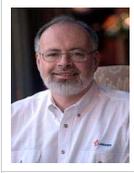


ABOUT THIS BLOG



BILL ST. ARNAUD

This blog is focused on the concept of user controlled and managed processes that will have a profound effect on the way we do science, education and business over the Internet. The use of web services, service oriented architecture and Web 2.0 technologies will permit various process to be accessible across the Internet and be manipulated by users, much in the same way that users today can manipulate and link pictures, text and images across web pages. An early example of this is the work we are doing with User Controlled LightPaths (UCLP) where users can setup, configure and manage their own IP networks, virtual routers, switches, instruments and attached devices on top of a common optical substrate. It is my belief that the network of the future will not be controlled, or owned by the telcos, cablecos or municipalities - but by users themselves.

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UPCOMING EVENTS ON MY CALENDAR

- [National Telecommunications Netherlands - June 19](#)
 - [SOA and User Controlled Light Path- OFC March 27](#)
 - [Collaborative ICT - Canada & EU - Mar 5,12, 14](#)
 - [ISOC Board Meeting -Prague- Mar 23-25](#)
 - [Neptune CDR review meeting- Victoria -March 15](#)
 - [Optical Internet in North America - Feb 26 - San Diego](#)
 - [Broadband and ICT issues Canada - Ottawa Feb14](#)
 - [Future of the Interent in Canada - Ottawa - Feb 6](#)
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WEDNESDAY, MARCH 7, 2007

International Grid battles Malaria

For more information on this item please visit my blog at <http://billstarnaud.blogspot.com/>

[Excerpts from www.gridtoday.com- BSA]

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



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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. 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."

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.

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.

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Posted by Bill St. Arnaud at [11:45 AM](#) .