

THE UNIVERSITY



OF HONG KONG

Department of Mathematics

## Seminar

# The Magical Journey from Structural Biology to Semi-Definite Programming

**Dr. Mingxu HU**

Shenzhen Medical Academy of Research and Translation, Frontier Research Center for Biological Structures at Tsinghua University

Date: October 20, 2023 (Friday)

Time: 5:00 - 6:00pm

Venue: Room 210, Run Run Shaw Bldg., HKU

### Abstract

Since the discovery of the DNA helix's role in genetic information storage and transmission, structural biology has become pivotal in biology. The 2015 “resolution revolution” in cryogenic electron microscopy (cryo-EM) significantly advanced structural biology, making the determination of biological macromolecule structures more routine and greatly enhancing our understanding of biological principles and targeted drug development. Cryo-EM combines numerous transmission images to derive high-resolution 3D structures of these macromolecules. While their inherent symmetry aids in interpreting images from multiple perspectives, processing that incorporates this symmetry can obscure asymmetric features. Addressing this, we introduce a novel method to determine orientations with molecular symmetry. By applying non-unique games tools, we simplify our non-convex formulation into a semi-definite programming problem and present a new rounding procedure for representative value determination. Our experiments show this approach reliably finds global minima and accurate representatives. We've made our method available as the open-source Python package, pySymStat. Using pySymStat, we successfully visualized an asymmetric feature in an icosahedral virus, a task conventional 2D classification in RELION couldn't achieve.

*All are welcome*