# EXASCALE

Newsletter of Forschungszentrum Jülich on Supercomputing

JÜLICH FORSCHUNGSZENTRUM

Issue: 3 | October 2011



Member of the Helmholtz Association

## A United Europe

The world of supercomputing is in flux. In June 2011, Japan was once again top of the league: the K Computer with 8 petaflop/s knocked China's Tianhe-1A from first position in the list of the 500 most powerful computers in the world. Despite this, the USA continues to set the pace, dominating the Top500 with 255 listed computers.

Europe boasts a total of 126 systems. However, only a small proportion of these are actually also built there. Yet, all the signs point towards an offensive. Exaflop/s is the ultimate aim – a computing power that is around a thousand times faster than is currently possible. Several European initiatives have already been launched. The latest step involves setting up a European Technology Platform. It aims to bring leading technology companies together with supercomputer users from industry and research, to combine resources, and to improve the competitiveness of Europe. The partners have agreed to draw up an agenda before the end of the year outlining the most important research projects for high-performance computing (HPC). This will be used to help the European Union set the necessary priorities.

The project is closely associated with the PROSPECT consortium, which – together with French partners – aims to further develop the European technology platform. More than thirty companies, research centres and user organizations from seven countries in Europe are members of the association. Another European large-scale project is the Partnership for Advanced Computing in Europe (PRACE), which grants European scientists access to supercomputers throughout Europe. As one of the leading institutions in Europe, Forschungszentrum Jülich is among the driving forces behind these activities, coordinating PRACE with around ninety partners.

Prof. Achim Bachem
*Chairman of the Board of Directors*
*of Forschungszentrum Jülich*

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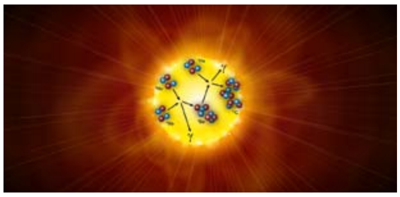
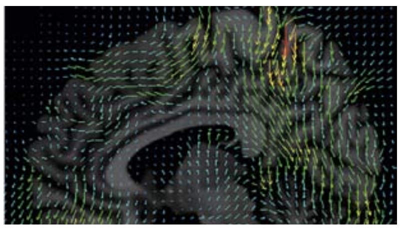








www.fz-juelich.de/ias/jsc/EN

# World-Record with Three Trillion Particles

Around eleven minutes is all it takes supercomputer JUGENE at Forschungszentrum Jülich to calculate a vast system comprising three trillion particles – a world record! This was made possible by optimizing the fast multipole method (FMM), which is one of the top ten algorithms for scientific simulations. Scientists at Jülich refined this method to allow a much greater number of particles to be simulated than was possible in the past.

FMM is used to determine long-range interactions between particles, such as the propagation of light. However, the total number of interactions that have to be considered can take on extreme proportions depending on the system. A supercomputer such as JUGENE, for example, would need 32,000 years to directly calculate all of the interactions between three trillion particles. The fast multipole method gets around having to account for each individual interaction by combining particles that are far apart to form clusters. Up to now, however, simulations using FMM were limited to a few hundred billion particles.

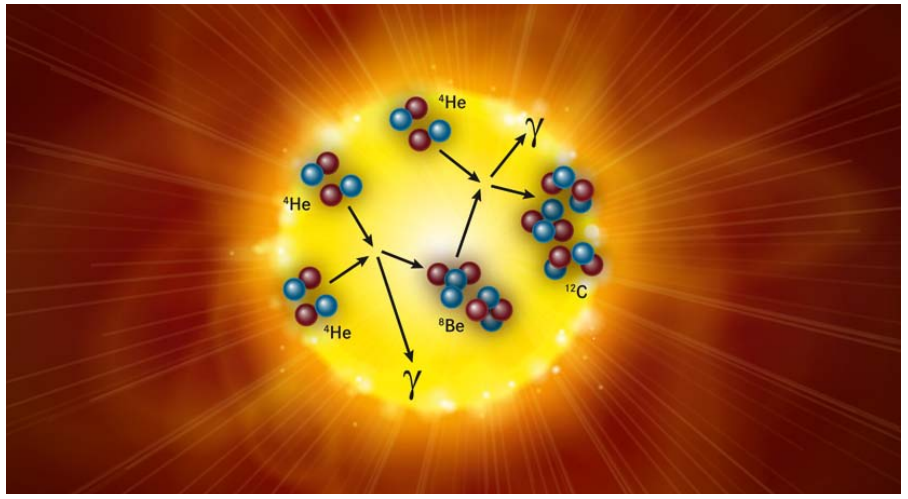
In order to push this boundary back, Ivo Kabadshow and Dr. Holger Dachsel from the Jülich Supercomputing Centre developed an algorithm that automatically checks for errors and reduces the computing time. "Supercomputers have limited storage per processor, which is why the number of particles tends to be more restricted by storage than by processor performance," says Kabadshow. The computing time required depends on three different parameters. The FMM optimized by the Jülich researchers adjusts these parameters continuously during the simulation, which significantly reduces the computing time involved.

*Simulating more particles thanks to optimized algorithm*

www2.fz-juelich.de/jsc/fmm

# Calculating the Basis of Life

One of the greatest scientific mysteries is the origin of life. Would we exist if different physical laws prevailed in the universe? A group of physicists headed by Prof. Ulf-G. Meißner at the Nuclear Physics Institute and the Institute for Advanced Simulation at Forschungszentrum Jülich are working on providing a partial answer. Using the Jülich supercomputer JUGENE, they succeeded in solving a puzzle that had eluded scientists for fifty years. They calculated what is known as the Hoyle state in its entirety, which is one of the basic prerequisites for the origin of life.




*Rarely successful: stable carbon-12 is formed from helium-4*

The base material for organic life is carbon, which is most commonly found in the universe in the form of the carbon-12 isotope. It is created by the fusion of three helium nuclei in massive stars, albeit not directly. First, a high-energy intermediate state is formed for a brief instance – the Hoyle state, which was predicted back in 1954 by astronomer Fred Hoyle. This state tends to decay, breaking up into beryllium-8 and helium-4. Stable carbon-12 is formed in only about four in ten thousand cases.

The Jülich supercomputer JUGENE needed almost a week to reproduce the Hoyle state. "To do so, we needed a new computing technique and a supercomputer capable of implementing it," says Meißner. Now, the researchers can investigate the important fusion processes in detail. "The Hoyle state is a prime example of the anthropic principle, according to which the natural constants of our universe behave in such a way that it allows us to exist as observers," explains the physicist. His team now want to change various parameters and see what happens. If the energy of the Hoyle state was to change in response, for example, no carbon-12 would be produced – and neither would life.

Physical Review Letters DOI: 10.1103/PhysRevLett.106.192501
www.fz-juelich.de/SharedDocs/Meldungen/PORTAL/DE/2011/11-05-12meissner.html





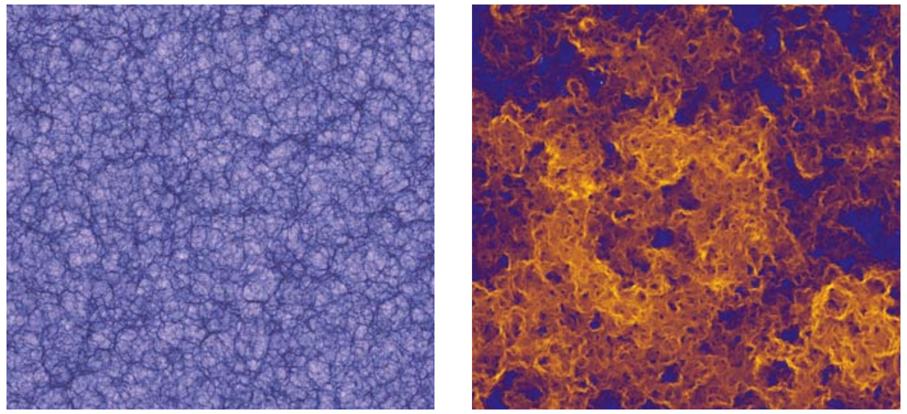
# The Cosmos in Time Lapse

Experts believe that in the universe there is about six times more dark matter than visible matter. The name "dark matter" was coined because this type of matter has not yet been directly detected by the observation instruments used in astrophysics – it is basically invisible. However, the majority of astronomers still believe that it exists because the mass of the planets and the stars is itself not enough for them to form galaxies by mutual attraction.

Prof. Volker Springel, head of the research group "Theoretical Astrophysics" at the Heidelberg Institute for Theoretical Studies (HITS) hopes to throw some light on dark matter. Within the project "Millennium XXL", he uses the Jülich supercomputer JUROPA to simulate the development of the universe from a time shortly after the big bang to the present day. In so doing, he works together with fellow researchers from the Virgo Consortium – a collaboration of astrophysicists who perform simulations on supercomputers.

The starting point for "Millennium XXL" is cosmic background radiation. It originated around 380,000 years after the big bang and can still be measured today. It is also the basis of our knowledge of the universe back then. The simulation begins at this point in time and calculates the development of the universe over the following 13.6 billion years right up to today. As the entire universe cannot be accounted for in the simulation, Springel's group simulates a representative section of the universe – a space cube with an edge length of around 10 billion light years and around 300 billion particles. This makes the project the biggest cosmological simulation in the world.

"The simulation allows us to investigate the extremely complex relationships between the galaxies and the distribution of matter in more detail," says Springel. The researchers can learn more about the properties of dark matter, for example, and test the underlying cosmological model. To do so, they map out step by step how the visible universe developed around the dark matter.



*Distribution of matter in space: projected density of dark matter in a cross section of the simulation (left), large-scale potential fluctuations in the simulated early universe (right).*

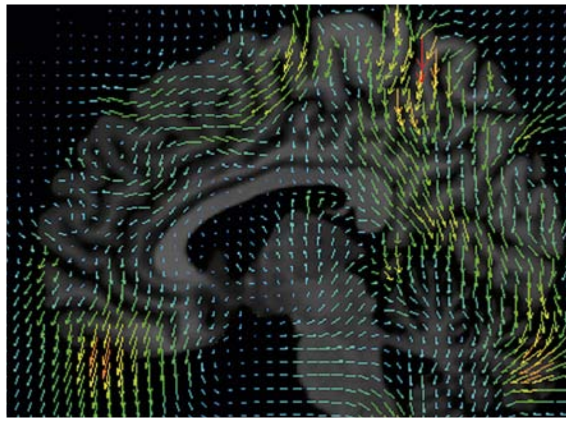
www.h-its.org/english

# A Thousand Times Faster with Booster

Simulation scientists are faced with increasingly challenging tasks. They model entire biological organs and develop evermore multifaceted models of the climate, the universe or the complex building blocks of matter. To do so, they need increasingly more powerful computers. However, the existing concepts cannot be infinitely expanded without causing the effort and costs to increase disproportionately. What Forschungszentrum Jülich is planning to achieve with the research project DEEP (Dynamical ExaScale Entry Platform), which will be funded with € 8 million from the European Commission, is therefore nothing less than the dawn of a new generation of supercomputing.

DEEP aims to create a new computer architecture that will make exascale a reality in around ten years – or to put it another way, to facilitate a computer performance of one exaflop/s. This is around a thousand times faster than supercomputers today. Researchers at Jülich want to optimize hardware networks and to integrate new cooling systems. For the project they have joined together with fifteen partners from research and industry, including companies such as Intel and ParTec with whom they also operate an ExaCluster Laboratory.

Two important elements in DEEP will be new MIC processors specially developed by Intel for parallel computing with fifty plus cores on one chip, and a network for parallel computers known as Extoll, which was developed at Heidelberg University. "Basically, we want to make parallel computers even more parallel," says Dr. Norbert Eicker from the Jülich Supercomputing Centre. The networked MIC processors will create a new type of booster. In addition to a cluster of conventional processors, the idea is that they will accelerate massively parallel applications and program components and thus increase the performance of the system as a whole.



*Technology for the future: brain simulation*

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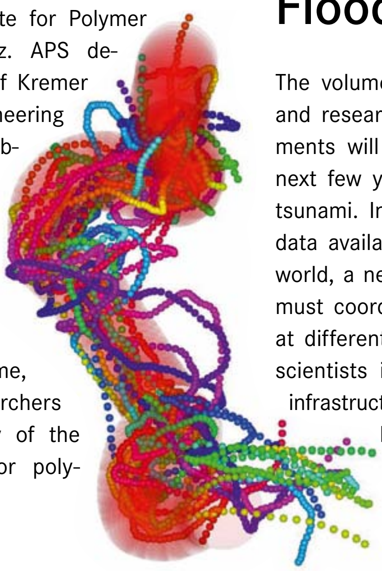
## NEWS IN BRIEF

# Unique Even Twenty Years Ago

Former Jülich solid-state researcher Prof. Kurt Kremer and Gary S. Grest from Sandia National Laboratory in Albuquerque were jointly awarded the Polymer Physics Prize by the American Physical Society (APS). The society paid tribute to their work on one of the first supercomputers at Forschungszentrum Jülich more than twenty years ago. "Back then, 1500 Cray X-MP hours was an enormous amount of time. Such calculations were only possible in Jülich; some of our fellow researchers even considered that to be impossible," says Kremer looking back. Today, Kremer is Director of the Max Planck Institute for Polymer Research in Mainz. APS described the work of Kremer and Grest as a pioneering contribution to establishing numerical simulations as a tool on an equal footing with theory and experiment in the field of polymer science. At the time, the two researchers proved the validity of the reptation model for polymers.



# Demand for Jülich's Know-How in the USA

The Jülich Supercomputing Centre (JSC) is the only institution outside of the USA involved in the creation of the Extreme Science and Engineering Discovery Environment (XSEDE). The cooperation of sixteen American computing centres provides more than 10,000 scientists from different scientific disciplines with easy access to computing time on supercomputers for their simulations. The project is the largest in the USA involving distributed computing infrastructure and was launched in July 2011. The US National Science Foundation (NSF) is funding XSEDE to the sum of $ 121 million over the next five years.

XSEDE uses the open-source software UNICORE to allow users to access the various supercomputers via the web. JSC is coordinating the development of the access software. It is responsible for all tasks arising from the use of UNICORE within the project, such as adapting the software to meet the needs of the users and the computing centres. "Our involvement in XSEDE reflects how successful our activities are in the area of standardization, which we pursue in developing UNICORE," says Daniel Mallmann, head of the Jülich group "Federated Systems and Data". www.unicore.eu

# Controlling the Flood of Data

The volume of data generated by science and research using computers and experiments will increase substantially over the next few years. Experts talk about a data tsunami. In order to make the plethora of data available to scientists throughout the world, a new infrastructure is necessary. It must coordinate access to data generated at different places and facilitate usage for scientists in other locations. This type of infrastructure is what the EUDAT (European Data) project launched in October aims to build within the next three years. One of the key partners in the project supported by the European Union is the Jülich Supercomputing Centre. It is developing both basic functions, such as the management of access rights and long-term data storage, as well as working environments for groups of users from various disciplines. www.eudat.eu

PUBLICATION DETAILS

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## UPCOMING EVENTS

Introduction to the programming and usage of the supercomputing resources at Jülich
24–25 November 2011
Jülich Supercomputing Centre

The course provides an overview of the supercomputer resources at Forschungszentrum Jülich and explains how efficient use can be made of allocated resources.

Instructors: JSC employees and representatives of IBM, Intel and ParTec

www.fz-juelich.de/ias/jsc/events/sc

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Introduction to parallel programming with MPI and OpenMP
28–30 November 2011
Jülich Supercomputing Centre

The course, which will be held in German, provides an introduction to parallel processing in technical and scientific computing. The focus is on the two most commonly used programming models for modern supercomputers: MPI and OpenMP.

Instructor: Dr. Rolf Rabenseifner, High Performance Computing Center Stuttgart

www.fz-juelich.de/ias/jsc/events/mpi-en

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GPU programming
5–7 December 2011
Jülich Supercomputing Centre

Participants will be introduced to CUDA, OpenCL, and multi-GPU programming. One of the topics is the optimization and tuning of scientific applications.

Instructors: Dr. Jan Meinke, Jochen Kreutz, Willi Homberg, JSC; Suraj Prabhakaran, GRS; Kevin Drzycimski, FH Aachen

www.fz-juelich.de/ias/jsc/events/gpu

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NIC-Symposium 2012
7–8 February 2012
at Forschungszentrum Jülich

The sixth NIC Symposium will give an overview of the activities of the John von Neumann Institute for Computing (NIC) and of the results of NIC projects over the last two years. Fifteen speakers will talk about work in eleven different scientific fields.

www.fz-juelich.de/ias/jsc/events/nic-symposium

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You can find an overview of events at the Jülich Supercomputing Centre at:
www.fz-juelich.de/ias/jsc/events