



UK, Thai Researchers Enlist NVIDIA Tesla GPUs to Fight the Next H1N1 Epidemic

ISC'12 - NVIDIA today announced that its GPUs are playing an integral role in research that's shedding new light on ways to prevent future epidemics of the deadly H1N1 influenza virus.

A major difficulty in combating H1N1 has been the frequent and rapid onset of new virus mutations that rendered anti-influenza drugs, such as Tamiflu® (*oseltamivir*) and Relenza® (*zanamivir*), ineffective.

However, using computer simulation, researchers at the [University of Bristol](#) in the United Kingdom, and the [Bansomdejchaopraya Rajabhat](#) and [Chulalongkorn](#) Universities in Bangkok, have observed how H1N1 mutations can cause changes in the chemical and biological structural dynamics of a key enzyme of the virus, revealing, for the first time, the mechanism of resistance to existing anti-influenza drugs. With this breakthrough, it will be possible to identify new ways in which inhibitor drugs can be quickly designed to address these mutations, and possibly reduce the deadly impact of future epidemics.

Using a small cluster equipped with high-performance [NVIDIA® Tesla® GPUs](#) running advanced simulations using the [AMBER molecular dynamics application](#), the research team uncovered the H1N1 mechanism of resistance in half the time and using one-fifth the servers that it would have taken using a CPU-only cluster.⁽¹⁾

A paper detailing the researchers' findings has been published in a recent edition of [Biochemistry](#).

"The four-node, eight-GPU cluster allowed us to quickly run and repeat a much larger number of complex simulations than otherwise would have been possible to perform," said Dr. Christopher Woods, lead investigator of the U.K. research team. "This enabled us to exhaustively explore all virus mutations of interest, building up a detailed picture that allowed us to quickly identify the key steps in the mechanism of resistance. A comparable CPU-only system with 16 to 24 CPUs would have taken twice as long, at best. And, it would have been practically impossible for our team to monopolize all this time on the cluster, given the high demand for compute cycles by other researchers across the university."

Following the outbreak of H1N1 influenza cases in 2009, which infected as many as 89 million people and killed up to 18,300,⁽²⁾ researchers worldwide have been racing to discover how virus mutations led to the ineffectiveness of leading anti-influenza drugs. However, studying viruses in laboratory experiments is difficult because reactions are often too fast and delicate to capture. And, advanced computer simulations of these systems have previously been beyond the reach of researchers without access to expensive, high-powered supercomputers.

"Until now, the use of computer simulations for drug discovery and disease prevention has been limited because of the large, expensive supercomputers required to study the biological systems," said Sumit Gupta, senior director of the Tesla business at NVIDIA. "Today a small, affordable GPU-based server gives researchers dedicated access to a high-performance system in-house to power a range of scientific discovery."

To help more researchers experience the power of GPU-accelerated research, NVIDIA has launched the GPU Test Drive program. It enables computational chemists and biologists to experience GPU acceleration of their molecular dynamics simulations for free on a remotely hosted GPU cluster. To learn more or to register, visit the [GPU Test Drive website](#).

About NVIDIA Tesla GPUs

NVIDIA Tesla GPUs are massively parallel accelerators based on the NVIDIA CUDA® parallel computing platform. Tesla GPUs are designed from the ground up for power-efficient, high performance computing, computational science and supercomputing, delivering dramatically higher application acceleration for a range of scientific and commercial applications than a CPU-only approach.

More information about NVIDIA Tesla GPUs is available at the [Tesla website](#). To learn more about CUDA or download the latest version, visit the [CUDA website](#). More NVIDIA news, company and product information, videos, images and other information is available at the [NVIDIA newsroom](#). You can also follow us on [Twitter](#) ([@NVIDIATesla](#)).

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(1) The research team ran 10 simulations on the H1N1 mutations, which took approximately one month to complete vs. two months on CPUs.

(2) Source: CDC.gov: http://www.cdc.gov/h1n1flu/estimates_2009_h1n1.htm

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