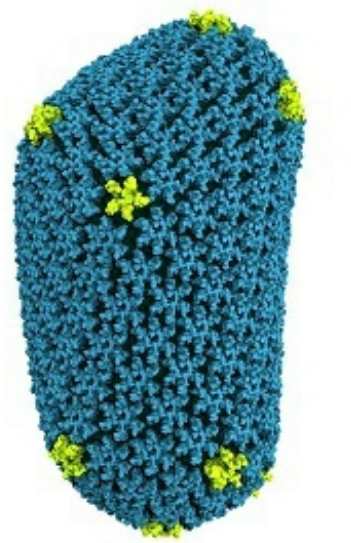
Nvidia GPUs Assist in Battling HIV

By Damon Poeter May 29, 2013 01:50pm EST 2 Comments

A "major breakthrough" in battling HIV was achieved with the help of Nvidia's Tesla GPU accelerators in Cray's Blue Waters supercomputer, the graphics chip maker said Wednesday.

A "major breakthrough" in battling HIV was achieved with the help of Nvidia's Tesla GPU accelerators, the graphics chip maker said Wednesday.



Researchers at the University of Illinois at Urbana-Champaign (UIUC) have "determined the precise chemical structure of the HIV 'capsid,' a protein shell that protects the virus's genetic material and is a key to its virulence," Nvidia said in a statement describing how the team conducted an "all-atom simulation of HIV" on the Tesla-powered Blue Waters supercomputer.

Blue Waters is a Cray XK7 supercomputer with 3,000 Nvidia Tesla K20X GPU accelerators. The research team, which published its findings in the current issue of *Nature*, ran the "largest simulation ever published" on Blue Waters, an experiment that involved mapping an incredible 64 million atoms to simulate the HIV capsid (pictured).

"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. We started using GPU accelerators more than five years ago, and GPUs have fundamentally accelerated the pace of our research," Klaus Schulten, a professor of physics at the University of Illinois, said in a statement.

Schulten and his colleagues said that understanding the structure of the HIV capsid "may hold the key to the development of new and more effective antiretroviral drugs to combat a virus that has killed an estimated 25 million people and infected 34 million more" around the world.

While no current HIV drugs target the HIV capsid, it is seen as "an attractive target for the development of new antiretroviral drugs" because scientists have discovered that the disruption of capsid functioning via a protein produced by Rhesus monkeys has given them an immunity to HIV.

Sumit Gupta, general manager of Nvidia's Tesla Accelerated Computing Business Unit, said GPU-accelerated supercomputers give researchers like Schulten and his colleagues the ability to run much more complicated computer simulations at a faster rate than was possible with older, CPU-only systems.

"GPUs help researchers push the envelope of scientific discovery, enabling them to solve bigger problems and gain insight into larger and more complex systems. Blue Waters and the Titan supercomputer, the world's No. 1 open science supercomputer at Oak Ridge National Labs, are just two of many GPU-equipped systems that are enabling the next wave of real-world scientific discovery," Gupta said.

Nvidia introduced its CUDA programming language several years ago in an effort to help supercomputer firms like Cray incorporate GPU-based parallel processing functionality in the world's most powerful computer systems. Today,

a great deal of the top supercomputers in the world use CPUs and GPUs to better perform the computing tasks best suited to each particular type of processing unit's strengths.

For more, check out the UIUC team's video below, which describes the discovery and how it was achieved.