WAYNE STATE UNIVERSITY

Annual Research Cluster Grant Competition

HPC provides a powerful and flexible new tool to be shared by computation-intensive interdisciplinary collaborative research teams

SILICON MECHANICS
SERVERS • STORAGE • HPC

WAYNE STATE UNIVERSITY

2014 Recipient:
Wayne State University, Detroit, MI
Website: https://wayne.edu/
Hardware and software partners:
Intel, NVIDIA, HGST
Mellanox Technologies, Supermicro
Seagate, Kingston Technology
Bright Computing, LSI Logic
HPC Cluster:

- Eight compute nodes
- One head node
- Intel® Xeon Phi™ coprocessors
- NVIDIA® Tesla® GPUs
- InfiniBand and gigabit Ethernet networking
- Bright Cluster Manager

"We are thrilled to be a recipient of Silicon Mechanics' generous grant program. Our research faculty are pushing the boundaries of discovery, and this high performance computing equipment will help accelerate innovative work across our campus."

Hilary Ratner, PhD
Vice President for Research
Wayne State University

For more informaiton about other Silicon Mechanics customer successes, please visit:
http://www.siliconmechanics.com/casestudies

Overview of the institution

Wayne State University, located in downtown Detroit, is one of the nation's 50 largest public universities, with nearly 30,000 students. Thirteen colleges and schools offer more than 370 undergraduate, graduate, post-graduate and specialist academic programs. WSU's School of Medicine is the nation's largest single-campus medical school.

Already known as a powerhouse research university with urban roots and a global reputation, WSU's mission is to be a premier urban research institution, working on solutions to the pressing economic and health problems that plague the nation and the world.

WSU has annual research expenditures of nearly $260 million and is among only 3.5 percent of U.S. universities with the highest research classification from the Carnegie Foundation for the Advancement of Teaching.

IT infrastructure expanded to make the best of both types of parallel computing

WSU has a robust IT infrastructure, with a central HPC grid, including more than 4,500 processing cores and 1.2 petabytes of data storage, filling ten racks, each seven feet tall.

As befits a premier research university with the motto "Aim Higher," the university is always looking to improve its IT resources, which play a role in determining the work WSU's researchers can do and in the quality of faculty and students the university attracts.

Although there are a number of individual graphics processing unit (GPU) computing efforts, there is no centralized support or infrastructure for these research endeavors. The new HPC cluster donated by Silicon Mechanics combines multiple compute and GPU nodes to make the best of both types of parallel computing, making it a significant update to WSU's current computing grid.

The new cluster will provide resources that will be shared by a variety of the most computation-intensive research groups on campus, making WSU's research infrastructure even more competitive.

Using the same operating system and job scheduler for all compute resources makes it easy for central IT staff to modify jobs to make use of the powerful new GPUs and Phi coprocessors.

"Detroit industry is diversifying and this cluster gives us the necessary processing power to tackle even larger, computation-intensive problems in healthcare, bioinformatics and genomics, as well as in advanced manufacturing and materials science."

Patrick Gossman, PhD
Deputy CIO, Community, Research and Special Projects
Wayne State University

"WSU stood out in the competitive field of applicants, based on the high level of collaboration across departments, the clear and convincing description of the need for the cluster, as well as specific applications that would use the processors, GPUs, and Phi co-processors. We were also impressed with the extremely high level of positive impacts to faculty, students, and the greater Detroit community."

Art Mann
Education/Research/Gov't Vertical Group Manager
Silicon Mechanics

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Examples of cutting edge research HPC cluster will facilitate

The Research Cluster Grant application was submitted jointly by two interdisciplinary collaborative research teams, which include both computer scientists and domain scientists focusing on chemistry, mathematics, physics, and biology, along with cancer and biomedical research. The application teams were supported by WSU's Computing & Information Technology Department.

Researchers from these teams are lining up to take advantage of the cluster's powerful new parallel processing capabilities. One example is Andrés Cisneros, Assistant Professor in the Chemistry Department, who leads a team that will use the cluster in its work developing and applying computational chemistry methods for the simulation of chemical and biochemical systems. The group is a member of the AMBER development team; AMBER is a popular molecular dynamics (MD) software program for biomolecular simulations and one of the first MD software packages to tap the power of GPUs.

The group uses computational simulations to investigate several biomolecular systems, including DNA repair and cancer-related proteins. One example, being conducted in collaboration with researchers in the chemistry and engineering departments, and the Karmanos Cancer Institute, is using the cluster to speed up the development of novel radiolabeled agents for Galectin-3 (Gal-3), a protein involved in such cancers as pancreatic ductal adenocarcinoma. The development of an imaging agent specific for Gal-3 will enable detection of early stage pancreatic ductal adenocarcinoma.

Another project, led by Zhi-Feng Huang, Associate Professor, Department of Physics and Astronomy, currently makes use of parallel computation with multiple GPUs to solve and simulate two-dimensional polycrystalline and/or nanostructured material systems that are important in developing new experimental tools used to understand grain growth dynamics, crucial to the control of hardness and strength of a wide range of engineering materials. The team will extend this to three-dimensional models with the new cluster.

These large dynamic systems are usually inaccessible to studies using conventional methods, and simulations and computations using multiple GPUs will allow the team to tackle these complex systems and identify the mechanisms inside, including grain growth and defect dynamics in polycrystals and quantum dots evolution in thin film growth.

A final interesting example, led by Jeffrey Potoff, a Professor in the Department of Chemical Engineering and Materials Science, will use the cluster's state-of-the-art hardware, particularly the NVIDIA K40 and Intel PHI co-processor, to enhance the development of WSU's novel GPU Optimized Monte Carlo simulation engine, known as GO-MC.

The research group will be able to perform high throughput computational screening of porous materials for CO_2 sequestration, develop novel materials for the stabilization of drug dispersions, predict phase behavior of polymers and polymer composites, and provide molecular level insight to such fundamental biological processes as membrane fusion.