Cryohub: A User-Friendly, Web-Based Platform for Command-Line Scientific Research Tools Specializing In Cryo-EM Analysis

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Recent improvements in software design and computing infrastructure have driven the integration of computational tools and conventional laboratory science. However, many software tools are designed to run in the command line interface (CLI) and are not straightforward for bench scientists to use. These programs can not only be difficult to use but also very computationally demanding, especially those involving high-throughput data processing. Cryogenic electron microscopy (cryo-EM) dataset processing serves as a prime example of this; high quality cryo-EM protein structures provide invaluable information to structural biologists, yet most free cryo-EM software remains challenging to implement. The disparity between software engineers and bench scientists inhibits research efforts and often results in powerful tools not reaching their full potential.

CryoHub offers a solution to this problem by providing an interactive, informative, web- based GUI to manage CLI jobs. It aims to streamline the process of submitting CLI jobs to a computing cluster by displaying a curated list of program options, with descriptions for user clarification, and queueing the job on behalf of the user. CryoHub not only assists in submission of CLI jobs but also allows for observation of job status and visualization of various output file types. The flexible backend framework allows for plugin of many CLI tools with minimal effort. We ultimately hope to improve the flow of scientific research by simplifying the use of software tools for bench scientists.