EGEE BATTLES MALARIA WITH GRID WISDOM

The first biomedical data challenge for drug discovery, which ran on the EGEE grid production service from 11 July 2005 until 19 August 2005, has been hailed a success. Entitled WISDOM (*Wide In Silico Docking On Malaria*), the challenge saw over 46 million docked ligands during that period – the equivalent of 80 years on a single PC. Usually *in silico* docking is carried out on classical computer clusters resulting in around 100,000 docked ligands. This type of scientific challenge would not be possible without the grid infrastructure - 1000 computers were simultaneously used in 15 countries around the world.

The Drug Discovery application, where scientists carry out *in silico* docking, was initiated and implemented by Fraunhofer Institute for Algorithms and Scientific Computing (SCAI) in Germany and the Corpuscular Physics Laboratory (IN2P3) of Clermont-Ferrand in France. It has been running on the EGEE production service since December 2004. *In silico* docking enables researchers to compute the probability that potential drugs will dock with a target protein and is one of the most promising approaches to speed-up and reduce the cost to develop new drugs to treat diseases such as malaria. The WISDOM data challenge demonstrated how grid computing can help drug discovery research by speeding up the whole process. The sheer amount of data generated indicates the potential benefits of grid computing for drug discovery and indeed, other life science applications.

This first biomedical data challenge on the EGEE production service is a step towards a full *in silico* drug discovery platform – to propose new inhibitors for the targets implicated in malaria by using a docking approach. By deploying an application that generated a large data flow – millions of files adding up to a few Terabytes (one million megabytes, the equivalent of around 1500 CDs) – it was possible to successfully test the grid infrastructure and services.

Dr. Martin Hofmann, Supervisor of the Drug Discovery Application at SCAI, said: “The biomedical data challenge has shown that we are able to dock an impressive number of ligands thanks to the EGEE grid and indeed, the commitment and dedication of the project’s biomedical staff as well as the institutes that took part. The next step now is to analyse the huge quantity of results provided by this experiment which will require significant data mining effort.”

The next steps for the drug discovery application include sorting through the large amounts of data to identify potential drugs to treat a range of diseases and to reduce the gap between virtual screening and real world drug development.

“We have already set-up a consortium of *in silico* researchers and pharmaceutical laboratories experienced in this area and we plan to chemically synthesize and test at least some of the “virtual drug candidates” we generated in the Grid-based, virtual screening. This could result in a significant number of physical drug candidate molecules which can then be further developed into real therapeutic compounds. These are exciting times in the drug discovery world,” added Dr. Martin Hofmann.

The Drug Discovery application was developed to enhance the ability of both pharmaceutical companies and academic research institutes to share diverse, complex and distributed information on a given disease for collaborative exploration and mutual benefit. This also contributes to lowering the barrier to

engagement in such significant interactions in order to produce cheaper drugs and insecticides, thereby addressing diseases that affect third world development.

The EGEE project has developed an international computing Grid infrastructure which provides scientists with access to major computing resources world-wide. To date, the EGEE project has established a broad portfolio of applications across a wide range of industrial and academic sectors including High Energy Physics, Life Sciences, Earth Sciences, Astroparticle Physics and Computational Chemistry. There are over 20 different applications now running on EGEE.

The partners in the WISDOM data challenge include: IN2P3-LPC, CNRS, IN2P3, SCAI, the ACCAMBA and AUVERGRID projects. The following institutes contributed computing resources to the data challenge: ASCC (Taipei); IPP-BAS, IMBM-BAS and IPP-ISTF (Bulgaria); CYFRONET (Poland); ICI (Romania); CEA-DAPNIA, CGG, IN2P3-CC, IN2P3-LAL, IN2P3-LAPP and IN2P3-LPC (France); SCAI (Germany); INFN (Italy); NIKHEF, SARA and Virtual Laboratory for e-Science (Netherlands); IMPB RAS (Russia); UCY (Cyprus); AUTH FORTH-ICS and HELLASGRID (Greece); RBI (Hungary); TAU (Israel); CESGA, CIEMAT, CNB-UAM, IFCA, INTA, PIC and UPV-GryCAP (Spain); BHAM, University of Bristol, IC, Lancaster University, MANHEP, University of Oxford, RAL and University of Glasgow (United Kingdom).

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Note to Editors:

1. For more information about the Drug Discovery application, visit: http://public.eu-egee.org/pr/ to view the press release. The current drug discovery and development process is long and expensive. Only one compound out of 10,000 makes it to the market and it can take upwards of 15 years and $800 million to commercialise a single drug. The challenge of the Drug Discovery application is to reduce product development costs, decrease time to market, and increase the probability of success for the most promising leads.

2. The Enabling Grids for E-sciencE project (EGEE) is funded by the European Commission. The project aims to provide researchers in both academia and industry with access to major computing resources, independent of their geographic location. For more information about EGEE, visit http://public.eu-egee.org ;

3. The definition of a ligand in this context is: a molecule, as an antibody, hormone, or drug, that binds to a receptor;

4. For more information about EGEE in general, contact Joanne Barnett, EGEE External Relations Officer, telephone: +31 (0)20 530 4488 or email: Barnett@terena.nl ;

5. For more information about WISDOM or other applications running on EGEE, contact Vincent Breton, EGEE Applications Manager, telephone: +33 4 73 40 72 19 or email: Breton@clermont.in2p3.fr .