



Case Study

Ames Laboratory

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Feng Zhang Assistant Scientist, Division of Materials Science & Engineering, Ames Laboratory

Their Challenge

The Ames Laboratory is a government-owned, contractor-operated national laboratory of the U.S. Department of Energy (DOE), operated by and located on the campus of Iowa State University in Ames, Iowa for over 65 years.

Key areas of expertise are materials design, synthesis and processing; analytical instrumentation design and development; materials characterization; catalysis; computational chemistry; condensed matter theory; and computational materials science and materials theory.

Both Ames Laboratory and DOE have been Ace Computers cluster clients for many years. Right now, Ames is using clusters primarily for deep learning. Most recently Ames contacted Ace Computers Business Development Manager Barry Spiegel to add an additional node and 8 GPU cards in order to increase processing speed.



The Ames Laboratory

The Project

Feng Zhang Assistant Scientist, Division of Materials Science & Engineering at Ames and his colleagues are working on a project titled, *Structures and Dynamics in Condensed Systems*. The project is designed to bring simulation methods together with theory and critical experiments in order to investigate structural selection dynamics in highly driven systems. They are developing a research program that is focused on the multi-scale structural dynamics of metallic liquids, glasses, and crystalline phases under far-from-equilibrium conditions. This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

Ames contacted Ace Computers Business Development Manager Barry Spiegel to add an additional node and 8 GPU cards in order to increase processing speed.

"We planned to use the node and cards in our simulation liquid and alloy systems," Feng said. "We wanted to create some models and run molecular dynamics simulations and we needed the GPU cards to accelerate the simulations. Traditional CPU cards are too slow."

Our Solution

Ames purchased the node and 8 NVIDIA® Tesla® M40 GPU cards from Ace Computers, an NVIDIA Preferred Partner.

The M40 GPU is the world's fastest accelerator for deep learning training; it is purpose-built to dramatically reduce training time. Training neural networks requires significant GPU memory; the Tesla M40 is built to handle these workloads for more accurate speech and image recognition and deeper understanding of video and natural language content. Before the M40, deep learning models typically required days to weeks to train, forcing data scientists to compromise between accuracy and time to deployment.

Barry also helped Ames implement a Slurm scheduling system. Slurm is an open source, fault-tolerant, and highly scalable cluster management and job scheduling system for large and small Linux clusters. Slurm requires no kernel modifications for its operation and is relatively self-contained. As a cluster workload manager, Slurm allocates exclusive and/or non-exclusive access to resources (compute nodes), for a period of time, to users so they can perform work. "We did have some minor issues with scheduling tasks on the M40s, but working together we were able to resolve them quickly," Barry said.

Their Success

In the end the solution achieved what Feng hoped it would and more. "It is doing more than what we needed it to do," he said. "We are able to process data 6-8 times faster. We are very happy with the new system."

Barry looks forward to a continuation of the long successful relationship with Ames. "The people at Ames are easy to work with," he said. "They are world-class experts in a number of fields involving HPC clusters and always have several interesting deep learning applications in the works."

The Ames team has already contacted Ace Computers about another similar order. "In addition to the solution itself, I am also very happy with the customer service," Feng said. "Barry has been very responsive. He answers our emails and calls promptly and takes care of our concerns effectively—those 2 things are the most important to us. I would definitely recommend Ace Computers because of the customer service and the price. I have had a very positive experience."

About Ace Computers

Leading custom computer builder and HPC cluster specialist, Ace Computers currently holds the following contracts: SEWP V, CCS-2, GSA, WSIPC, PEPPM, State of Wis., State of Ga. The company is a Woman-Owned Small Business custom technology systems manufacturer and reseller for the public sector as well as the commercial sector. Channel partners include Intel, Supermicro, NVIDIA, Mellanox and Samsung among others. An industry leader since 1983, the company is a multi-year HPCwire Readers' Choice Award finalist. In addition to some of the finest academic institutions in the U.S., long-term clients include the U.S. Department of Energy and the U.S. Department of Defense. In addition to our Greater Chicago headquarters, Ace Computers has locations in New Jersey, Pennsylvania, Virginia, and Nevada. To contact Ace Computers, call 1-877-223-2667 or 1-847-952-6900 or visit <http://www.acecomputers.com/>.