

THE HONG KONG UNIVERSITY OF SCIENCE & TECHNOLOGY

Department of Mathematics

PHD STUDENT SEMINAR

PF-ABGen: A Reliable and Efficient Antibody Generator via Poisson Flow

By

Miss Chutian HUANG

<u>Abstract</u>

An antibody is a special type of protein in the immune system to recognize and neutralize pathogenic targets, including bacteria and viruses. Antibody design is therefore valuable for the development of new therapeutics, while experimental- based methods are generally inefficient and expensive. Despite the fruitful progress in protein design with generative neural networks, including diffusion models, they still suffer from high computational costs. In this work, we propose **P**oisson **F**low based **AntiBody Gen**erator (PF-ABGen), a novel antibody structure and sequence designer. We adopt the protein structure representation with torsion and bond angles, which allows us to represent the conformations more elegantly, and take advantage of the efficient sampling procedure of the Poisson Flow Generative Model. Our computational experiments demonstrate that PF-ABGen can generate natural and realistic antibodies in an efficient and reliable way. Notably, PF-ABGen can also be applied to antibody design with variable lengths.

Date : 3 May 2024 (Friday) Time : 2:00pm Venue : Room 5562 (Lifts 27/28)

All are Welcome!