

# Grid computing offers new hope in race against bird flu

October 5 2007

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Last month a collaboration of European and Asian researchers launched a new attack against the deadly bird flu virus, harnessing the combined power of more than 40,000 computers across 45 countries to boost the pace of anti-viral drug discovery.

Called Enabling Grids for E-science, the computing grid connects ordinary PCs to form a super-sized supercomputer that is being used during this challenge to analyse the potential of more than 500,000 drug-like molecules over the next few weeks.

This effort comes as new data released last week by Peking University in Beijing, China, shows that the H5N1 bird flu virus can pass through the placenta of pregnant women to the unborn fetus, and can infect organs other than the lungs in adults. A rapid response to any pandemic outbreak of the virus would be essential to its control.

Dr Ying-Ta Wu, biologist at the Genomics Research Center of the Academia Sinica, says computing grids like EGEE are the fastest and cheapest way to discover new drug leads.

“We are using EGEE to find new molecules that can inhibit the activities of the influenza virus,” Dr Ying-Ta Wu explains “During previous challenges using the EGEE grid we discovered about 200 molecules with the potential to become drugs against bird flu.”

The EGEE computing grid powers drug discovery software that allows

researchers to compute the probability that a drug-like molecule will dock with active sites on the virus and thus inhibit its action. Using the results of such in silico screening, researchers can predict which compounds are most effective at blocking the virus. This accelerates the discovery of novel potent inhibitors by minimising the non-productive trial-and-error approach in a laboratory.

“Asian flu remains a threat to world health and we are well aware that any pandemic could quickly spread throughout Europe” said Viviane Reding, European Commissioner for Information Society and Media. “I am pleased that the European project EGEE has found such an important application for computer grid technology as speeding-up drug discovery against neglected and emerging diseases. Collaboration between Europe and Asia is essential if we are to address world wide threats to public health”.

At the EGEE’07 conference in Budapest, Ulf Dahlsten, Director of “Emerging Technologies and Infrastructures” in the Information Society and Media Directorate-General of the European Commission, used the example of EGEE’s success with bird flu to illustrate the potential contributions of e-Infrastructures to science. “Computer Grids have achieved a productivity increase of more than 6000% in the identification of potential new drugs” he said. “300,000 molecules have already been screened using the EGEE grid. Of these, 123 potential inhibitors were identified, of which seven have now been shown to act as inhibitors in in-vitro laboratory tests. This is a six percent success rate compared to typical values of around 0.1 percent using classical drug discovery methods.”

Source: CERN

Citation: Grid computing offers new hope in race against bird flu (2007, October 5) retrieved 24 April 2024 from <https://phys.org/news/2007-10-grid-bird-flu.html>

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