

18th LCDS meeting: Electron Nanoscopy & Data Science

Abstracts

Single Particle Analysis cryo-EM Image processing - Dr Roman Koning (LUMC)

In Single Particle Analysis cryo-EM from many different projection images, containing identical protein molecules, 3D reconstructions can be made and atomic models can be calculated. An introduction of cryo-EM, a short overview of methods and recent developments in the field will be discussed, while computational aspects and needs will be explained.

LLSC: A cluster computer for bio-science - Dr Kristian Rietveld (LIACS)

The LIACS Life Science Cluster (LLSC) is a cluster computer that is used for the development and deployment of bio-science software. Examples include tomographic reconstruction, OPT image reconstruction, DNA analysis and High Throughput Screening. By means of parallelization across multiple compute nodes we aim to increase the performance and throughput of such software. Furthermore, we are working to provide smart and easy-to-use user interfaces for the end users that automate upload of data to the cluster and execution of compute jobs. In this talk, we will describe the architecture of the LLSC and discuss several applications that have been realized on the LLSC. We conclude by sketching our vision and aims for the (near) future.

A semantic-based metadata validation for an automated High-Throughput Screening workflow: Case study in CytomicsDB - Dr Enrique Larios (LIACS)

High-Throughput Screening (HTS) techniques are typically used to identify potential drug candidates. These type of experiments require to invest in large amounts of resources. The appropriate data management of HTS experiments has become a key challenge in order to succeed in the target validation. Current developments in imaging systems have to cope with computational requirements due to the significant increment of volumes of data. However, no special care has been taken to ensure the consistency, integrity and reliability of the data managed in HTS experiments. The appropriate validation of the data used in an HTS experiment has turned to be a key success factor in the target validation, thus a mandatory process to be included in the HTS workflow. This paper describes our research in the validation process as performed in CytomicsDB. This system is a modern RDBMS-based platform, designed to provide an architecture capable of dealing with the strict validation requirements during each stage of the HTS workflow. Furthermore, CytomicsDB has a flexible architecture which supports easy access to external repositories in order to validate experiments data.