for studying the geometry embedded in those data. Furthermore, I will also show a new framework of materials informatics by combining statistical and machine learning methods with persistence diagram.

Then, motivated from materials TDA project, I will also present a recent result [3] about convergence of persistence diagrams on stationary point processes in R^N. Several limit theorems such as strong laws of large numbers and central limit theorems for random cubical homology are also shown [4].

[1] Y. Hiraoka, T. Nakamura, A. Hirata, E. G. Escolar, K. Matsue, and Y. Nishiura. Hierarchical structures of amorphous solids characterized by persistent homology. Proceedings of the National Academy of Sciences of the United States of America 113 (2016), 7035–7040.
[2] Mohammad Saadatfar, Hiroshi Takeuchi, Nicolas Francois, Vanessa Robins, and Yasuaki Hiraoka. Pore configuration landscape of granular crystallisation. Nature Communications. 8:15082 (2017), DOI: 10.1038/ncomms15082.
[3] T. K. Duy, Y. Hiraoka, and T. Shirai. Limit theorems for persistence diagrams. arXiv:1612.08371.
[4] Y. Hiraoka and K. Tsunoda. Limit theorems for random cubical homology. arXiv:1612.08485.



Persistence diagrams of SiO2. Left: Crystal, Middle: Glass, Right: liquid.