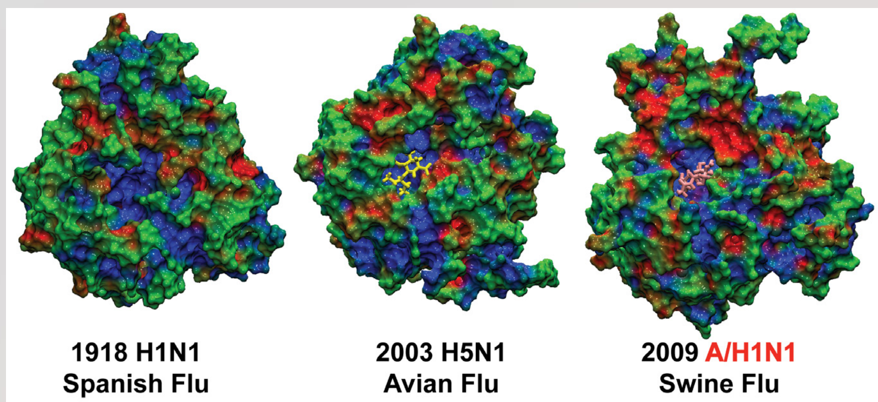
THE UNIVERSITY OF TEXAS AT AUSTIN
TEXAS ADVANCED COMPUTING CENTER

TACC's Ranger supercomputer enlisted to combat the H1N1 pandemic

The A/H1N1 virus, also known as the 'swine flu,' first surfaced in Veracruz, Mexico, in April 2009. With more than 400,000 cases and approximately 4,500 fatalities reported as of October 2009, the virus has questioned our readiness to confront virulent forms of the flu, and other diseases that might come in the future.

When information emerged that the virus might be resistant to Tamiflu, the most common antiviral flu medication, the race to find strategies to fight the virus became even more urgent. In response, researchers Klaus Schulten from the University of Illinois at Urbana-Champaign, and Thanh Truong from the University of Utah, mobilized a team to combat this worldwide health threat.



Computational models show Spanish H1N1 with no drugs bound, Avian H5N1 with Tamiflu bound, and Swine A/H1N1 with Relenza bound.

"Our study marks a historic moment, namely that supercomputers are being used in direct response to a pandemic emergency situation," Schulten said. "Prior to this moment, computational tools were employed to shape drug development strategy. This time, researchers were granted computing resources right away to start work on a pharmacological defense strategy."

The research team began by determining the 3-D structure of the neuraminidase protein of the virus. Neuraminidase is the most quickly evolving part of the virus' reproductive cycle and the main target for antiviral drugs.

With priority access to Ranger, the research team employed 2,000 to 3,000 processors (or the equivalent of 1,000 laptops) continuously over two weeks. Using an atomic-level 3D modeling program, the scientists modeled how the neuraminidases proteins of the Spanish, Avian and Swine flu interact with the two most prescribed flu-fighting medicines (Tamiflu and Relenza), two trial drugs (Peramivir and A-315675), and Sialic acid, their natural target on the human cell. These simulations revealed the pathway by which drugs normally bind to the neuraminidase protein and illustrated how changes to the A/H1N1 protein could cause drug resistance.

The research team learned that, while the current strain of A/H1N1 swine flu is not yet drug resistant, the virus' resistance to these drugs is not far off, underscoring the need to know precisely how mutations make the flu immune to antiviral therapies.

This research was conducted in Spring 2009.

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