Fall 2024

MATH 725-748: Independent Study I

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Math 725-748 – Fall 2024

Title: Applications of Computational Topology in Materials Science

Course Description: Computational topology is finding new and exciting applications in a variety of systems. The course will focus on applications in the field of materials science and will also include significant parts related to mathematical methods, data analysis, in addition to materials science.

Literature:

(available in the library or from the instructor)

1. Kaczynski, Mischaikow, Mrozek: Computational Homology; ISBN 978-1-4419-2354-7, Springer (2003)
2. Edelsbrunner, Morozov, Persistence Homology, in the Handbook of Discrete and Computational Geometry, Goodman, O'Rourk, Toth (editors), CRC Press (2017)
3. Allen, Tildesley: Computer Simulation of Liquids; ISBN 19-855645-4, Oxford (1991)
4. Selected research articles and reviews, including:
   - Albert, Barabasi, Rev. Mod. Phys. 74, 47 (2002)
   - Boccaleti etal., Phys. Reports 424, 175 (2006)
   - Morone etal, Physica A 516, 172 (2019)

Course Goals:

- Develop basic understanding of computational topology;
- Develop familiarity with the outstanding issues in materials science that could be considered using the methods emerging from computational topology.

Course Outcomes:

- Ability to work with existing computational topology software packages and interpret the results;
- Ability to start working on research projects involving analysis of the data obtained in simulations and experiments of materials science systems.

Grading policy:

Class Participation: 30%;
Midterm Project: 30%;
Final Project: 40%.

Course Outline

Week 1: Basics of Computational Topology

Week 2: Persistent Homology: Introduction

Week 3: Graph Theory & Persistent Homology on Graphs

Week 4: Computing Persistence on Graphs

Week 5: Persistence: Application to Image Processing

Week 6: Persistent Topology of Materials Systems;

> **Midterm Report**: Analysis of software packages for persistence computations with application to test data sets

Week 7: Modeling Materials using Discrete Element Methods (DEM)

Week 8: DEM applied to Repulsive and Cohesive Particulate Systems

Week 9: Graphs in Particulate-based Materials Systems

Week 10: Persistence Diagrams for Two and Three Dimensional Data Sets

Week 11: Extensions of Persistence diagrams: Persistence Landscapes

Week 12: From Graphs to Images: Application of Persistence to Experimental Data

Week 13: Introduction to K-core Analysis of Materials Systems

Week 14: Final Project: Computing Persistence Diagrams of K-cores