

## **Chemistry Grid and its application for air pollution forecast**

Recently, Grid systems are becoming more and more popular. In such systems, large number or very powerful resources are interconnected in order to solve complex problems. The aim of this project is to investigate three important aspects of Grids and to achieve practical results in those areas. These aspects are as follows.

*(a) Establishment of a Chemistry Grid: using the Grid for supporting a specific science area.* One of the goals of this project is to provide access for chemist partners for both the Hungarian computational Grid resources (Hungarian Cluster Grid) and the European wide chemistry Grid infrastructure being established as a result of the EU funded COST project called SYMBEX.

*(b) The Grid as a very high performance computational resource.* The MTA SZTAKI Research Institute has elaborated a unique integrated parallel program development environment, called P-GRADE, that supports the parallelization process of sequential applications in a very efficient and convenient way by means of its high level graphical user interface and special correctness and performance debugging and analyzing tools. In this project, we will further develop P-GRADE to provide dedicated support for efficient execution of parallel programs in Grids, i.e. we want to solve the problem of migrating the application across the Grid resources according to the actual load and availability conditions. The P-GRADE system will be used by all chemist partners, within both the current and the related SYMBEX project, to parallelize their sequential applications with high computational demand and to run them afterwards in Grids.

*(c) The Grid as an informatics system for supporting complex collaborative work and its application for air pollution forecasting (elaboration of smog alarm plans). We will elaborate a collaborative application that will run on a supercomputer to forecast air pollution in Hungary in an operative manner. The same application will be run on Grid as well to simulate former smog events and to analyze the efficiency of smog alarm plans and the prospective effects of various potential measures against air pollution. The application will also serve as a demonstrative example showing how complex collaborative problems can be efficiently solved by means of Grid.*