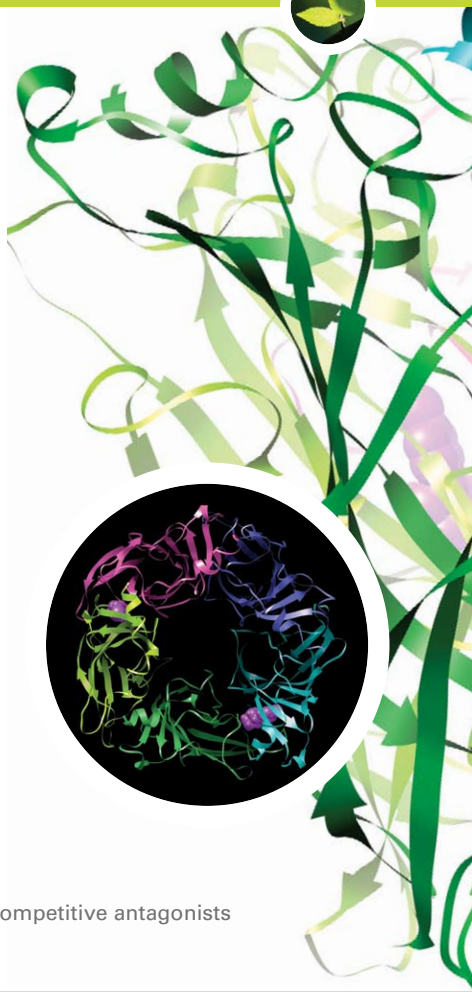
Finding treatments for neurological diseases



A treatment, or perhaps even cure, for neurodegenerative disorders such as Parkinson's, Alzheimer's or autism could lie in managing a specific family of proteins that control messages sent to the brain.

The proteins, called neuronal nicotinic acetylcholine receptors (abbreviated nAChRs), are often located at nerve endings. They selectively bind to certain chemicals and are responsible for sending multiple types of signals to the body.

To look for medications or substances that will bind with a specific member of the nAChR family of proteins and block the damaging signals, Ohio State University biochemists are modeling the activities of known nAChR antagonists — chemicals that thwart nAChRs' messages to the brain.

"Through this computationally intensive process, we are identifying — for the first time — which specific sites on the nAChR proteins will bind with a novel class of antagonistic compounds," said Chenglong Li, Ph.D., an assistant professor in OSU's College of Pharmacy. His collaborators are colleagues Ryan Pavlovicz and Dennis McKay, Ph.D.

Using the Ohio Supercomputer Center's IBM Cluster 1350, they are building and studying, through molecular dynamics simulations, the functions of various nAChRs. Then, they computationally let molecular partners "dock" to each other and predict how one molecule will bind to another to form a functional complex.

"We can then use virtual, high-throughput screenings [millions of compounds] and fragment-based designs [thousands of specific compounds] at these sites to optimize and design new, highly selective and potent compounds that will better inhibit the debilitating actions of nAChRs, with minimum side effects," Dr. Li added. ■

Project lead: Chenglong Li, Ph.D., The Ohio State University
Research title: Computational evaluation, design & discovery of nicotinic acetylcholine receptor noncompetitive antagonists

Visualization builds window to understanding

Ohio State's Graphics and Visualization Research Group embodies the proverb that "a picture is worth a thousand words." These researchers specialize in scientific visualizations — the science of translating data analysis into cutting-edge renderings.

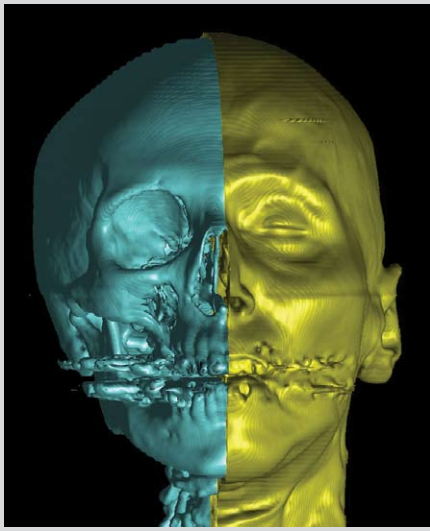
The graphics hardware market has advanced exponentially; commodity-based graphical processing units (GPUs) have become more programmable and easier to use for general applications. To empower research in this area, the Ohio Supercomputer Center's GPGPU/Visualization Cluster provides 36 graphical processing units capable of 11,800 peak gigaflops. The cluster's level of memory, speed and programmability is a necessity for realistic graphics.

"We have relied on the Ohio Supercomputer Center's GPGPU/Visualization Cluster to develop high performance, scalable parallel visualization algorithms targeted at very large data sets, as well as verify our research results," said Han-Wei Shen, Ph.D., an associate professor in computer science and engineering at The Ohio State University.

Parallel processing increasingly plays a more important role in the area of scientific visualization, especially as the size of data increases. Although many parallel visualization algorithms have been developed in the past, the complexity and scale of the data generated by terascale simulations demand even greater advancement in fundamental visualization algorithms and system designs.

Dr. Shen and his colleagues also tap OSC resources for flow visualization, time-varying data visualization and real-time applications, such as those used in medical surgical simulations. While each area uses different computational methods, all strive to create effective — and powerful — images to better illustrate the science behind the art. ■

below: Using OSC computers, Dr. Han-Wei Shen detected a symmetry plan from the data of a skull's three-dimensional CT scan. He then applied different visualization techniques to the two halves of the skull.



Project lead: Han-Wei Shen, Ph.D., The Ohio State University
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