

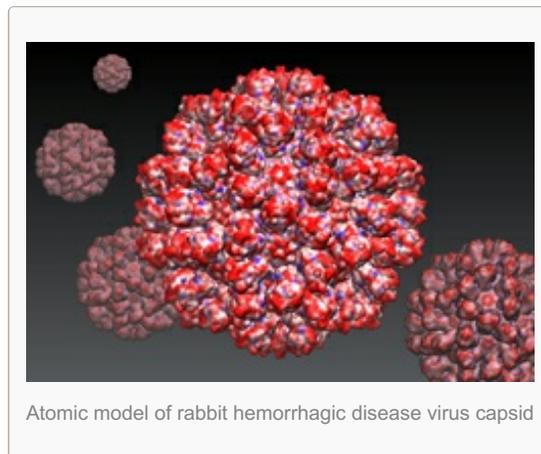
U.S.-China team determines structure of virus with Blue Waters

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Simulations carried out using the Blue Waters petascale supercomputer have determined the structure of the rabbit hemorrhagic disease virus (RHDV), which causes a highly infectious and often fatal illness in domestic and wild rabbits.

This research, carried out collaboratively by researchers at the University of Illinois at Urbana-Champaign, the University of California-San Diego, and several Chinese research institutions, has been published in *PLOS Pathogens*.

RHDV belong to the Lagovirus genus, and the detailed structure of any lagovirus has yet to be determined. The study published in *PLOS Pathogens* used a cryo-electron microscopic reconstruction of wild-type RHDV and the crystal structures of two domains of its capsid, the protein structure that encases the virus' genetic material. These data were used to build a complete atomic model of the RHDV capsid. According to the researchers, this “provides a reliable, pseudo-atomic model of a Lagovirus and suggests a new candidate for an efficient vaccine that can be used to protect rabbits from RHDV infection.”



University of Illinois biophysicist Klaus Schulten, a co-author of the published study, says the computational power of Blue Waters and the NAMD molecular dynamics code developed at Illinois were vital to achieving this result.

“The structure of the capsid of RHDV could only be achieved through a 9,891,665-atom NAMD simulation. The computational strategy adopted would have been inconceivable before the advent of Blue Waters due to the needed large simulation size,” he said. “This study demonstrates clearly that Blue Waters is a research instrument for mainstream life science!”

Schulten received a Petascale Computing Resource Allocation from the National Science Foundation that enabled his research team to prepare NAMD for extreme-scale supercomputers and to tap into the computing and data power of Blue Waters. His group is currently using Blue Waters to conduct a 24 million-atom simulation of a photosynthetic membrane that harvests sunlight and a 65 million-atom simulation of another capsid, this time the protein capsule that encases HIV.

For more information about how Blue Waters is used for a wide range of science and engineering research by investigators across the country, visit <http://www.ncsa.illinois.edu/BlueWaters>.

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Image courtesy Yanxin Liu and Klaus Schulten, Beckman Institute, University of Illinois at Urbana-Champaign; Fei Sun, Institute of Biophysics, Chinese Academy of Sciences.