Bielefeld University Case Study

Bielefeld University selects ScaleMP for molecular physics research

Molecular Magnetism Research Group at Bielefeld University's Physics Department Chooses vSMP Foundation to Accelerate Research and Decrease IT Management and System Costs

Universität Bielefeld

BUSINESS BENEFITS

- Reduced capital expen diture requirements since the purchase of a proprietary SMP system was not required.
- Improved performance resulting in the group's ability to more quickly achieve results in research projects.
- Increased calculation speeds enabling the research group to address more complex mathematical problems.
- Helped group maintain its leadership in the theoretical description of highly symmetric magnetic molecules.

Objective:

The Molecular Magnetism Research Group working within the Department of Physics at Bielefeld University needed a symmetric multiprocessing system (SMP) to address the computation and diagonalization of large matrices of physical quantities. The goal was to find a solution that would allow the group to perform timely local supercomputer calculations while staying within the university's allotted budget.

Approach:

Professor Jürgen Schnack, a faculty member in the Department of Physics at Bielefeld University and head of the Molecular Magnetism Research Group, investigated the purchase of a proprietary SMP before learning about ScaleMP from a vendor. His research group selected vSMP Foundation for SMP because it met their budget requirements and provided them with the amount of RAM and CPU power they require to complete their compute intensive calculations.

Customer Background:

Bielefeld University in Bielefeld, Germany, combines classical academic tradition with innovative research and teaching. Founded in 1969, Bielefeld University has attained an outstanding position among national and international academic institutions on the strength of its research achievements and unique courses of study.

As part of the university's Department of Physics, the Molecular Magnetism Research Group conducts theoretical research in quantum mechanics, specifically investigating magnetic molecules by quantum mechanical modeling. The goal of the research group is to predict and understand how molecules behave within magnetic fields and how specific molecule reactions may be useful for future functional materials.

With many research fields within the university, each research group is responsible for identifying and purchasing technologies that are relevant to their research goals and methods used. The university provides housing in its central data center for any machines purchased and ensures the necessary power, cooling and networking requirements to support it, but each group is responsible for its own IT operations. Composed of 10-15 scientists at any given time and without a dedicated IT staff to help deploy and manage their computing architecture, the Molecular Magnetism Research Group needed to deploy a technology that was not only easy to install, but also easy to manage and maintain.

Prior to ScaleMP, the research group was mostly using an SGI Altix 4700 with 4864 dual-core Intel Itanium2 processors, 40 TB RAM from the Leibniz Supercomputing Center (LRZ), one of Germany's large computer centers which supplies free CPUs and compute power to organizations that submit and qualify. In addition to these resources, the team locally ran the group's research on three smaller servers with up to 64 GB RAM.

IT IMPROVEMENTS

- Access to a reliable, high-performance, scalable compute infrastructure.
- Easy-to-use solution with low maintenance costs which is ideal since the research group has no dedicated IT staff.
- Easy-to-program using OpenMP rather than using MPI.
- Ability to solve problems in a timely manner with local resources.

CUSTOMER SOLUTION QUICK VIEW

Hardware Stack

- 16 x Intel Servers
- Processor: 32 x Xeon X5550 (@2.67GHz)
- Memory: 384GB RAM, RHEL 5.5

Virtualization Layer

- vSMP Foundation

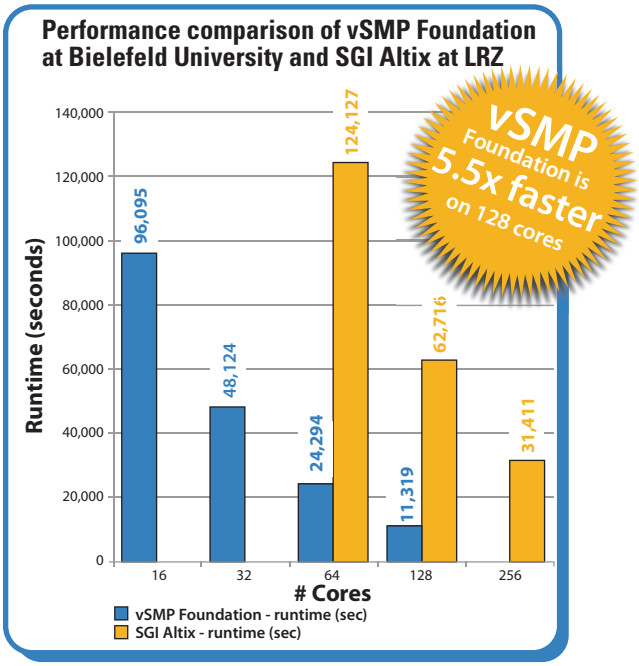
Software Stack

- Red Hat Enterprise Linux (RHEL) 5
- OpenMP home-grown codes

Customer Challenges

One of the main challenges the Molecular Magnetism Research Group faced was that they were using computing resources from the Leibniz Supercomputing Center which – although they were free – were not flexible enough to allow them to run timely smaller projects. Although LRZ is very useful for large and long-term projects, Professor Schnack's group needed a complementary local solution without the restrictions of queues and job classes.

"Although we were able to use the Leibniz Supercomputing Center resources for free, we often needed the numerical solutions faster than the Supercomputing Center could deliver since those resources are valuable and in such demand," said Professor Schnack.



A key challenge the research group faced was the limited amount of memory on their local servers. The group's large matrices require large amounts of RAM to be run and calculated. Additionally, because the group was running such large, memory-intensive applications, the stability of the resources is a major issue.

"We use high performance computers for our calculations but don't produce much data so don't have large disc storage needs," said Professor Schnack. "What we really need is large amounts of RAM because we work with large matrices and run mathematical simulations with them. To work with these matrices, we need to use an SMP machine."

Solution Selection Process

The Molecular Magnetism Research Group first learned about ScaleMP from Bull, the French infrastructure company from whom the group purchased its servers. Since the group needed more memory, Bull recommended that Professor Schnack and his team take a closer look at ScaleMP's server virtualization for aggregation hypervisor. After speaking with ScaleMP, Professor Schnack realized that ScaleMP's technology could provide the group with the large amounts of memory and high-core-count they required, which led him to adopt and deploy the technology in October of 2009. He ultimately chose ScaleMP's vSMP Foundation for SMP technology because he found it to provide a stable, large memory solution, and a lot of computing power, while being much more cost effective than purchasing a proprietary system for 200,000 Euros.

"Since all of our projects are funded by grants, we need to be cognizant of the amount of funding we apply for and spend on a technology solution," said Professor Schnack. "We were definitely looking for the best solution for the amount of money we had, which was not enough to spend on one of the more expensive, proprietary systems available on the market. Based on the recommendation from Bull, we were excited to learn more about ScaleMP and ultimately apply for the funding to purchase and deploy the solution."

The Molecular Magnetism Research Group deployed vSMP Foundation for SMP along with Intel Xeon Quad Core Nehalem processors for a total of 128 cores and 384 GB of RAM. Although the group was previously running their research on Intel Itanium II processors, they found Nehalem processors to be less expensive and to provide better performance. Since the group does not have a dedicated IT staff on hand to deploy and manage technology investments, a large benefit the group recognized from its deployment of vSMP Foundation for SMP was the fact that it was extremely easy to deploy and use.

"I'm a physicist and I solve physics problems," said Professor Schnack. "I want to focus my time on research projects, not on learning details about the underlying IT infrastructure we are using to run our simulations. With vSMP Foundation, I am able to focus on my physics problems without worrying about IT management taking time away from my research. As it turns out, Bull's recommendation of ScaleMP was very beneficial to us, and has allowed us to do what we need, without spending time on managing the infrastructure."

Benefits:

With vSMP Foundation, The Molecular Magnetism Research Group at the Department of Physics at Bielefeld University has recognized the following key benefits:

- Accelerated research by offering an on-premise, easy-to-access SMP: Since vSMP runs on local hardware, the research group can complete timely problems locally in a much shorter time. Today only very large long-term projects are submitted to the Leibniz Supercomputing Center.

- Increased amounts of memory to support high performance workloads: vSMP Foundation allows the research group to scale up memory and CPU power for its matrices, all while leveraging existing server infrastructure.

- Improved quality and impact of research: vSMP Foundation allows the research group to increase calculation speeds and solve larger problems than they were ever able to before. Now, they can do high priority problems locally and submit problems that have a longer timeline or need more resources to the Leibniz Supercomputing Center.

- Ease of programming: vSMP Foundation provides researchers with programming model of choice. Contrary to clusters, researchers can use OpenMP and scale their programs to utilize all the available CPU cores.

- Decreased time spent on management: vSMP Foundation enables the research group to spend more time focusing on its research and less time managing the technology used to run their simulations.

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