The Gene Center of the University of Munich (LMU)

Mini-Supercomputer in a Box:
512 Cores, 4 TB DRAM in 10 Rack Units and 3.5 KW

Website
http://www.genzentrum.lmu.de/

Background
The Gene Center is a central research facility of the Ludwig-Maximilians University (LMU) of Munich. The Center houses 15 labs with 250 personnel. Research is focused on structural biochemistry, genome maintenance and the regulation of gene expression using cryo-electron microscopy, x-ray crystallography, deep sequencing, and computational biology.

Applications
Genomic Deep Sequencing, Cryo-Electron-Microscopy Maps, 3-D Molecular Modeling, HHsuite, High Performance Computing (HPC), SPIDER, Relion, NAMD, Gromacs, Infiscale, Scientific Linux

Challenges
- Computing constraint due to power limitations in server rooms
- Poor message passing interface (MPI) scaling to more than a few nodes
- High CAPEX to purchase HPC server clusters, supercomputers, or integrated clusters

Solution
- SeaMicro SM15000-OP (AMD Opteron™) and SM10000-XE (Intel® Xeon®) high density servers
- 1,024 computing cores in 30 rack units or 52.5 inches (1.3 meters)
- 1.28 Tbps SeaMicro Freedom™ Supercompute Fabric

Results
- Supercomputer-like performance with up to 90 percent MPI scaling
- Eliminated the need for InfiniBand® and 10 GbE switches
- 2X computing density compared to blade servers
- 50 percent savings in power and space

As a leading life sciences research center, the Gene Center at LMU has invested over $1 million Euros in computing and IT infrastructure. The research requires intensive computational capability that has traditionally been only found in custom built, highly expensive high performance computing (HPC) clusters or supercomputers. A small supercomputer costs around $500,000[1], requires a minimum of one full rack and requires up to 25KW of power[2]. Researchers have turned to these high performance clusters because of their computing density and high bandwidth interconnects and maintenance.

The Gene Center at LMU has been growing, and as the number of research projects increased, additional computing capacity was required. HPC clusters were one option, however, due to the complexity and operational overhead, a more integrated solution was desirable. The Gene Center narrowed its decision down to the Dell™ PowerEdge™ M1000 blade server and AMD's SeaMicro server. Most server rooms only had 10KW to 12KW of power, and one of the key criteria was the highest computing capacity in the densest form factor fitting within this power budget. After extensive testing and analysis, the SeaMicro server was selected due to its power efficiency, computing density, and the ability to deliver supercomputer performance at a fraction of the cost.

[1] Cray press release, Cray Expands Line of Cray XC30 Supercomputers with New Technical Enterprise System, May 7, 2013.

[2] Cray XC30-AC Supercomputer datasheet

[3] Ronald Beckman, et al. "Structures of the human and Drosophila 80S ribosome." Nature, May 2, 2013.

SeaMicro SM15000™ Enables World's First 3D Structural View of Human Ribosome

AMD's SeaMicro servers have accelerated the Gene Center's research in understanding biomolecular structures and have resulted in the acceleration of research related to analyzing the ribosome of higher eukaryotes, such as humans. The findings were published in the May 2013 edition of the prestigious journal *Nature* in an article titled *Structures of the human and Drosophila 80S ribosome*[3]. Using over 800,000 images to create a 3-D image, the researchers discovered that metazoan-specific ribosomal RNA and ribosomal proteins co-evolved and revealed the presence of two additional structural layers in metazoan ribosome. The findings advance the understanding of how bacteria ribosomes can be broken down without harming human ribosomes, similar to how some antibiotics work.

The Gene Center also develops and runs general bioinformatics services such as protein homology searches, which help to understand unknown proteins. The most demanding task in running these services is computing the Findex databases that drive the searches. This, as well as the actual searches, which are crucial to the accuracy of sequence-based protein

> "AMD's SeaMicro servers provide a computational edge by delivering supercomputer-like performance in the industry's smallest form factor. It is really a mini-supercomputer in a box, and it is accelerating my research and allowing us to do analysis and break new ground in the field of structural biochemistry."
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> **Ronald Beckmann**
> Professor, Gene Center at LMU

function and structure predictions, can now be scaled better and run much faster thanks to the bandwidth and SeaMicro Freedom™ Fabric features offered such as, mapping all drives to all compute nodes. The tool developed by the Gene Center has 50–100 percent higher sensitivity than other tools and generates more accurate alignments while being orders of magnitude faster when run on the SeaMicro SM15000.

Scaling Message Passing Interface (MPI) — Eliminating the Need for InfiniBand

One particular challenge in computational analytics in the HPC field is the nonlinear scaling of MPI. MPI is the de facto standard for communication among processes that model a parallel program running on a distributed memory system, most commonly found in supercomputers. With other interconnect technologies, researchers at the Gene Center often saw MPI scaling inefficiencies, but with AMD's Freedom Fabric technology with 1.28 Tbps bandwidth, they found this interconnect bandwidth constraint could be removed and they now experience MPI scaling of up to 90 percent. The SeaMicro system with its supercompute fabric eliminated the need for 10 Gbps InfiniBand, which costs as much as 20,000 euros.

The groundbreaking work at the Gene Center has the potential to make medications safer and more effective, while unlocking the secrets of how life works on the molecular level. Some newer drugs breaking
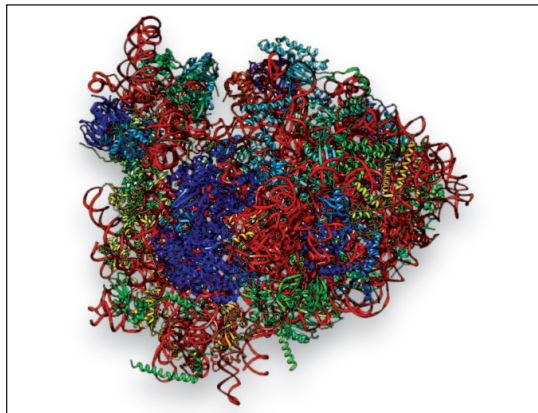
Structure of the D. melanogaster 40S ribosomal proteins — The asymmetric unit for this structure is composed of multiple PDB entries: 3J38, 3J39, 3J3C, and 3J3E. Image from the RCSB PDB (www.pdb.org) of PDB ID 3J38 (Anger AM, Armache JP, Berninghausen O, Habeck M, Subklewe M, Wilson DN, Beckmann R. (2013) Structures of the human and Drosophila 80S ribosome Nature 497: 80-85).

> "AMD's SeaMicro mini-supercomputer is simple to deploy, easy to manage and provides the industry's best price to performance value. I deployed 128 servers consisting of 512 computing cores, and the systems have run flawlessly."

Andreas Hause
Scientific Computing Expert at the Gene Center at LMU

down the bacterial ribosome have only been allowed for adults for now. Hopefully research like this helps bring these sometimes more effective medications to a wider range of use without side-effects. This is all enabled by creating 3-D images to understand the ribosome structure to see how a protein is built. Once this is understood, it will ultimately lead to the development of new, more effective cures that can more effectively break down the ribosome of bacteria.

AMD's SeaMicro server product family currently supports the next generation AMD Opteron™ ("Piledriver" core-based) processor, Intel® Xeon® E3-1260L ("Sandy Bridge") and E3-1265Lv2 ("Ivy Bridge") and Intel® Atom™ N570 processors. The AMD SeaMicro SM15000 also supports the Freedom Fabric Storage products, enabling a single system to connect with more than five petabytes of storage capacity in two racks. This approach delivers the benefits of expensive and complex solutions such as network attached storage (NAS) and storage area networking (SAN) with the simplicity and low cost of direct attached storage.

For more information about AMD and the SeaMicro family of high density, low power servers, please visit **www.seamicro.com**.