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Grid computing and cryo-EM

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Throughout the last 25 years, single particle cryo-electron microscopy (cryo-EM) has continuously evolved into a powerful modality for determining the 3D structure of radiation-sensitive biological macromolecules, culminating in the award of the recent Nobel prices in Chemistry 2017. This development has been enabled by constant maturation of image processing algorithms in concert with the emergence of direct electron detectors, improvements in electron optics, stage stability and microscope automation, resulting in ever-growing image data volumes. I will give a brief overview of the state-of-the-art single particle cryo-EM workflow and the process of 3D reconstruction from images. Although the data volume generated by a single modern cryo electron microscope is still far from what detectors in particle physics produce each day, the growing interest and combined word-wide deployment of these facilities have already created bottlenecks in data storage and processing capacity. I will outline the resulting challenges faced by cryo-EM labs, describe the current modus operandi and a road map to grid computing in this field, which may enable institutions without expensive local infrastructure to benefit from distributed compute resources.

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