

The Grid-enabled NMR spectroscopy.

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The laboratory equipment used for experimental work is very expensive and unique as well. Only big regional or national centers could afford to purchase and use it, but on a very limited scale. That is a real problem that disqualifies all other research groups not having direct access to these instruments. Therefore the proposed framework plays a crucial role in equalizing the chances of all research groups.

The Virtual Laboratory (VLab) project focuses its activity on embedding laboratory equipments in grid environments (handling HPC and visualization), touching some crucial issues not solved yet. In general the issues concern the standardization of the laboratory equipment definition to treat it as a simple grid resource, supporting the end user under the term of the workflow definition, introducing the accounting issues and prioritizing jobs which follow experiments on equipments. Nowadays, we have a lot of various equipments, which can be accessed remotely *via* network, but only on the way allowing the local management console/display to move through the network to make a simpler access. To manage an experimental and post-processing data as well as store them in a organized way, a special Digital Science Library was developed.

The project delivers a framework to enable the usage of many different scientific facilities. The physical layer of the architecture includes the existing high-speed network like PIONIER in Poland, and the HPC and visualization infrastructure. The application, in fact the framework, can be used in all experimental disciplines, where access to physical equipments are crucial, e.g., chemistry (spectrometer), radio astronomy (radio telescope), and medicine (CAT scanner). The poster presentation will show how we deployed the concept in chemistry, supporting these disciplines with grid environment and embedding the Bruker Avance 600 MHz and Varian 300 MHz spectrometers.

For more information please visit our webpage at: <http://vlab.psnc.pl/>.