

### THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

## **Department of Mathematics**

# PHD STUDENT SEMINAR

# Detect conformation change by template matching in cryo-em images

By

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#### **Abstract**

Cryo-EM detects protein conformations froze in solution, and thus provides a promising way to characterize these conformational changes. In order to detect the conformational change, we developed a new algorithm to obtain multiple conformations and their populations from Cryo-EM datasets. In our algorithm, we constructed our "basis set" (as templates) by applying Molecular Dynamics (MD) simulations to widely search the conformational space, and then perform the fast assignment of experimental Cryo-EM 2D images to a set of reference 2D images generated by these basis-set structures. We find that our algorithm holds promise to be widely applied to elucidate the dynamic ensemble of protein conformations from Cryo-EM datasets.

Date: 14 May 2020 (Thursday)

Time : 5:00pm – 6:00pm

Zoom Meeting: <a href="https://hkust.zoom.us/j/98675423362">https://hkust.zoom.us/j/98675423362</a>

All are Welcome!