



## OPEN DAY: THE GRID AND NEGLECTED DISEASES

Those working in the field of neglected diseases should not miss the opportunity to meet with like-minded scientists to discuss the next step in grid computing, the major driving force for new approaches towards collaborative large scale science. An open day to discuss the future of grid computing and drug discovery is taking place on Friday 16 December 2005 at Bonn-Aachen International Centre for Information Technology, Bonn, Germany.

In the biomedical community, grid computing has already initiated several projects on large scale *in silico* drug screening approaches. The project WISDOM (Wide In Silico Docking on Malaria) was amongst the first in the public domain that made use of grid enabled *in silico* docking to simulate the interaction of potential drugs with target proteins on the Enabling Grids for E-scienceE (EGEE) grid infrastructure. *In silico* docking is the first step in the virtual screening process, which is one of the most promising approaches to help speed-up and reduce the costs of the development of new drugs. The DENGUE project is also using *in silico* docking to identify new potential compounds directed against proteins that mediate essential functions for dengue virus infection and replication. The AFRICA@home project is a grid based project aiming at improving epidemiological monitoring of Malaria in Africa. These grid projects have the potential to transform into true e-Science projects, integrating *in silico* research with experimental biology and chemistry.

Dr. Martin Hofmann, Drug Discovery Application Supervisor at Fraunhofer-Institute for Algorithms and Scientific Computing (SCAI), said: "This open day is the first in a series of planned events to set up a framework that coordinates and supports these initiatives and projects. In particular, we aim to develop concepts for the integration of experimental biology and chemistry labs to ensure proper follow-up of the *in silico* screening in the real world." He added: "Moreover, we want to bring together all the stakeholders to discuss the perspectives of our research activities for health management in those countries affected by neglected diseases."

The Open Day will be of particular interest to those working in the following fields:

- Grid research
- Life science informatics
- Molecular biology and molecular parasitology
- Organic chemistry and pharmaceutical chemistry
- National and international health organisations
- National and international research organisations
- Private enterprises interested in fighting neglected diseases
- Private research foundations interested in fighting neglected diseases

To register (free) for the Open Day in Bonn, please visit:

<http://www.scai.fraunhofer.de/index.php?id=1654&L=1> .

For more information about the day, please contact either Dr. Martin Hofmann, email: [martin.hofmann@scai.fraunhofer.de](mailto:martin.hofmann@scai.fraunhofer.de) or Dr. Nicolas Jacq, email: [jacq@clermont.in2p3.fr](mailto:jacq@clermont.in2p3.fr) .

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## Note to Editors:

1. For more information about WISDOM, please visit: <http://wisdom.eu-egee.fr/> or <http://public.eu-egee.org/files/battles-malaria-grid-wisdom.pdf> or contact Martin Hofmann, email: [martin.hofmann@scai.fhg.de](mailto:martin.hofmann@scai.fhg.de) .
2. For more information about the DENGUE project, please visit: [http://www.swissbiogrid.com/project\\_and\\_proof.html](http://www.swissbiogrid.com/project_and_proof.html) or contact Torsten Schwede, email: [Torsten.Schwede@unibas.ch](mailto:Torsten.Schwede@unibas.ch) .
3. For more information about the AFRICA@home project, please visit: <http://www.africaathome.org/> or email Francois Grey, email: [Francois.Grey@cern.ch](mailto:Francois.Grey@cern.ch) .
4. 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/> . For more information about EGEE in general, contact Joanne Barnett, EGEE External Relations Officer, telephone: +31 20 530 4488 or email: [barnett@terena.nl](mailto:barnett@terena.nl) .