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Joining the world's supercomputing league: New Leibniz Computing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities was inaugurated with the introduction of the new national supercomputing system SGI Altix 4700, on July 21, 2006

On Friday, July 21 2006, Federal Minister for Education and Research Dr. Annette Schavan, the Bavarian Minister President Dr. Edmund Stoiber, and the Bavarian Minister for Science, Research and the Arts Dr. Thomas Goppel inaugurated the new building of the Leibniz Computing Centre in Garching near Munich (budgeted at ca. 45.2 Million Euros). At the same time the new national supercomputing system (budgeted at ca. 38 Million Euros) started operation.

The new system will not only strengthen LRZ's standing in the area of high performance computing, but will also ensure improved competitiveness of the Munich area as well as Bavaria on an international level with respect to scientific computing capability. The new, extensible building, the technical infrastructure, the existing know-how, the firm foundation in many application areas and the nationwide unique combination of economic, industrial and scientific surroundings combine in an ideal manner in favour of LRZ. As a consequence, LRZ is a serious candidate for becoming a European supercomputing centre.

The newly erected building which now houses the Leibniz Computing Centre of the Bavarian Academy of Sciences and Humanities is the most modern and - due to its 5700 m² floor space and 5000 m^2 system floor space – the largest computing centre building in Germany. The building, which was designed by the building enterprise Herzog & Partner BDA, is architecturally divided into three major parts:

1. Compute Cube: National supercomputing system, servers for network and IT infrastructure, the Linux cluster and the extensive data backup and archiving facilities as well as the expensive infrastructure providing electricity and cooling are housed in a remarkable, cube-shaped building measuring 36 meters in each dimension. Within this area increased security measures are enforced, and hence no public access is possible. An electrical power of nominally 4.8 MVA can provide up to 2 Megawatts to the compute systems, and a further 2 Megawatts to the cooling systems. Uninterruptible power supplies are provided. The cooling of the national supercomputing system requires an air throughput of 400,000 m³/hour. Sophisticated security and fire extinguishing equipment protect the technical infrastructure. Further extension due to future demands from additional cooling, electricity or compute systems can easily be performed.

- 2. *Institute Building:* The offices and labs of the 170 LRZ staff members are located in the institute building. The ground floor also provides public access (reception, PC-equipped work places for students, offices for help desk and telephone hotline). The three upper stories house the staff offices, labs, conference rooms and the central control room.
- 3. *Lecture and Conference Building:* The new building provides a lecture room with 120 seats and a number of seminar rooms of varying sizes. This area of intense public access will mainly be used by students and scientists of the universities in Munich for LRZ presentations (e.g., workshops for computational sciences, DEISA, D-Grid), for series of lectures, or for short-term courses.

The new building was completed within only two years. The cost of around 45.2 Million Euros was borne by the German Federation and the State of Bavaria in equal parts, based on the HBFG (Hochschulbauförderungsgesetz). It would not have been possible to install the new supercomputing system within the old LRZ building in the centre of Munich (Barer St. 21) due to an aged and insufficient infrastructure; furthermore more office space was needed for a staff which is considerably increasing because of new areas of responsibility and recent successes in starting third-party funded projects.

The new supercomputing system replaces the previously used Hitachi SR8000, which was retired on June 30, 2006 after more than six years of user operation. The investment budget for the new system, which is deployed as a nation-wide supercomputing system, is 38 Million Euros. This budget is also provided via the HBFG, and hence is covered in equal part by Federal Republic and the State. The new system will be placed at around rank 13 in the Top500 list of the fastest computers worldwide. With respect to sustained performance, i.e. the performance achieved by the actual scientific users' application profile running on the system, it can be numbered among the fastest systems available worldwide.

Based on a Europe-wide tendering procedure which yielded a number of interesting offers, SGI's Altix 4700 system which makes use of Intel's Itanium2 processors was selected, since it promised to deliver the highest application performance. A special feature of the selected system consists in its large, uniformly addressable shared memory. This significantly eases the programming of parallelized applications. Due to the well-balanced ratio between compute and I/O performance, the wealth of available software tools and applications, and the usability-targeted embedding into the computing centre's infrastructure the new national supercomputing systems throughout Germany.

The *performance* of the new computer is impressive. Phase 1 which is starting operation now, is comprised of 4096 Madison9M processors which are coupled via a ccNUMA fabric, and provides a peak performance of 27 trillion floating point operations per second (27 TFlops). In Phase 2, to be installed in summer 2007, this number will increase to more than 60 Teraflops. The size of the main memory is presently 17 TBytes, and will be increased to ca. 40 TBytes. The presently available 300 TBytes scratch disk space will be later increased to 600 TBytes. For the user's home directories 40 TBytes of NAS storage (later 60 TBytes) will be available. Connection to the outside world is provided by the German scientific network using 10 Gigabit/s ethernet technologies.

All common programming languages, tools, and parallelization paradigms (from pure OpenMP parallelization on up to 252 processors in a shared memory up to pure MPI parallelization using more than 4000 CPUs as well as any hybrid combination of the two) will

be available. As a result, new orders of magnitudes of computability will open up in many areas of scientific investigation.

The new system will be mainly deployed for simulations of complex systems and processes in physics, materials science, fluid dynamics, astrophysics, chemistry as well as in geo- and biosciences. Examples are: the investigation of turbulence, of flows in porous media, of the interaction of flows with deformable structures, the generation and propagation of acoustic waves, high temperature superconductivity, materials with form memory, chemical reactions during catalytic and combustion processes, the propagation of seismic waves and earthquakes, as well as investigations of sequence, structure and function of proteins. A prerequisite for usage of the system is a positive assessment of the prospective user's project by a committee of experts.

Leibniz Computing Centre of the Bavarian Academy of Sciences and Humanities

Leibniz Computing Centre (LRZ) is an institution of the commission for informatics at the Bavarian Academy of Sciences and Humanities. Nowadays, it employs 170 staff members. LRZ understands itself as a service-oriented enterprise for scientific institutions. Via the Munich scientific network, which is also operated by LRZ, all central servers and systems of the universities in Munich as well as from other scientific institutions (e.g., the Bavarian Academy of Sciences and Humanities, the Max-Planck Institutes, the Fraunhofer society etc.) are interconnected. In its role as a centre for technical and scientific supercomputing, LRZ operates an HPC system for state-wide usage, and since March 2000 also one of three national supercomputing systems, which can be used by scientists throughout Germany. Apart from investigations in the area of scientific supercomputing and IT management LRZ also is a nation-wide competence centre for data communication networks, collaborating with other scientific institutions and industrial partners within a number of pilot projects.

Bavarian Academy of Sciences and Humanities

The Bavarian Academy of Sciences and Humanities was founded in Munich in 1759. With a full-time staff of 350 and an annual budget of 35 Million Euros it is the largest of the seven scientific Academies in Germany. Its main focus is on interdisciplinary basic research, long-term research projects in the arts and humanities as well as the natural sciences, for example the compilation of scientific dictionaries, publication indices, and critical complete editions, which provide an essential basis for scientific teaching and research. The Academy maintains international contacts and arranges symposia on present research activities, e.g. in the area of ecology or medicine. The 39 commissions encompassed by the Academy presently supervise 129 research projects. Two of the commissions additionally operate scientific institutions in Garching: Leibniz Computing Centre and the Walther-Meißner institute for low-temperature research.