EXTENDING TANGO CONTROL SYSTEM WITH KEPLER WORKFLOW, PRESENTED ON AN X-RAY CRYSTALLOGRAPHIC APPLICATION

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Abstract

Nowadays there is a growing need for user friendly workflow editors in all fields of scientific research. A special interest group is present at big physics research facilities where instrumentation is mostly controlled by a robust and reliable low level control software solution. Different types of specific experiments using predeter-mined automated protocols and on-line data processing with real-time feedback require a more flexible and ab-stract high level control system[1]. Beside flexibility and dynamism, easy usability is also required for researchers collaborating from several different fields. Tentatively, to test the ease and flexible usability, the Kepler workflow-engine was integrated with TANGO[2]. It enables researchers to automate and document experiment protocols without any programming skill. The X-ray crystallography laboratory at the Biological Research Center of Hungarian Academy of Science (BRC) has implemented an example crystallographic workflow to test the integrated system. This development was performed in cooperation with ELI-ALPS.

TANGO – Kepler Integration

A generic Tango Client has been integrated into Kepler workflow environment. It is browsing the Tango Database and enables an intuitive configuration to have access to instrumentation services. By integrating instrument control with online data analysis in the same workflow, users can easily build or modify their experiment protocols in Kepler. The created workflow serves as a documentation of the experiments performed and supports reproducible science by facilitating the reproduction of the experiment and the related data analysis steps.

Virtual Beamline Simulator

Virtual reality allows testing for potential collision during the movement of a planned trajectory of instrumentation. This information can be used to verify if the planned experiments can be performed and enables their optimization. Applying path finding algorithms can allow users to easily move between experiment setups without being distracted by planning and carefully executing complex trajectories.

Instrument Monitoring

VBS comes with a Tango control interface and mimics all instrumental motions. The virtual reality scene is configured to match hardware setup and allows the automatic adjustments of the configuration settings if appropriate calibration procedure is set up. The 3D scene enables users to investigate the geometry of the experiment remotely.

Collision Avoidance

Virtual reality allows testing for potential collision during the movement of a planned trajectory of instrumentation. This information can be used to verify if the planned experiments can be performed and enables their optimization. Applying path finding algorithms can allow users to easily move between experiment setups without being distracted by planning and carefully executing complex trajectories.

Kappa Strategy

After the analysis of initial diffraction patterns which provides the current orientation of the crystalline sample, optimal data collection strategy can be computed which may require the reorientation of the sample between data collection scans. Kepler supports the design of such complex experiments where instrument control and online data analysis must be coupled into one workflow.

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