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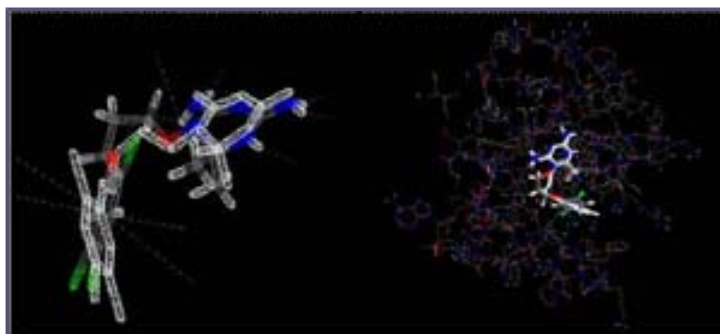
WISDOM fights malaria - with help from GridPP

Fri 2 Feb 2007

The UK particle physics Grid has again played a leading role in EGEE's latest biomedical data challenge searching for potential drugs against malaria. Malaria kills more than one million people each year, most of them young children living in Africa. 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 using GridPP providing nearly half of the computing hours used.

This challenge of the international WISDOM (World-wide In Silico Docking On Malaria) initiative ran from 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.

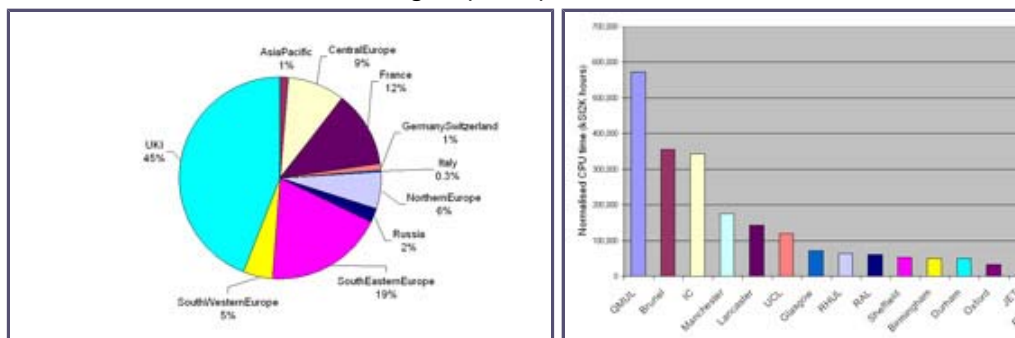
"The impact of WISDOM goes much beyond malaria," declared Doman Kim, Director of the Bioindustry and Technology Institute at Jeonnam National University in Korea. "The method developed can be extended to all diseases and this opens exciting industrial perspectives. Until now, the search for new drugs 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."



Docking of the WR9-molecule into the structure of a target protein of the Malaria parasite (quadruple-mutant DHFR of Plasmodium Falciparum). This figure was generated using the FlexV software from BioSolveIT.

The charts below show the CPU hours used in the challenge from each EGEE region (on the left) and contribution from each UK site (on the right). The UK provided 45% of CPU hours overall, with the largest proportion coming from Queen Mary University of London, who provided 27% of the UK's CPU hours.

Normalised CPU hours from each region (k.SI2k) Normalised CPU hours from each UK site



Professor Tony Doyle, GridPP Project Leader, commented, "Although our Grid was built to analyse physics data, when we have spare capacity we're able to share it with other scientists worldwide. In fact, we're happy to have contributed more than two million hours of computer time to help find drugs against malaria." 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 GBytes of useful data.

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 profile 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 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 Lemmer, 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." Following the initial success of the data challenge, the company even decided to extend the FlexX license for six 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 Embryo 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.

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