

## **Supporting Anti-cancer Drug Discovery by a Private SZTAKI Desktop Grid System**

**Jozsef Kovacs**

MTA SZTAKI, Hungary

SZTAKI Desktop Grid (SZDG) is an extension of BOINC in order to make it more flexible, versatile and scalable. BOINC infrastructure gives the possibility to gather huge amount of resources to run computation, while SZDG - through a set of tools - provides a framework to ease application development, porting and workunit creation. In the CancerGrid EU FP7 project a private Desktop Grid infrastructure has been built based on SZDG to perform chemistry-related computations on the field of drug design. The applications are combined into workflows to support descriptor calculation, model building, and property prediction. The workflows are managed and processed by a web portal called WS-PGRADE where the users can also maintain their compounds, models, properties, descriptors. The resulting portal-szdg pairing is a general framework that can be specialised to any research area by adding applications, workflows and web portlets as plugins.

