

UK, Thai researchers work on H1N1 mutations

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Singapore: 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. NVIDIA 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.

Using computer simulation, researchers at the University of Bristol in the UK and 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 for running advanced simulations using the AMBER molecular dynamics application, the research team discovered 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.

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 UK 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, 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."