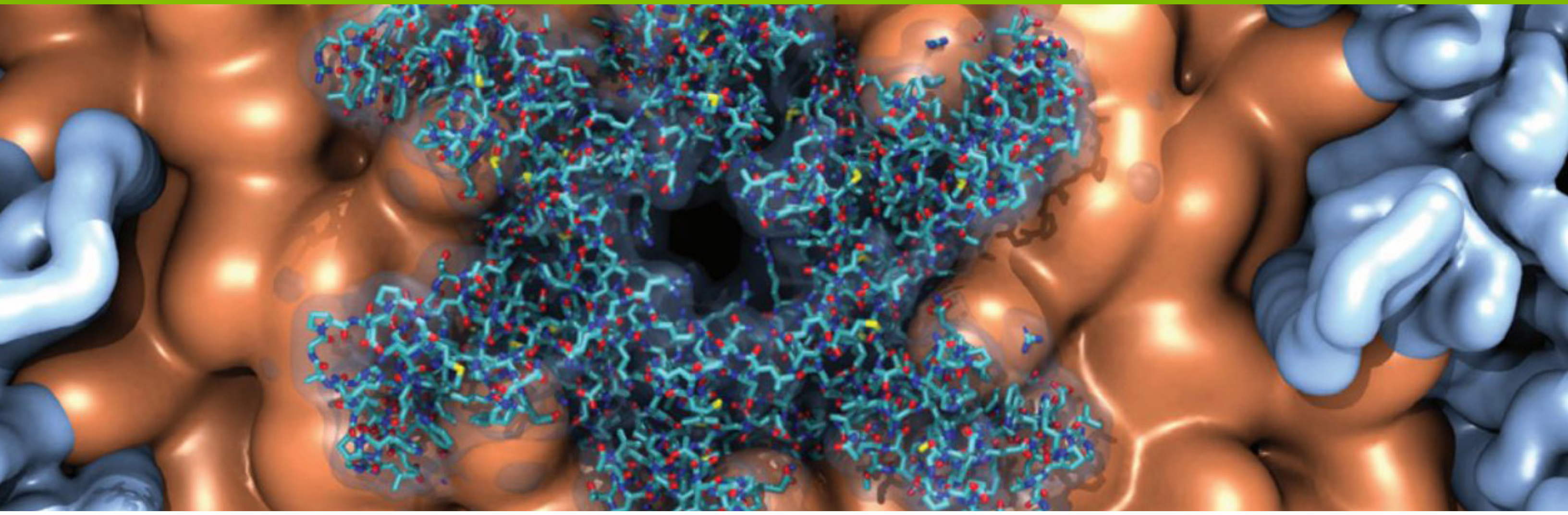
SUCCESS STORY | THE BECKMAN INSTITUTE, UIUC

OPENING NEW FRONTIERS IN THE BATTLE AGAINST HIV/AIDS

Adding GPU acceleration has allowed the Beckman Institute to model the entire HIV capsid.



NVIDIA® Tesla® GPUs enable researchers to understand the interaction between the dynamic HIV structure and the human protein to help develop new therapeutic drugs.

AT A GLANCE

CUSTOMER PROFILE

Customer: The Beckman Institute for Advanced Science and Technology at the University of Illinois

Industry: Research

Locations: Urbana, IL

Size: 1,500 researchers from more than 40 different University of Illinois departments

System: ORNL TITAN, the #2 Supercomputer on the November 2015 Top500 List

SUMMARY

> This interdisciplinary research institute is devoted to research in physical sciences, computation, engineering, biology, and neuroscience.

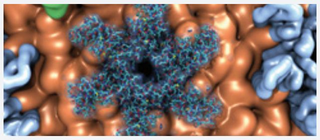
> Researchers use NAMD to simulate HIV capsid.

> NAMD runs on CPU-only systems but is limited to small models and slow speeds.

> 1024 GPUs on ORNL's TITAN supercomputer are used to simulate 26 million atoms of the HIV capsid.

REASONS FOR THE NVIDIA TESLA K80

1. There are 400+ GPU-accelerated applications.
2. A single Tesla K80-powered server replaces up to eight CPU-only servers.
3. Higher throughput leads to more discoveries.



Cover: VMD close-up rendering of the atomic structure of the HIV-1 capsid. *Source: John Stone, UIUC*

The Beckman Institute for Advanced Science and Technology at the University of Illinois is an interdisciplinary research institute. It is devoted to leading-edge research in physical sciences, computation, engineering, biology, and neuroscience.

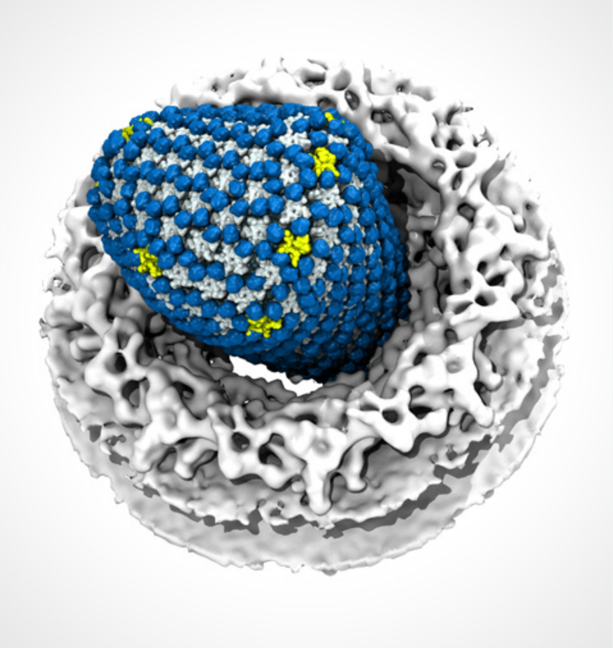
CHALLENGE

The mechanism by which human protein, Cyclophilin A (CypA), assists the capsid has been unclear, despite knowing the crystal structure of CypA and CA proteins. Computational biologist have shown that the interaction of CypA with the capsid are both structural and dynamic; both the shapes of the individual proteins and the ever-changing shape of the entire capsid make it difficult to develop drugs that can effectively neutralize these moving targets. Furthermore, the enormous size of the HIV capsid has stymied attempts at simulating the entire capsid.

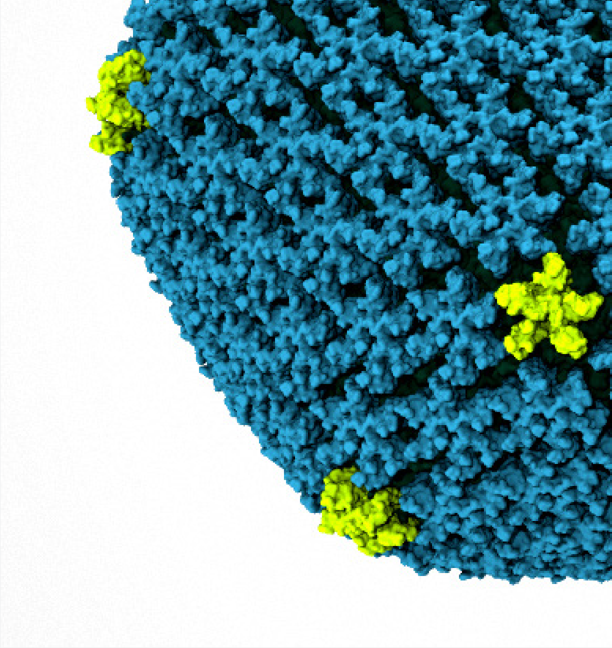
SOLUTION

Researchers at UIUC are using NAMD, a biomolecular simulation application, to understand the structure and explain the behavior and interactivity of the systems at an atomic level. NAMD enables researchers to study dynamics of molecular systems in a very efficient way.

"Thanks to NAMD, we were able to identify a previously unobserved binding point between CypA and CA," said Klaus Schulten, computational biophysicist and Swanlund Professor of Physics at the University of Illinois. "Moreover, running NAMD on GPUs has enabled us to perform statistically significant analysis by using more samples and trying different experimental conditions."



Left: HIV capsid simulated with 26M atoms.
Source: Beckman Institute, UIUC.



Right: A rendering of the HIV capsid with pentamers (yellow) and hexamers (blue)—the building blocks of the capsid.
Source: Beckman Institute, UIUC.

NAMD can run on CPU-only systems but is limited to small models and slow speeds. "The GPU-accelerated version of NAMD has enabled us to simulate 26 million capsid atoms, a difficult task to achieve on a CPU system," said Juan Perilla, Postdoctoral Research Associate at UIUC. This simulation run used 1,024 Tesla GPUs, delivering over 4PFlops of single-precision performance.

IMPACT

Since 2000, 38.1 million people have been infected with HIV, and 25.3 million people have died of AIDS-related illnesses. A well thought-out drug therapy is essential to saving HIV/AIDS patients.

Better understanding of CypA's structural and dynamic interaction with CA will help develop new therapeutic drugs that inhibit the binding of CypA to the capsid and other cellular proteins.

THE NVIDIA GPU-READY APP QUICK START GUIDE

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