Nvidia supercomputer powers HIV breakthrough

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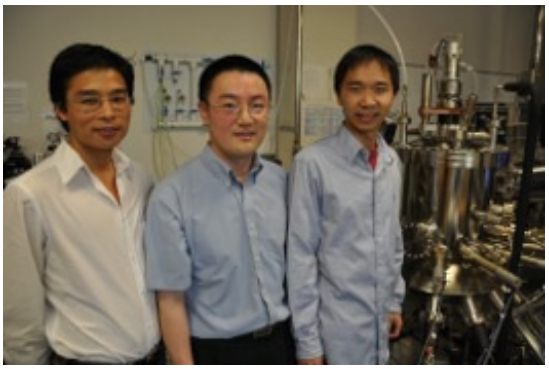
Nvidia's Tesla GPU accelerators are being used to help fight the spread of HIV.



The company has said its technology is being used by researchers at the University of Illinois at Urbana-Champaign (UIUC) who have teamed up with the University of Pittsburgh School of Medicine. The team claim in the latest issue of science journal, *Nature*, that they have for the first time determined the precise chemical structure of the HIV capsid.

For those without a PHD, this is a protein shell that protects the virus's genetic material and is a key to its virulence.

The researchers said that the findings could hold the key to the development of new and more effective antiretroviral drugs to conquer the virus - which has killed an estimated 25 million people and infected 34 million more.

UIUC researchers used the brains of the Blue Waters Supercomputer to run what they claim is the first all-atom simulation of HIV.

The computer is powered by 3,000 NVIDIA Tesla K20X GPU accelerators, which the company says is the highest performance, most efficient accelerators ever built and gave researchers the computational performance to run the largest simulation ever published, involving 64 million atoms.

Klaus Schulten, professor of physics at the University of Illinois, said it would have been "very difficult" to run a simulation of this size without the power of GPU-accelerated supercomputing in the Blue Waters system. He added the GPUs had "fundamentally accelerated the pace of [the] research".

The system could enable further breakthroughs with the planned addition of more GPUs. As a result UIUC researchers expect to increase simulation times, providing additional insight into the structure and behavior of the HIV capsid.

The capsid has become an attractive target for the development of new antiretroviral drugs. This is said to be largely due to the discovery that Rhesus monkeys have developed an immunity to HIV through a protein that disrupts capsid functioning.

The capsid is the protein cell of a virus, containing the virus's genetic material. It protects and "smuggles" the genetic material into the human host cell. Once inside, it uncoats the material and initiates the infection.

Currently there are no HIV drug treatments designed to target the capsid.

However, it is hoped that by providing a better understanding of the structure of the HIV capsid, pharmacologists will have more information to help them develop new and potentially more effective antiviral HIV drugs.