The introduction of HunGrid and its application for air pollution forecast

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The purpose of this article is to introduce the Hungarian Virtual Organisation, HunGrid, established within the EGEE project. The article briefly reviews the current infrastructure of EGEE, with more than 9000 processors the largest Grid of the world. The most important components of the EGGE Grid middleware (LCG-2) are also exposed. The article also touches the role and organisation of the virtual organisations (VO), then continues to fully introduce the development of the Hungarian VO, the set up of HunGrid and the infrastructure of the participating institutions, respectively.

HunGrid is not simply a virtual organisation of LCG-2, rather more than that, containing new elements not listed in the original LCG-2 system. Such expansions are the P-GRADE Grid portal and the Mercury Grid monitor. P-GRADE Grid Portal works out the web-based entry point of HunGrid, through which one can use HunGrid without the need of learning long and difficult commands. The portal allows the users to easily create and run complex workflow applications on HunGrid. With the help of Mercury Grid the realisation of monitoring parallel Grid applications at process-level comes true.

The article introduces how to put HunGrid in practice for the potential users, including the process of obtaining the necessary Grid licenses. HunGrid can be dynamically expanded with any university or academic resources. The article describes the method of joining for the participating institutions. According to the current plans, the article would like to provide information through the demonstration of a generic image, on the future organisation of HunGrid, realising the full Hungarian LCG-2 based Grid, which is open for all who does academic research or education.

In this decade the Grid systems are becoming more and more popular in natural science. In such systems, large number of heterogeneous resources can be interconnected in order to solve complex problems. One of the main aims of a joint national project, ”Chemistry Grid and its application for air pollution forecast” is to investigate the Grid as a high performance computational infrastructure and to find practical results in the field of chemistry.

MTA SZTAKI has elaborated a family of development tools, called P-GRADE, P-GRADE portal and MERCURY that support the reengineering process of sequential and also legacy applications in an efficient and clear way by means of their high level graphical approach as well as the performance debugging and execution of applications on parallel and Grid platforms. As a new achievement, these tools support the creation of workflow to execute complex programs in various Grids. The presented tools are available for Hungarian universities and academic institutes to easily parallelise sequential simulations having high computational demands and afterwards to make them run on Grid systems including the new HUNGRID as well.

As a joint effort of MTA SZTAKI and Department of Physical Chemistry, Eötvös University (ELTE), P-GRADE, P-GRADE portal and MERCURY monitoring system have been successfully applied to make grid-enabled an existing simulator for chemical reactions-diffusion-advection systems in the frame of the chemistry Grid project. The developed application can be accessed via P-GRADE portal, where each component (parallel or sequential job) is able to collaborate in the Grid based on P-GRADE workflow concept to provide efficient air pollution forecasting e.g. in case of the dispersion of radioactive nuclides.

Furthermore, in this paper we briefly introduce the fundamentals of reaction-diffusion-advection systems and their simulation with P-GRADE programming environment and P-GRADE portal in details through the design, the performance analysis and execution phases. Furthermore, the experimental results of executions on HUNGRID are also presented in order to demonstrate the efficient use of P-GRADE portal.