



# MAX PLANCK *News*



Photo: IBM

**MORE POWER FOR THE GWDG AND  
THE GARCHING COMPUTER CENTER**

## **Computers for Complex Simulations**

Both the Garching Computer Center and the GWDG computer and competence center in Göttingen are enhancing their computing performance. At the Center in Garching, the Max Planck Society is installing an IBM supercomputer that will increase the present supercomputing system's capacity up to 20 times, to over 100 billion operations per second. This will help provide answers to a host of research questions, from the origins of the universe to nanophysical relationships. Two new parallel computing systems that were commissioned in March have already brought a five-fold increase in performance at the GWDG.

At the moment, it is still a case of wait and see: the new IBM supercomputer will be ready to help Max Planck scientists perform complex and intricate simulations beginning in 2008. "Our researchers will then be able to undertake competitive, cutting-edge work in the field of numerical simulations," says Stefan Heinzl, Director at the Garching Computer Center, where the new facility will be located. The Computer Center in the Munich suburb of Garching is operated by the local Max Planck Institute for Plasma Physics on behalf of the Max Planck Society as a whole. With 45 years of experience in the field of supercomputing, the Garching Center is one of the world's lon-

Shawn Hall, a member of the IBM research team, is seen here taking measurements at a type Blue Gene/L supercomputer. "The next generation of this system should help us in preparing, developing and optimizing applications at the level of petascale computing," hopes Hermann Lederer of the Garching Computer Center.

gest-standing civil centers of its kind.

The IBM supercomputer will be of great value to researchers in a wide range of scientific disciplines, including, for example, materials science. It is anticipated that it will contribute to a better understanding of the characteristics and functions of nano, polymer and colloid systems and membranes. In addition, it will also be employed in the field of computer-aided material design, as well as for 3D pattern recognition in macromolecular systems.

Scientists at the Max Planck Institute for Plasma

Physics will use the new system to simulate turbulence in fusion plants as part of their research contribution to the global fusion project ITER. Astrophysics projects will simulate the origins of the structure of the universe, complex interaction processes in supernovae and their effects on cosmology, gravitational fluctuations and collapse, and other cosmological tests designed to reveal the secret of dark matter. The supercomputer is also expected to provide fresh findings in the field of quantum mechanical computation models, referred to as quantum computing, by helping scientists research the equilibrium characteristics of new quantum phases in subordinate quantum systems.

The new Power Processor-based system installed by the Max Planck Society is designed for a maximum performance of more than 100 teraflops, equal to 100 billion program steps per second. Once installed, it will rank among the most powerful supercomputers in Europe, with up to 20 times the capability of the supercomputing system currently in use. It features IBM's new Power6 technology, the next step forward in the IBM Power microprocessor family, which makes this an exceptionally powerful system. In fact, this was one of the main reasons why, after a Europe-wide invitation to tender, the Max Planck Society finally decided on IBM's offer.

"This new system is another link in the long chain of pioneering IBM supercomputers, which extends from Deep Blue and ASCI White to ASC Purple. It also represents a major step forward in the field of supercomputing in Europe," explained Dave Turek, Vice President of IBM Deep Computing. "As a committed partner, our company is keen to support the Max Planck Society in resolving some of mankind's most important scientific problems."

In addition to the new supercomputer, the Max Planck Society is also taking delivery of the next



generation of IBM's Blue Gene system. This technology is optimized for the use of highly scaleable and communication-intensive applications. "Even more important," says Hermann Lederer, head of application support at the Garching Computer Center, "is the fact that the next generation of the Blue Gene system will help us in preparing, developing and optimizing applications at the future-oriented level of peta-scale computing." Peta-scale means computing performance on the order of peta-flops per second – that's a trillion program steps per second.

The Garching Computer Center is not the only one to upscale its computing performance: the Gesellschaft für wissenschaftliche Datenverarbeitung Göttingen (the GWDG computer and competence center) is also acquiring new high-performance parallel computing systems. One of the principal tasks of the GWDG is to provide state-of-the-art high-performance computing services for scientists of the Max Planck Society and the University of Göttingen. In contrast to the Computer Center in Garching, the experts in Göttingen are already enjoying the benefits of the increased computing power: their two new systems were commissioned at the end of March. For applications with extensive storage and communication requirements, they now have a shared memory processor (SMP) system at their disposal. And for applications with a medium to low communication requirement, a cluster system is available.

With an overall computing power of almost 10.5 teraflops per second, these two multicompilers are among the most powerful of their kind in the state of Lower Saxony. They represent a five-fold increase in the computing performance available for research purposes from the GWDG, enabling scientists to carry out numerical simulations of complex systems with a degree of accuracy not previously achievable.

Here, too, the benefits of enhanced computing power will be felt in many different fields. Astrophysicists are keen to simulate the magnetic fields and atmospheres of planets in greater resolution, while materials scientists aim to trace the surface characteristics of everyday materials back to forces at an atomic level, thereby improving the materials' properties. These new high-performance computers are also able to calculate the reaction mechanisms of molecules, and scientists intend to use this facility to optimize technical processes and pharmacological properties. ●

Bits and bytes and teraflops: One of the two new computing systems for the GWDG.

PHOTO: GWDG

## MAX PLANCK DIGITAL LIBRARY OPENS FOR BUSINESS

### Help in the Data Jungle

Since the beginning of the year, the Max Planck Society has had a new central service unit: The Max Planck Digital Library (MPDL), located at Amalienstrasse 33 in Munich. From here, the library staff coordinates the web-based supply of scientific information for the research organization as a whole. This includes not only the operation of the electronic infrastructure, but also the development of new components necessary to tie individual Max Planck institutes into the global scientific communications network.

"Our work begins with the question: 'What information do scientists need?'" says Laurent Romary. He is the computer linguist in charge of the Max Planck Digital Library, and as such, heads up a service unit whose function is to help Max Planck scientists keep their heads above water in the deluge of data. A Frenchman by nationality, Romary previously worked at the Centre national de la recherche scientifique (CNRS). His task at the Max Planck Digital Library is to merge two previously separate units into one: Section VIIb at MPS Administrative Headquarters

(the Electronic Library) and the Heinz Nixdorf Center for Information Management in the Max Planck Society (ZIM).

The organizational structure of the Max Planck Digital Library reflects these twin roots: the Information Supply department essentially comprises the former Section VIIb headed by Ralf Schimmer. This department will continue to support Max Planck institute libraries by providing them with literature, and will take charge of the MPS's Digital Library Services. Well-established services, such as the Electronic Journals Library (EZB), the Max Planck Virtual Library (vLib) and the Linking Service (SFX), will continue to be operated by this department. The counterpart Research and Development department under the leadership of Malte Dreyer will pursue projects initiated by the ZIM, including the eDoc server, which is the digital archive of the MPS, and also the Living Reviews series of journals.

However, the Max Planck Digital Library is intended to be far more than just the sum of its pre-existing parts, as Romary emphasizes: "The

new organizational structure is bound to deliver synergies. But most importantly, there is now a central unit that coordinates all e-science services within the Max Planck Society and that is perceived by the institutes as a competent partner and point of contact."

In answer to the question 'What is e-science?', Ralf Schimmer explains: "There is a radical change taking place in the environment in which scientists work, as new opportunities for communication and a torrent of data hugely accelerate the

exchange of information. We need to develop digital services that will keep us more closely in touch with Max Planck researchers, and think of ourselves as a kind of support agency. By providing them with innovative data processing tools, we are helping scientists create new knowledge." Given its role, the new service unit has a rather unusual format. Legally, the Max Planck Digital Library has the status of a Project Group and is initially limited to a five-year term.

In addition to already existing projects, the Max Planck Digital Library intends primarily to promote the concept of free access to electronic scientific resources.

And then there is eSciDoc – in the coming years, this name will come to stand for a high-performance integrated information and communication platform serving the Max Planck Society as a whole. Laurent Romary also attaches particular importance to cooperation with the institute libraries of individual Max Planck institutes, whose decentralized service is irreplaceable.

He also intends to work closely with the Information Retrieval Services (IVS) operated by the Chemistry, Physics and Technology Section and the Biology and Medicine Section, which offer assistance in subject-specific research. There are also plans to develop digital databases particularly for scientists working in the humanities and social sciences – a complex undertaking, as Romary well knows, given that the range of sources can be highly specialized – from art objects and historic legal texts to audiovisual media. "Particularly when dealing with audiovisual data inventories, it is crucial to be careful not to infringe on personal rights." In that sense, life is easier for astrophysicists: galaxies rarely complain about invasions of their privacy. ●



Head of the Max Planck Digital Library: Laurent Romary

PHOTO: CNRS/PHOTOHEQUE/CHRISTOPHE LEBEDINSKY

## COOPERATION WITH FRAUNHOFER INSTITUTES

## From Biomass to Fuel Cell

Fuel cells are predominantly powered by hydrogen. In the future, rather than continue to use fossil fuels as in the past, greater use is to be made of biomass as the source of this hydrogen. In a new research project entitled ProBio, scientists at the Max Planck Institute for the Dynamics of Complex Technical Systems in Magdeburg are working together with colleagues from two Fraunhofer Institutes to investigate how such renewable raw material can be effectively used to generate electricity without harming the environment.

PHOTO: P. FÖRSTER



Kai Sundmacher, Spokesman for the joint ProBio project and Director at the Max Planck Institute for the Dynamics of Complex Technical Systems, with a stack of PEM fuel cells that are powered by hydrogen.

combustion chambers to provide heat, or in gas engines to generate electricity.

Researchers at the Fraunhofer Institute of Ceramic Technologies and Systems (IKTS) in Dresden are studying the application of this gas in a high-temperature fuel cell. In parallel, scientists at the Max Planck Institute in Magdeburg are investigating the use of combustible gases in low-temperature fuel cells, after the gas has been purified by these newly developed methods. Fuel cells convert chemically stored energy directly into electrical energy in a process that yields significantly higher levels of efficiency than conventional power station technologies.

The results of experiments by all partners in the project are being collated at the Max Planck Institute for the Dynamics of Complex Technical Systems. The data is then used by Max Planck scientists to simulate the generating plant as a whole. The results of the simulation are also expected to prompt improvements in the design of equipment components and the materials and energy transfer methods by which these are connected.

At the very latest following the publication of the latest study by the Intergovernmental Panel (IPCC) in February 2007, it became clear that climate change is unstoppable. However, its effects can be mitigated. Hopes are pinned particularly on regenerative energy sources and fuel cell technology, and all the more so when the two are combined. "We intend through ProBio to discover the most efficient and environmentally friendly way of generating electricity from biomass," relates Kai Sundmacher, Director at the Max Planck institute, describing the aims of the research project.

The scientists are currently working on the optimum constellation of individual processes in readiness for the subsequent development of a quasi-industrial pilot plant. When biomass, such as wood or straw, is gasified, the resulting combustible gases are rich in hydrogen. However, before the gases can be fed into the fuel cell, they must undergo special treatment and purification processes. The Fraunhofer Institute of Factory Operation and Automation (IFF) in Magdeburg is developing such processes for ProBio, based on the principles of fluidized solids technology. Most significantly, the combustible gas thus produced has a variety of uses – not just in fuel cells, but also in

Provided an evaluation of the first phase of the project proves successful, a second three-year research phase is planned. After that, the theoretical and experimental findings should help to develop and operate a quasi-industrial pilot plant. The three institutes involved have their sights set on jointly building and running the plant in Magdeburg. Michael Schenk, Institute Director of the Fraunhofer IFF, commented: "With the energy sector developing at a headlong pace, industry in Germany urgently needs plants like this." His colleague in Dresden, Alexander Michaelis, Director of the Fraunhofer IKTS, is of the same mind: "Our research results are designed for direct practical application to support the process of innovation."

As part of the Pact for Research and Innovation, both the Max Planck Society and the Fraunhofer Gesellschaft have agreed to intensify their already existing diverse joint ventures. The joint projects undertaken by these organizations are intended to accelerate the process of innovation by closely integrating basic and applied research. ProBio is one of the first of these projects to get under way in Germany. The two societies are providing funding totaling 4.2 million euros – a clear sign of the commitment of these organizations to the research centers in the former East Germany. ●

## MPI FOR PLANT BREEDING RESEARCH (MPIZ)

## And the Winner Is ...

The MPIZ Innovation Award for non-scientific staff has been in existence since 2004. It is presented by the Max Planck Institute for Plant Breeding Research in recognition of ideas that might, for instance, simplify work processes or offer unusual solutions to technical problems. The award is currently unique among Max Planck institutes and compares most directly with the operational suggestions schemes common in industry. The prize money of 500 euros was donated by Max Planck Director Paul Schulze-Lefert.

There are scores of awards for scientists – they make an impression when applying for positions, add to one's reputation and, in some cases, yield substantial prize money. But beyond the glorious scientific breakthroughs in the academic world, there is a huge fund of creative potential at Max Planck institutes that plays a part in the leading-edge research of the MPS – the non-scientific staff.

That is why, back in 2003, Paul Schulze-Lefert, Director at the MPI for Plant Breeding Research in Cologne, had the idea of offering a prize for these employees to compete for – the Innovation Award. The prize money of 500 euros was donated out of his own pocket. Just what motivated him Schulze-Lefert now finds difficult to recall: "I honestly cannot remember. Possibly a guilty conscience after the rigorous restructuring of the institute at that time?! But seriously, I think it's great when staff have the courage to express their ideas and get involved – and I don't mean just scientists, I mean all employees."

The Award is unusual and is comparable at best with the prize for Employee of the Year most recently awarded by the MPI for Biophysical Chemistry in 2004. In that case, the prize was also initiated at the private behest of two Institute Directors, Peter Gruss and Herbert Jäckle. Back in 1999, they were awarded the German Future Prize and wanted to pass on a part of the prize money to their staff. To do this, they set up a foundation that annually presented awards to two institute employees – one scientific and one non-scientific. The criteria for the latter were to be an idea, a particular commitment or a piece of work that facilitated, simplified or significantly improved one or more aspects of the institute's research.

The Innovation Award at the Max Planck Institute for Plant Breeding Research has exactly the same object. And the idea itself has proved to be a winner: in late 2006, a diverse jury of Advisory Board members, Directors and technical employees met for the fourth time to decide who should receive the distinction. The victor was Amanda



Imaginative posters are one reason why the Innovation Award is successful: "Every time we passed one of the posters, my colleagues urged me to put my idea forward," says 2007 prize-winner Amanda Davis.

Davis, who was chosen for a suggestion that substantially simplified work in the laboratory. Her idea: to use sand as a substrate instead of an agar culture medium in the selection of *Arabidopsis* transformants.

*Arabidopsis thaliana*, an unprepossessing plant with the common name of mouse-ear cress, is the workhorse of plant genetics. In many laboratories, foreign genes are routinely introduced into *Arabidopsis* plants – and the seed is transformed. Laboratory staff then have to identify the *Arabidopsis* shoots in which the transformation was successful. Amanda Davis was able to simplify this work stage for antibiotic-resistant *Arabidopsis* transformants. She developed a standard procedure by which selection takes place on a sand substrate. Sterile conditions can be dispensed with, yet despite this, the risk of contamination, for example by fungi, is substantially reduced.

Although she was initially reluctant to submit her suggestion, Amanda Davis is convinced of the concept behind the Innovation Award: "Sometimes we technical assistants never even get to hear if someone in the laboratory next door has an inspiration. Thanks to the Award, there is now a much-improved exchange of ideas." So the Innovation Award ultimately benefits all of the staff at the institute – regardless of whether they are scientists or non-scientists. ●

PHOTO: MPI FOR PLANT BREEDING RESEARCH

**JOINT EXCELLENCE:** The Max Planck Society and the University of Heidelberg intend to work even more closely together. Max Planck President Peter Gruss and University Rector Peter Hommelhoff have concluded an agreement that summarizes the details of future cooperation, including dual appointments, Max Planck fellowships, International Max Planck Research Schools (IMPRS) and, of course, joint research projects. This is the first time such a package has been put together that simultaneously embraces four Max Planck institutes. "The promise of success inherent in this joint venture underscores the excellence of both partners, whose strengths are employed to full advantage here," commented President Gruss about the agreement. The Max Planck Society maintains Institutes for Astronomy, Nuclear Physics, Medical Research and Comparative Public Law and International Law in Heidelberg. In common with many other individual Max Planck institutes nationwide, they have been cooperating successfully with universities for a long time. Proof of this can be found in the results of the Excellence Initiative, in which both Heidelberg University and other similar establishments that are networked with Max Planck Institutes took leading positions.

proportions of young viewers, not least because of its popular German-language programs *Galileo* and *Wunderwelt Wissen*. As a result, MAX subject matter is now available to a wider audience. But max-wissen.de is also benefiting from this joint venture: in the first few months, visitor numbers grew 60 percent.

**MAX PLANCK INNOVATION**, the Max Planck Society's technology transfer unit, has signed a so-called co-licensing agreement with Stratagene, covering the exploitation rights to more than 150 microRNA sequences. This is the last license to be granted for the development of diagnostics. MicroRNAs play an important role in functions that are vital to the life of cells, and therefore probably also in the origins of various diseases, including metabolic disorders, infections and cancer. As a result, there is substantial interest on the part of industrial companies to use microRNAs as a basis for new diagnostic aids and treatments. In the interest of making rapid progress in this field, Max Planck Innovation has decided on a differentiated licensing strategy. "For research purposes, we grant broad, non-exclusive licenses to microRNA technology. For treatment purposes, we have issued a total of two co-exclusive licenses, and in

the field of diagnostics we have limited access to four partners," explained Jörn Erselius, Managing Director of Max Planck Innovation. The existence and function of microRNAs in vertebrates were discovered and first described in 2001 by Thomas Tuschl and his team at the Max Planck Institute for Biophysical Chemistry in Göttingen.

**PLUS 6 EQUALS 49:** The Max Planck Society has decided, in addition to the 43 International Max Planck Research Schools (IMPRS) already in existence, to establish six more in the course of the year. Three will special-

ize in aspects of the Humanities and Social Sciences, two will supplement the research of the Chemistry, Physics and Technology Section, and one will further the work of the Biology and Medicine Section. Since 2000, the IMPRS have become an established part of the Max Planck Society's support program for doctoral candidates. They are each the product of an initiative by one or more Max Planck institutes and work closely with universities and other research institutions, in some cases also abroad. They offer exceptionally gifted German and foreign junior scientists the opportunity to earn their doctorates under excellent research conditions. The individual Research Schools invite applications worldwide for their post-doc positions and grants. ●



**"WE LOVE TO ENTERTAIN YOU":** Since max-wissen.de went online in August 2005, the site has attracted around 200,000 visitors. The number of page views is running at over 40,000 per month. So far, however, the knowledge portal has been something of a secret in the data-filled vastness of the Internet. Now things are set to change as part of a media deal with TV broadcaster ProSieben. In January 2007, ProSieben launched a new knowledge channel on its website – and max-wissen is in on the act. Content managers at ProSieben on the lookout for suitable scientific content managed to hook up with the movers and shakers at max-wissen, who were keen to reach out to specific target groups. And ProSieben is second only to RTL in attracting one of the largest

Clever clicks: max-wissen.de now has a prominent place in the new knowledge portal operated by German TV broadcaster ProSieben.

Photo: MPS