

CryoEM image processing using ASGC integrated environment

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CryoEM single particle analysis often needs millions individual particles to successfully reconstruct the 3-dimensional map of interest target. High performance computational resources play crucial roles in accelerating 3D EM map reconstructions. With the implementation of powerful Nvidia graphic cards in popular cryoEM software such as RELION and cryoSPARC, time to obtain refined and sharpened 3D map has been significantly reduced. Although both software and hardware are highly improved to reduce time for whole reconstruction process, accessing high-end GPU workstation or large-scale CPU cluster remains as major problem for users. It might be affordable for one laboratory to build its own GPU workstations or min-sized clusters, however, substantial routine management and issues of cyber security will be the burden for a 5-10 person laboratory. Moreover, monster-scale data transfer and storage of cryoEM dataset (1-4TB) will be the headache of each laboratory to maintain high-speed bandwidth and enough backup space.

The Academia Sinica Grid Center (ASGC), the first tier 1 level grid center in Asia, is proud to provide cloud computation for the cryoEM society in Taiwan. The ASGC team closely collaborates with cryoEM users at Academia Sinica to build grid instances for cryoEM-related computation including 3 most popular software: RELION, cisTEM and cryoSPARC, supported by 200+ CPUs, 64+ GPUs and 1TB+ memory in total. Currently, 8 RELION 2, 8 RELION 3, 10 cisTEM, and 2 cryoSPARC instances are available for public. There will be more grid instances for cryoEM-related software built in the near future. This talk will briefly describe the system environment, user application, workflow and benchmarks of cryoEM software at ASGC.

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