PC grids to power hunt for new drugs

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The humble personal computer used to send e-mail or surf the Internet could quietly be finding a way to stop cancer, treat smallpox or counter a bio terror attack with anthrax spores.

Of limited power on their own, PC's when wired into so-called "grids" mimic the world's most powerful supercomputers but at a fraction of the cost.

Networks of Internet-linked computers - many in people's homes - are breaking the constraints that tight budgets and a lack of number-crunching power once imposed on researchers' quests for important new medicines.

Computer mice have not replaced laboratory mice as the proving ground for drugs, but the grids are helping scientists in their hunt for them.

In essence, grid computing parcels out tiny parts of a complex equation to lots of remote computers that seek digital needles in haystacks and then send the results back to the data centre to be reassembled in a useful form.

Grids can tackle in days complex problems that would take months or years to crack on costly conventional hardware.

The technique is perhaps best known from the SETI@home project that uses millions of networked computers - each examining just small samples of data - to search for extraterrestrial intelligence by poring over signals from space.

"When you turn on so much power, science guys who have limited their science based on real budgets and departmental boundaries and everything else really have to rethink what is truly possible," said Paul Kirchoff, vice president of marketing at United Devices, a Texas firm whose software makes grids run.

Supercomputers

United Devices (UD) rents out time on a commercial grid which it assembled from 7000 personal computers, a network that Kirchoff said ranked among the world's top eight supercomputers.

"Frankly at the moment I think we are limited more by our imaginations that we are by the technology"

Mike Brady,
Information Engineering professor at Oxford University

That is dwarfed by the 2.5 million computers hooked up to a global grid (www.grid.org) run by UD that crunches numbers for purely humanitarian causes, including the search for drugs to treat cancer, smallpox and anthrax.

A lot of the grid's machines - half at big companies, half in individual homes or offices - get turned off at night or are portables that go on or off the network, Kirchoff said, but the grid in theory has peak power of just over three petaFLOPS.

"To put that into perspective, it would be about 23 times the top 10 supercomputers in the world combined in terms of power. It is truly phenomenal," he said.

UD accepts only non-commercial projects for that giant grid, which depends on corporate sponsors to help defray costs.

The grid approach works especially well for screening tens of millions of known chemicals compounds to see if their shape lets them attach themselves to - and thus effectively switch off - proteins that are known to cause disease.

This whittles down huge chemical libraries to a few dozen promising compounds to be tested in animals and humans.

The grid.org search for smallpox drugs, for example, reduced Oxford University's library of 35 million compounds to 45 likely molecules in five months, a task that would have cost up to $75 million on the cheapest conventional hardware, Kirchoff said.

Research

Novartis is among the growing number of drug makers using in-house grids to search for new drugs.

It has 2700 PCs linked up now and aims to boost that to between 20,000 and 25,000 within two years, said Manuel Peitsch, the head of informatics and knowledge management at its drug research labs.

That would put the Swiss group's private grid in the same ballpark as the supercomputer that simulates earth's climate.

The first drug to be detected "in silico" is still years away from use in humans, but promising compounds found by the grid are now moving into the lab.

Peitsch said that is just the start.

In two years Novartis might be using the grid as a virtual chemist to design targeted new drugs.

"You have fertile ground and once you have that fertile ground you can start thinking about processes you have never thought about before," Peitsch said, such as simulating clinical trials or predicting how toxic new drugs might be in humans.

Powerful computers will never replace a scientist's flash of brilliance because you can't teach computers serendipity, he said, but the technology can change the way researchers work.

Treating diseases

"The big associations, the creative, crazy steps are taken by humans, not by machines," he said, but grids let scientists focus on creative things while machines do the drudgery.

Grid computing is also helping improve treatment of diseases such as breast cancer by creating huge databases that specialists can comb efficiently for useful information - for instance guidance on whether a biopsy might be warranted.

It was dream technology for Mike Brady, an Oxford professor of information engineering who had wondered how to share batches of data on cancer patients and still guard their privacy.

The e-Diamond grid project set up by Oxford and IBM solved the problem.

Radiologists could compare mammograms from other cancer screening centres, not just their own, creating a much more representative sample of cancer cases.

"I didn't see any way in which we could overcome all of that but actually the grid provides precisely the technology needed to do that," he said, adding that the technology lends itself easily to studying other kinds of cancers or brain disease.

"Frankly at the moment I think we are limited more by our imaginations than we are by the technology," Brady said.