Most powerful computer of its kind in western N.Y. available worldwide

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Local scientist Dr. Russ Miller is leading the rollout of "Magic," one of the most powerful computers in New York State to qualified users worldwide for solving computationally-demanding problems.

Cyberinfrastructure sits at the core of modern simulation and modeling, which creates new methods of investigation that allow scholars to address previously unsolvable problems, according to Miller who holds scientific appointments at both Hauptman-Woodward as a senior scientist and at the University at Buffalo as a Distinguished Professor of Computer Science and Engineering. The Miller Cyberinfrastructure Laboratory (MCIL) is taking advantage of recent advances in technologies in order to link distributed resources, including compute systems, data storage devices, visualization systems, sensors, and a wide variety of instruments and make those resources available worldwide.

"The work done by Dr. Miller's group, which was supported by an NSF grant that also providing funding to Niagara University (NU) provided us with the opportunity to acquire significant computing power and skills. It also allowed us to train students on creating and utilizing modern computing platforms," Dr. Mary McCourt, chair and professor of Chemistry at NU, said. "We are excited to have immediate access to this new state-of-the-art computing system, which enhances the resources of Niagara's Academic Center for Integrated Sciences."

"We have been working on grid computing efforts with Russ and his group for years," Dr. Charles M. Weeks, senior research scientist at

HWI, said. "These efforts have resulted in a number of joint research and funding efforts. We are particularly anxious to experiment with this new trend in high-performance computing as part of one of our jointly funded projects, especially for some of HWI's computationally demanding applications."

The Miller Cyberinfrastructure Laboratory (MCIL) was founded at the beginning of the 21st century by Miller who is widely recognized as a leader in parallel computing, grid computing, and cyberinfrastructure. Miller served as Founding Director of the UB Center for Computational Research (CCR) from 1998-2006. Under Miller's direction, and with primary funding from the National Science Foundation (NSF) and National Institutes of Health (NIH), a Buffalo-based grid was developed as an experimental way to create an institutionally-distributed platform that integrated information and computing. This led to the design, implementation, and deployment of the Western New York Grid (WNY Grid), which aggregated costly computational resources at institutions throughout WNY. The overwhelming success of the WNY Grid led to the MCIL-deployed New York State Grid (NYS Grid), based on the Open Science Grid set of grid software.

Magic is a state-of-the-art computer system located at UB's North Campus which consists of graphics processing units typically reserved for high-end gaming systems that are integrated into a traditional rack of computers. Magic was delivered in late 2008 and is now available to users worldwide. The system is cost-effective in solving large computational problems in areas including bioinformatics, computational chemistry, computational fluid dynamics, computational finance, medical imaging, weather and ocean modeling.

Led by Miller, MCIL worked on platforms for monitoring grid systems, for providing a single point-of-entry portal and for solving intricate problems involving node swapping, predictive scheduling and resource

management. MCIL has been responsible for grid-enabling critical applications in areas such as structural biology, bioinformatics, ground water modeling, earthquake engineering and computational chemistry.

"The new partnership with NVIDIA and our ongoing partnership with Dell have made possible the acquisition of a leading-edge machine, one of the fastest in New York for solving a large set of scientific, engineering and multimedia problems," Miller said. "In fact, due to the advances in heterogeneous computing, this machine cost approximately 1/1000th of the two machines in New York that have peak computing power exceeding this machine. In particular, Graphics Processing Unit (GPU)-based systems are affordable by many research groups and departments offering processing capabilities thousands of times faster than traditional systems, whereas traditional high-end clusters require extraordinary funds, space, cooling, and staffing. This is also the fastest machine on the MCIL Grid for solving many computationally-intensive problems."

Professor Jack Dongarra, one of the foremost authorities on high-end computing and director of the Innovative Computing Laboratory at the University of Tennessee said, "GPUs have evolved to the point where real-world applications are easily implemented on them and run faster than on multi-core systems. Future computing architectures will be hybrid systems with parallel-core GPUs working in tandem with multi-core CPUs."

"The Tesla GPU-based clusters used by the Cyberinfrastructure Laboratory are enabling its researchers to get supercomputing performance from smaller clusters at 1/100th the cost, significantly improving the scope and size of the research problems that they can solve. More importantly they can do this while consuming less electricity, reducing the carbon footprint required to power these systems and cool the data centers that house them," Andy Keane, general

manager, GPU Computing at NVIDIA, said.

The NVIDIA-based GPU-system was acquired with funds from the National Science Foundation's (NSF's) Collaborative Research Infrastructure (CRI) Program based on a joint proposal from UB (Miller), Niagara (McCourt), SUNY-Geneseo (Farian), and the Hauptman-Woodward Institute (Weeks). These funds have been used previously to acquire compute clusters at each of these institutions to support research, scholarship, and education at and between these institutions. In fact, at Niagara University, the Academic Center for Integrated Sciences, which will be housed in the new Thomas B. Golisano science building, has benefitted immensely from this collaboration in terms of intellectual and capital resources. The system was brought on-line by Kevin Cleary, systems administrator in the UB Department of Computer Science and Engineering, with guidance and assistance from Jon Bednasz, senior systems administrator in the UB Center for Computational Research.

Source: Hauptman-Woodward Medical Research Institute