EGEE SPEEDS UP HUNT FOR NEW MALARIA DRUGS

The Drug Discovery application running on the Enabling Grids for E-sciencE (EGEE) production service aims to find potential new drugs to combat malaria, a disease which kills a million people per year and affects 300 million more. The number of malaria cases and deaths has increased in many parts of the world, mainly because the most widely used drug (Chloroquine) has been rendered useless by drug resistance, and because the *Anopheles* mosquitoes that carry malaria have become increasingly resistant to common insecticides. In molecular biology research, parasite proteins have been identified which are potential targets for drugs against malaria.

The Drug Discovery application, where scientists carry out '*in silico*' docking, 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 - in this particular case that potential drugs will dock on the active site of one of the malaria parasite proteins. On a single computer, a study like this with 100,000 potential drugs would normally require six months to complete - but on the EGEE grid it was achieved in just two days. The next step is to increase the performance of the application and compute millions of potential drugs in only a few weeks – a real possibility with the EGEE grid. Working at this rate, researchers hope to take a significant step towards finding a new drug to treat this widespread disease which affects millions of people every year.

The application is currently used by the Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI) in Germany and the Corpuscular Physics Laboratory of Clermont-Ferrand in France, but potentially could also be used by further institutes to find cures for diseases, such as dengue fever.

Dr. Martin Hofmann, Drug Discovery Application Supervisor at SCAI, said: *"Without the grid, such large scale studies would be expensive and very time consuming. The grid allows biologists and chemists to focus their experimental work on the most promising potential drugs, reducing the time required to develop commercial drugs for malaria and indeed, other diseases."*

Martin Hofmann added: *"The Grid could be the catalyst for drug development that brings together the actors - biochemists, physicians and computational chemists - and pushes them ahead in the same direction."*

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.

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Note to Editors:

1. The current drug discovery and development process is long and expensive. Only one compound out of 10,000 makes it to 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. Docking is the first step towards *in silico* drug design. Basically, docking is about computing the binding energy of a protein target to a library of potential drugs using a scoring algorithm. The target is typically a protein that plays a pivotal role in a pathological process, e.g. the biological cycles of a given pathogen (parasite, virus, bacteria). The goal is to identify which molecules could dock on the protein's active sites in order to inhibit its action and therefore interfere with the molecular processes essential for the pathogen.

3. The Enabling Grids for E-sciencE (EGEE) project 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 see http://public.eu-egee.org/ .

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

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

6. For more information about the Drug Discovery application, contact Martin Hofmann, telephone: +49 2241 14 2802 or email martin.hofmann@scai.fhg.de .