

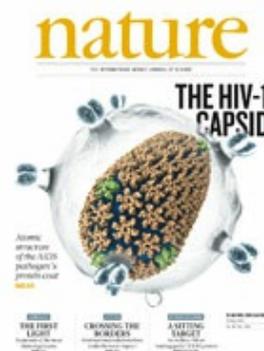
GPUs Help Researchers Uncover New Approach to Combating HIV Virus

Rich Brueckner

Today Nvidia announced that researchers using Tesla GPUs have achieved a [major breakthrough](#) in the battle to fight the spread of the HIV virus.

Featured on the cover of the latest issue of *Nature*, a new paper details how researchers from the University of Illinois at Urbana-Champaign and the University of Pittsburgh School of Medical Sciences have, for the first time, 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. Understanding this structure 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.

UIUC researchers uncovered detail about the capsid structure by running the first all-atom simulation of HIV on the Blue Waters supercomputer. Powered by 3,000 NVIDIA Tesla K20X GPU accelerators – the highest performance, most efficient accelerators ever built – the Cray XK7 supercomputer gave researchers the computational performance to run the largest simulation ever published, involving 64 million atoms.



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

While no existing HIV drug treatments are designed to target the capsid, by providing a better understanding of the structure of the HIV capsid, pharmacologists now have a wealth of new information to develop new and potentially more effective antiviral HIV drugs.

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