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How GPUs Are Helping Pin Down Shape-Shifting Retroviruses – and Their Diseases

By George Millington (https://blogs.nvidia.com/blog/author/george-millington/)

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Mutations. Infectious particles. Cell invasions. This isn't a zombie movie. It's daily life for a retrovirus.

The shape-shifting of viruses is a big part of why they're a global threat to human health. They go through a multistage process to produce infections, making them hard to analyze and treat. Until now.

University of Illinois researchers at the Beckman Institute for Advanced Science and Technology's theoretical and computational biophysics group, led by Professor Klaus Schulten, are accelerating simulations of immature retroviruses using GPU technology on some of the world's most powerful computers.

It's helping them pin down the shifty creatures.

When viruses burst forth from infected cells, they're in an immature state composed of a protein-coated RNA genome. The researchers are examining ways to prevent their spread by locking the viral particles in this non-infectious stage before they morph and mature.

"What we're doing is looking for ways to effectively disrupt the life cycle of the virus before it becomes infectious," said Juan Perilla, a postdoctoral researcher working on the project.

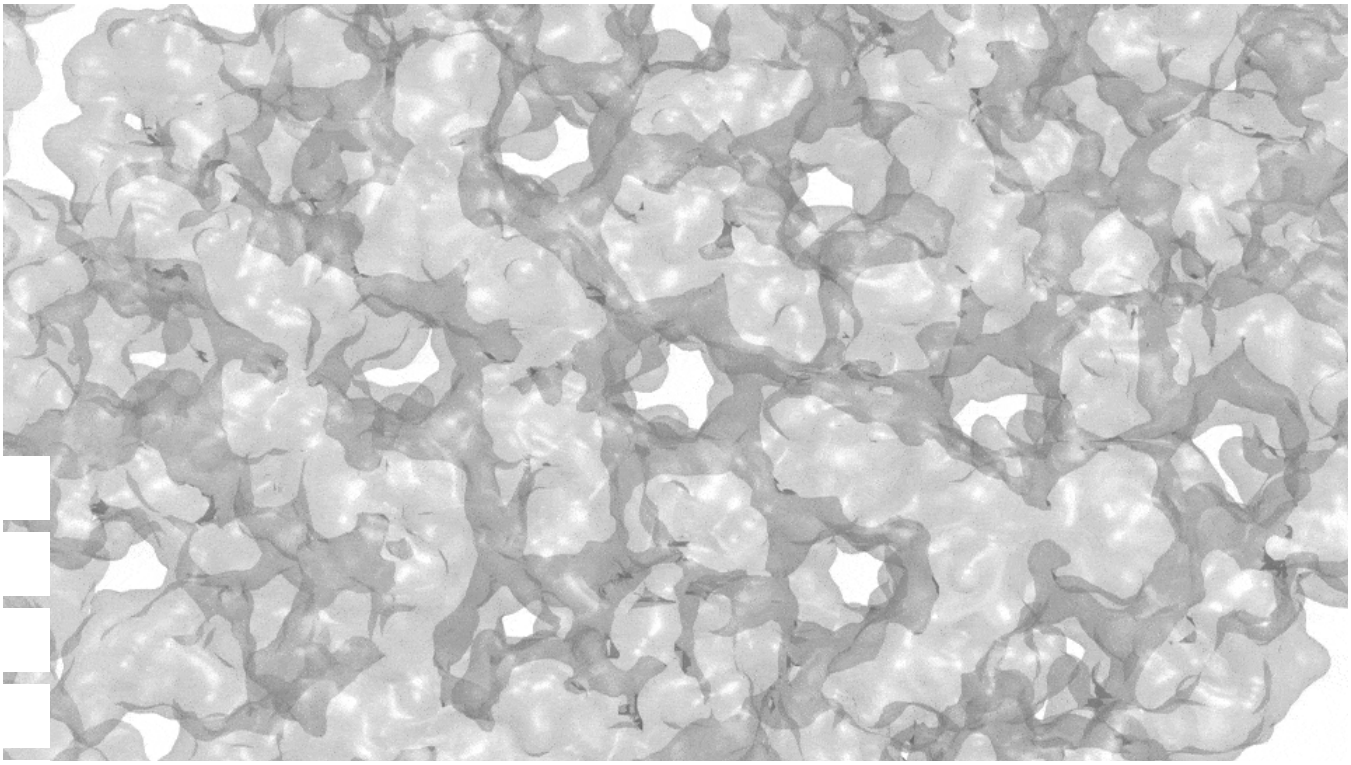
Until recently, their tiny, irregular shape made study of the atomic-level structure of the particles difficult.

"It's very clear when the retrovirus is immature because it goes into a very particular state before it becomes infectious," said Perilla. "But it's very tricky

(https://blogs.nvidia.com/wp-content/uploads/2015/11/ImmatureLatticeofRSVcrop.jpg)

A model of an immature retrovirus capsid of RSV.

to get at its structure.”



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An atomic model of the immature retrovirus was constructed by placing individual viral subunits into the density map rated by cryo-electron microscopy.

imulations at Supercomputing Speed

As viruses mature, they undergo a process — called reverse transcription — that rearranges viral proteins and activates the conversion of the RNA genome into DNA. The viral DNA then invades a host cell’s genome. The infected cell will release copies of the immature virus into the host’s bloodstream. These newly released viruses must in turn mature before they can infect other cells.

During this complex process, mutations can occur, which makes treating the retrovirus more complicated. A good model for studying this process is the structure of the Rous sarcoma virus, or RSV, which affects birds. High-resolution images of its immature stage have been hard to come by.

This led researchers to run simulations in some of the fastest, GPU-powered computers in the world, including Titan, at the Oak Ridge National Laboratory, and Blue Waters, at the National Center for Supercomputing Applications at Illinois.

“Using GPUs, we get 2X acceleration, which means the turnaround time on calculations is two times faster,” said Boon Chong Goh, a physics grad student at the university who works on the project. “Instead of two months waiting for a result, we can get it in a month.”

The simulations provided the first atomic-level structural model of the immature retroviral lattice of RSV earlier this year (http://www.cell.com/structure/abstract/S0969-2126(15)00220-8). The researchers have been studying the immature HIV virus on the Blue Waters supercomputer since January.

At the SC15 (http://sc15.supercomputing.org/) supercomputing conference in Austin, Texas, next week, the researchers will present a paper and video, “Chemical Visualization of Human Pathogens: the Retroviral Capsids (https://www.youtube.com/watch?v=FEWkd01HRMc&feature=youtu.be),” that

describes the techniques used to build, simulate, analyze and visualize the structures. These structures are considered unexploited targets for pharmaceutical intervention.

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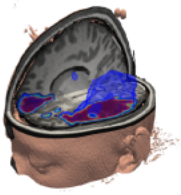

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