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Special Features:

From Sheffield to Singapore, International Grid Battles Malaria

Malaria kills more than one million people each year, most of them young children living in Africa. Now physicists in the UK have shared their computers with biologists from countries including France and Korea in an effort to combat the disease. Using an international computing Grid spanning 27 countries, scientists on the WISDOM project analysed an average of 80,000 possible drug compounds against malaria every hour. In total, the challenge processed over 140 million compounds, with a UK physics Grid providing nearly half of the computing hours used.

The computers are all part of EGEE (Enabling Grids for E-science), which brings together computing Grids from different countries and disciplines. During the challenge, the project used the equivalent of 420 years of computing power from a single PC. Up to 5000 computers were used simultaneously, generating a total of 2000 GB (2,000,000,000,000 bytes) of useful data.

Most of the UK's contribution came from GridPP, a computing Grid funded by the Particle Physics and Astronomy Research Council and built to process data from the world's largest particle physics accelerator, due to be turned on later this year in Geneva. Professor Tony Doyle, the GridPP Project Leader, explains, "Although our Grid was built to analyse particle physics data, when we have spare capacity we're able to share it with other scientists worldwide. In this case, we're happy to have contributed more than two million hours of computer time to help find drugs against malaria."

This challenge of the international WISDOM (World-wide In Silico Docking On Malaria) initiative ran between 1 October and 31 January. Its analysis of possible docking arrangements between drug compounds and target proteins of the malaria parasite will greatly speed up the search for drugs against malaria. WISDOM uses in silico docking, where computers calculate the probability that molecules will dock with a target protein. This lets researchers rule out the vast majority of potential drugs, so they can concentrate on the most promising compounds in laboratory tests. As well as speeding up the screening process, this reduces the cost of developing new drugs to treat diseases.

"The impact of WISDOM goes much beyond malaria," declared Doman Kim, Director of the Bioindustry and Technology Institute at Jeonnam National University in Korea. "The method developed can be extended to all diseases and this opens exciting industrial perspectives. Until now, the search for new drugs in the academic sector was done at a relatively small scale whereas the WISDOM approach allows a systematic inquiry of all the potentially interesting molecules."

UK computers were used from the Universities of Birmingham, Brunel, Cambridge, Durham, Edinburgh, Glasgow, Imperial College London, Lancaster, Manchester, Oxford, Queen Mary University of London, Royal Holloway University of London, Sheffield, University College London, CCLRC Rutherford Appleton Laboratory and the JET Facilities at Culham Science Centre.

This challenge was a consequence of the first, very successful, large scale in silico docking, which ran on the EGEE Grid in summer 2005. In that case, WISDOM docked over 41 million compounds in just six weeks, the equivalent of 80 years work for a single PC. The WISDOM team identified some 5000 interesting compounds, from which they found three families of molecules that could be effective against the malaria parasite. Laboratories at the University of Modena, CNRS in France and CNR-ITB

in Italy are now carrying out more advanced studies of the molecules using molecular dynamics. Following these studies, the enzymology laboratory of the Jeonnam National University in Korea will test them in vitro.

A second computing challenge targeting avian flu in April and May 2006 has significantly raised the interest of the biomedical research community. Laboratories in France, Italy, Venezuela and South Africa proposed targets for the second challenge against neglected diseases. The WISDOM researchers plan a further data challenge on avian flu later in 2007.

The WISDOM endeavour would be impossible without support from BioSolveIT, a German firm who provided more than 6000 free floating licenses for their commercial docking program FlexX. "The WISDOM programme is very interesting and BioSolveIT is happy to sponsor this work," says Dr Christian Lemmen, CEO of BioSolveIT. "The initiative takes full advantage of the speed and accuracy of FlexX -- demonstrating the potential of the virtual screening technique in the search for drugs against neglected diseases." Due to the initial success of the data challenge, the company even decided to extend the FlexX license for several weeks, which allowed studying a new target.

In addition to the computing power of the EGEE Grid (of which GridPP is a part), AuverGrid, EELA, EUChinaGRID, EUMedGRID and South East Asia Grid all provided additional resources. The Embrace and BioinfoGRID projects are contributing to the development of a virtual, in silico screening pipeline that will allow researchers to select, for any given target protein, the most active molecules out of the millions of compounds commercially available.

Source: Particle Physics and Astronomy Research Council (PPARC)

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