

國立中山大學應用數學系

學術演講

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講題：Computational methods for noisy high-dimensional images and application to Cryogenic Electron Microscopy (cryo-EM) workflow

時間：2021/03/04（Thursday）14:10 ~ 15:00

地點：理學院四樓理 SC 4009-1 教室

茶會：13:30 於理 SC 4010 室（系辦公室）

Abstract

Due to the recent advancement of GPU-accelerated computations and algorithms, cryo-EM has become an essential instrument for determining the 3D structures of macro-molecules at near-atomic resolution. Remarkably, the first dynamic movie of 2019-nCoV Spike trimer structure is derived from cryo-EM within 12 days using computational methods. This further demonstrated that cryo-EM had been a powerful technique with high efficiency to provide crucial medical insight for developing vaccines or drugs. However, the data characteristics of cryo-EM images include strong noise, huge dimension, large sample size and high heterogeneity with unknown orientations, have made analysis and inference very challenging. In the literature, dimension reduction and clustering play an essential role in overcoming the challenges above. The traditional methods employed in the field, however, are starting to encounter bottlenecks either in computation or performance due to the fast-growing rate of automatic data acquisition. In this talk, I will first address the importance of cryo-EM image processing in structural biology and the challenges of processing the dataset. Second, I will discuss our proposed dimension reduction strategy called two-stage dimension reduction (2SDR) and clustering approach called DRMRA, which alleviate the computation burden and improves performance over existing methods. Specifically, I will elaborate on utilizing our computational methods to enhance the workflow and present a unified framework that enables us to select the best processing steps to deliver a reliable 3D initial model and push the final resolution. Based on the initial model, I will describe how to perform 3D conformation analysis and enhance the results. Finally, future research directions in 3D conformation analysis will be given.

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