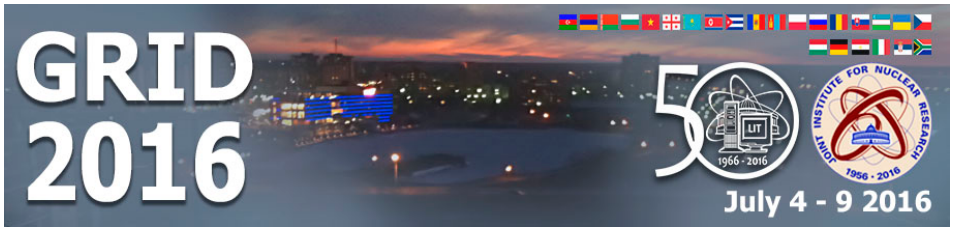

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Using General Lattice Program on the desktopgrid systems

Tuesday, 5 July 2016 14:30 (15 minutes)

The prediction of the crystal structure is an important area in the chemistry and physics. There are many software implementations for solving this problem. The report contains the overview of the main implementations. The specific theme of the report is to adapt the application GULP to the infrastructure.
The General Utility Lattice Program (GULP) is designed to perform a variety of tasks based on force field methods. The report contains the description of specifics of the functioning GULP application and various approaches to adapt it to the BONC system. Description of the experimental computing and various approaches to automated analysis of the calculation results and the generation of new jobs. The report contains recommendations on the organization of calculations of this kind.

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