DEISA

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Extreme computing in Europe

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DEISA is a consortium of leading national supercomputing centres that operates a production quality, distributed super-computing environment at continental scale.

The purpose of this research infrastructure is to enable scientific discovery across a broad spectrum of science and technology, by enhancing and reinforcing European capabilities in the area of high performance computing. National supercomputing platforms have been strongly integrated to provide transparent access to a pool of European computing resources for scientific end users and user communities. The joint and coordinated operation of this environment is tailored to provide enhanced computing power and resources for leading computational scientists, and to enable new, groundbreaking research activities in science and technology. DEISA operates as a virtual European supercomputing centre. Human competences are also pooled, to provide first class, substantial added value services to computational sciences. The DEISA Consortium receives funding from the European Community's Seventh Framework Programme (FP7) under the grant agreement n° RI-222919.

Distributed European Infrastructure for Supercomputing Applications

e-infrastructure

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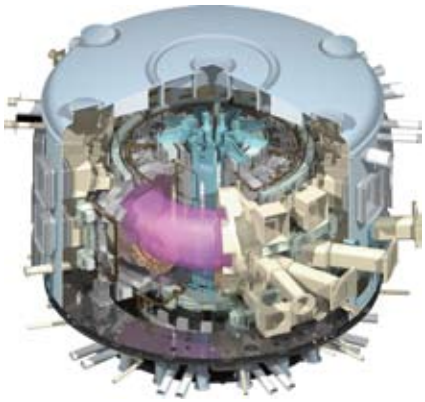
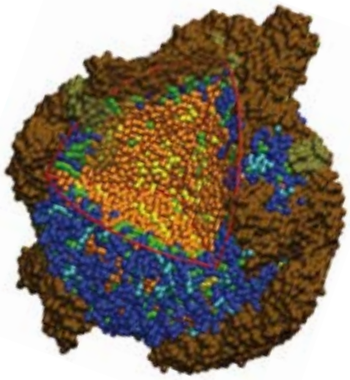
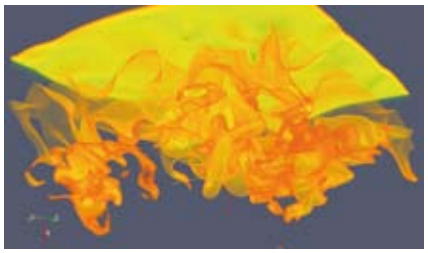
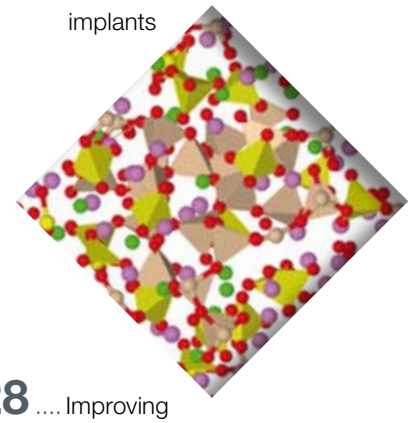
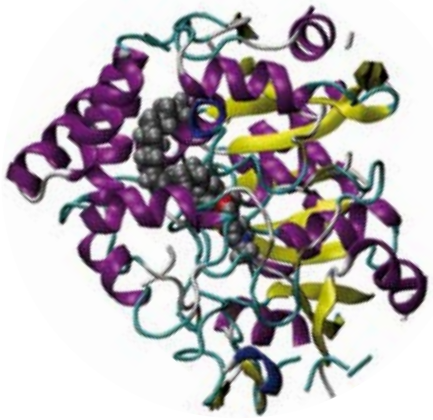










EDITORIAL

DEISA Extreme Computing is beneficial for science and industry

Hermann Lederer, (Deisa external relations and dissemination) RZG, Germany
Ari Turunen, Editor-in-Chief CSC, Finland

High Performance Computing and networking is becoming more and more important and beneficial for science and industry. Thus communication with potential users of HPC related information and the public is an increasingly important aspect of science. Unfortunately, it is not always understood by the general public what an important role supercomputer simulations are playing in the progress being made in research and technology. As a result, the benefits of computational sciences are not widely acknowledged. However, there is a constant and increasing demand for non-technical material about supercomputing results, especially for funders, decision makers and new potential customers in industry. Dissemination of research results has become almost as important as the generation of research.

DEISA, the Distributed European Infrastructure for Supercomputing Applications has published the second DEISA Digest Magazine, which concentrates on key results of the DEISA Extreme Computing Initiative (DECI), started in 2005, to enable “grand challenge” applications in all areas of science and technology. So far scientists from more than 180 research institutes and universities from 25 different European countries have benefited from DECI, with collaborators from North and South America, Asia and Australia. The selected scientific projects reported in DEISA Digest 2010 cover major areas of science including Astro Sciences, Earth Sciences, Engineering, Life Sciences, Materials Science, and Plasma Physics.

The applications can help to create environmentally and economically viable energy, better weather forecasts and predictions about earthquakes. Computer simulations can help prevent heart attacks, destroy cancer cells and develop better bone implants. The research done on resources provided by DEISA can also reveal details about star formation, what happens below the surface of the sun, or how the Milky Way has been formed. Another fascinating area is how to handle turbulence effects better when designing aeroplanes, with impacts on noise reduction and energy efficiency.

These leading, ground breaking applications must deal with complex, demanding and innovative simulations that would not be possible without the DEISA infrastructure, and which benefit from the exceptional resources provided by the Consortium. The DEISA applications are expected to have requirements that cannot be fulfilled by the national HPC services alone.

A European Call for Extreme Computing Proposals is published regularly. By selecting the most appropriate supercomputer architectures for each project, DEISA has opened up the most powerful HPC architectures available in Europe for the most challenging projects. This mitigates the rapid performance decay of a single national supercomputer within its short life cycle typically of about 5 years, as implied by Moore’s law.

The number of DECI proposals and accepted projects has increased from year to year. Supercomputing resources are awarded for scientific projects on the fastest supercomputers in Europe, accompanied by application enabling services, which are distributed over all partner sites, with access to the application specialists’ knowledge of each site.

Until the beginning of the third millennium, the European HPC landscape was fragmented. Then Europe started to take measures towards building up European-scale research infrastructures of strategic relevance, with the creation of ESFRI, the European Strategy Forum for Research Infrastructures, in 2002, and e-IRG, the eInfrastructure Reflection Group, in 2003. Also back in 2002, leading European supercomputing centers came together to start a close trans-national collaboration and proposed to build DEISA, The DEISA consortium started to deploy the distributed High Performance Computing infrastructure through EU FP6 support as of 2004, and continued its operation with an extension of services through EU FP7 support in 2008. ■

Acknowledgement
The DEISA Consortium thanks the European Commission for support in EU FP7 through contract RI-222919.

One step closer to ensuring the accuracy of weather models

Euan MacDonald

Scientists seeking to develop accurate weather, climate and air quality prediction models have long been confronted with a difficult yet important problem: how to accurately forecast the height of the atmospheric boundary layer as it develops during daytime heating. Using DEISA resources, a team of scientists from the Delft University of Technology in the Netherlands, Imperial College London and the National Center for Atmospheric Research in Colorado initiated the PINNACLE project in order to resolve this longstanding controversy.

The atmospheric boundary layer (ABL) is the part of the atmosphere in which we live. It is the essentially turbulent lower layer of the atmosphere, connecting the Earth's surface to the free atmosphere (troposphere). A typical daytime boundary layer (also known as the "convective boundary layer") grows from a few hundred meters in the morning to one kilometre or more in the afternoon. The top of the boundary layer is clearly identifiable by a so-called capping inversion, a steep increase in the temperature profile. Due to solar heating of the surface, hot air will be formed which, due to its lower density, will rise in the form of thermals all the way to the top of the boundary layer. Owing to the large Reynolds number (a dimensionless number used in order to represent how many scales of motion are involved in the turbulence under study) associated with atmospheric flow, the motion in the boundary layer is highly turbulent. Understanding the atmospheric boundary layer is of crucial importance if scientists are to be confident in the accuracy of the weather and climate predictions that they make.

This is a photograph of a real inversion, as taken by a glider pilot. The inversion is topped by very small cumulus clouds; however, the "misty" band that is associated with the top of the boundary layer can clearly be identified here.

"Turbulence in the atmospheric boundary layer mixes heat, momentum, and bio(chemical) species originating on the surface throughout the entire boundary layer; any inaccurate calculation of the boundary layer height will result in flawed predictions of – for example – temperature and pollutant concentrations," notes Dr. **Harm Jonker** of the Delft University of Technology in the Netherlands, and the lead researcher on the PINNACLE project. "Therefore, for weather, climate, and air quality models, it is of vital importance to

correctly forecast the height of the boundary layer as it develops under daytime heating. To put it bluntly: if a model cannot get the boundary layer height correct, it cannot get anything correct."

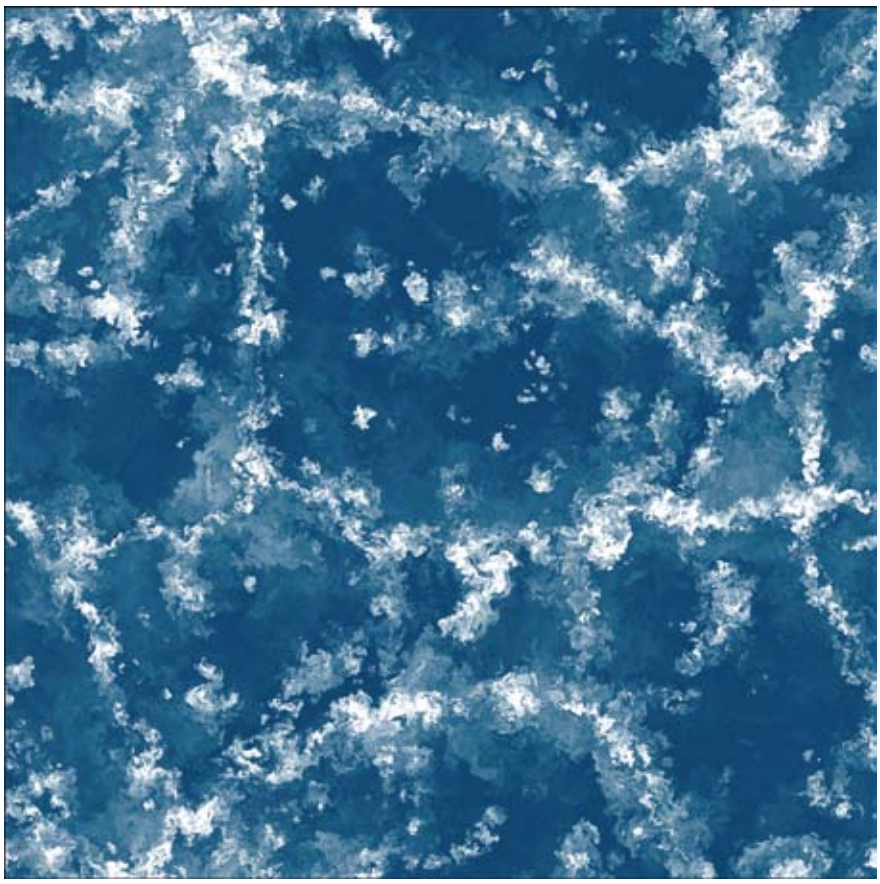
Ascertaining the growth-rate law of the atmospheric boundary layer: A longstanding problem

A key issue in weather modelling is, therefore, the so-called "growth-rate law" for the evolution of the daytime atmospheric boundary layer; this, however, remained a highly controversial question.

"The most widely employed growth rate law for the atmospheric boundary layer is riddled with controversy," continues Jonker. "Results from atmospheric observations, large-eddy simulations and laboratory experiments are mutually inconsistent, and display substantial scatter; which, of course, renders predictions of the boundary layer height based on these results of somewhat questionable accuracy."

The PINNACLE project was carried out in order to confront this controversy directly. The project, led by Jonker, brought together a number of other scientists from the US and Europe: Dr. **Maarten van Reeuwijk** of Imperial College London, who co-developed the computer code used in the project, and Dr. **Peter Sullivan** and Dr. **Ned Patton** from the National Center for Atmospheric Research (NCAR) in Boulder, Colorado, whose years of experience with high-performance computers was essential to its success. The project was largely carried out between June 2008 and January 2009, when Jonker was a visiting researcher at the NCAR.

"Our goal was to put an end to this controversy by conducting "ground truth" (that is, departing from first principles) Direct Numerical Simulation (DNS) of convective boundary layers. DNS employs no empirical rules whatsoever and explicitly calculates the full spectrum of turbulent motions in three dimensions. Of course, it is simply not possible at present to simulate the high Reynolds number of atmospheric turbulence; this would require the simultaneous simulation of kilometre-sized motions and millimetre-sized motions and every size in between (that is, cover six orders of magnitude of scale in three directions). However, current computing capabilities do enable us to accurately simulate the classical laboratory experiments on the basis of which the existing growth-rate laws for the atmospheric boundary layer were proposed – indeed, we can now reach Reynolds numbers that are some ten times higher than those of the original experiments. Our hope was that, by varying the Reynolds number over three orders of magnitude and analysing in detail its impact on the growth-rate law, many of the key controversies could be resolved."



Both figures display the simulated temperature field: The first figure (above) is a horizontal (xy) cut, while the second (below) figure 2 is a vertical (xz) cut. Darker colours represent cooler zones. In the horizontal cut, the large-scale organization of the temperature field can be observed, whilst in the vertical cut a thermal can be seen impacting upon the inversion (on the left), lifting it up and generating lateral motions.

A controversy laid to rest

"The PINNACLE project was a tremendous success, as it explained why the previous experimental results had yielded apparently confusing and inconsistent results," notes Jonker. "It showed that, in general terms, the original experiments had been well conducted; but also, however, that the common assumption that fluid >>>

Doctor Harm Jonker, taking a break from the PINNACLE project in the Colorado mountains. The project was largely conducted while he was a visiting researcher at the National Center for Atmospheric Research there during 2008.

properties play only a minor role on the growth of the boundary was demonstrably false."

"Most importantly, the project revealed which of the competing growth-rate laws was, in fact, the correct one in the context of atmospheric boundary layers. This law can now be used with full confidence in weather, climate and air quality models. Secondly, the project results also shed light on why different laboratory experiments, conducted in the past by various groups using different methods, gave different growth-rate laws. By mimicking these experimental conditions in our simulations, we were able to exactly reproduce those historical experiments and get insight into how the properties of the fluid in question (in particular its viscosity, conductivity/diffusivity) had influenced previous findings on the boundary layer growth-rate."

"Indeed, one of the most interesting outcomes of the project is our finding that the experiment that historically was most influential in the field was actually right – but for the wrong reasons. In that experiment, the fluid used was heated water in a tank. Compared to the atmosphere, the Reynolds number was too low; however, compared to the fluid in the atmosphere (air), the water's conductivity was also too low. We found that these two elements effectively cancelled each other out, so that the correct 'atmospheric' growth law emerged – somewhat fortuitously – from the experiment."

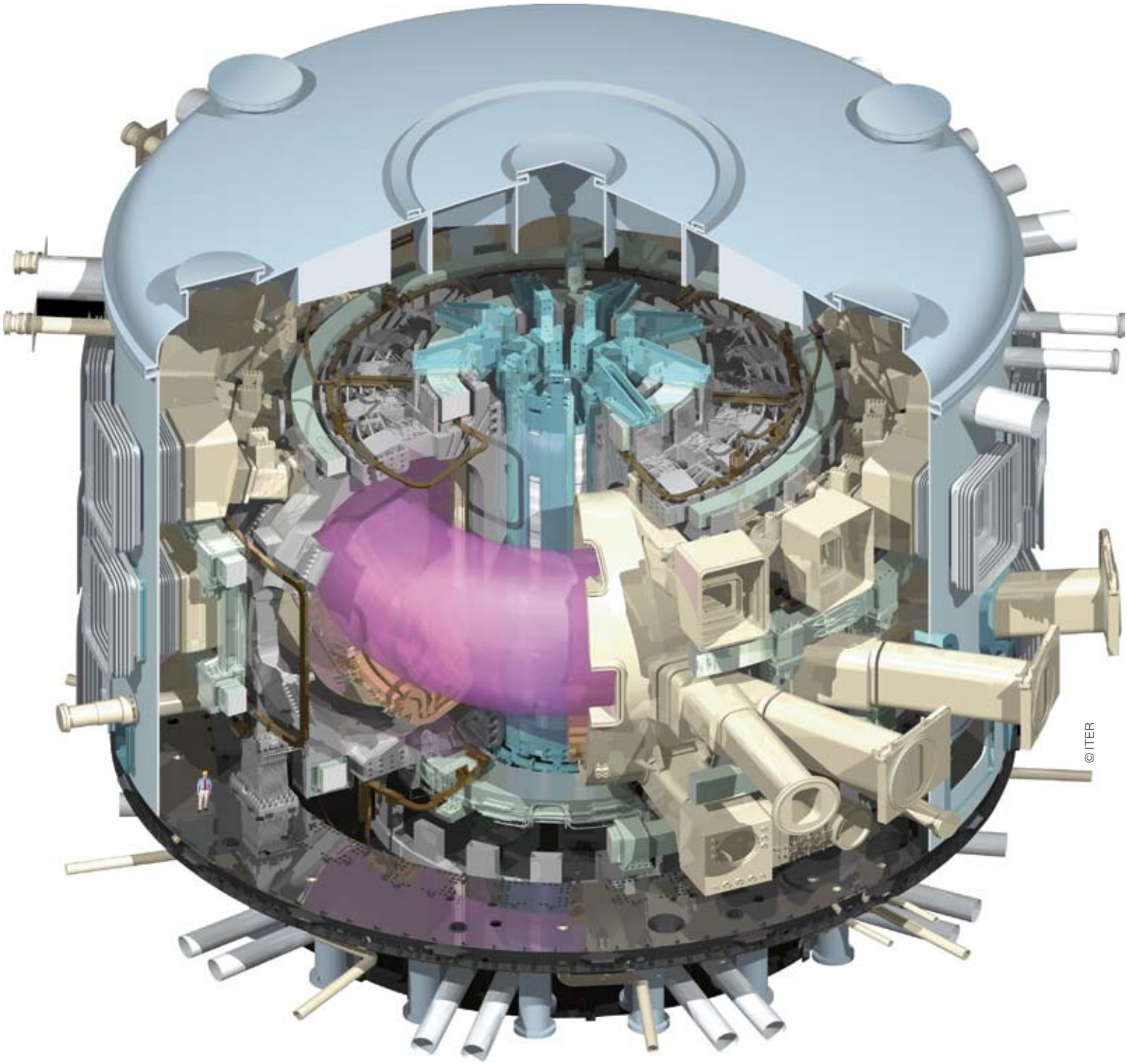
The PINNACLE project is now almost entirely complete: all that remains to be done is some final post-processing, before the results are written up for publication in an academic journal. "The next step," according to Jonker, "is to apply the same strategy to the more complex atmospheric situations in which wind shear (difference in wind speed and direction over relatively short distances) and/or the presence of boundary layer clouds (cumulus or stratocumulus) are known to significantly alter the growth-rate of the boundary layer. Simulations of this sort will be even more computational resource-heavy than those we carried out in the PINNACLE project; but the new generation of supercomputers will, we think, be equal to the task." ■

For more information:
www.deisa.eu/science/deci/projects2007-2008/PINNACLE

DEISA Resources: Essential to the PINNACLE project's success

The DEISA framework was crucial to the PINNACLE project as the total computational cost of the simulations exceeded by far anything that can normally be requested at the national level.

The resource allocation was the equivalent of 1.9 million CPU-h (IBM Power5, 1.9 GHz). It was equally divided over a number of different supercomputing centres that constitute the DEISA consortium: SARA (Amsterdam, the Netherlands); CINECA (Bologna, Italy); EPCC (Edinburgh, Scotland); FZJ (Jülich, Germany); and LRZ (Munich, Germany). When, during the course of the project, it transpired that it would be necessary to conduct at least one massive simulation that exceeded the resource allocation on each individual platform, the researchers were able to overcome this problem by transferring the resources allocated at EPCC to FZJ's new IBM Blue Gene/P super-computer. In this "super-size" run, 32 768 processors were used (i.e. half of the machine's full capacity).



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Europe plays a leading role in the field of fusion research

Sanna Pyysalo

To develop safe, sustainable, environmentally responsible and economically viable energy: this is the goal of European fusion research. Different organizations work together to meet the needs of developing fusion energy.

Given that fossil fuel resources are depleted, and that burning them pollutes the atmosphere, energy has become the most important issue for the long-term sustainable development of the world's economy.

"To maintain the way of living enjoyed in developed countries, mainly in Europe, North America and Japan, we will need a mix of energy sources to replace the depleting reserves of fossil fuels," argues **Duarte Borba**, responsible officer of the European Fusion Development Agreement (EFDA).

The goal of European fusion research is simply to develop fusion power as a safe, sustainable, environmentally responsible and economically viable energy source to meet the needs of a growing world population. In Europe, all EU member states are collaborating in a joint >>>

Duarte Borba works as a responsible officer at EFDA, the European Fusion Development Agreement.

effort carried out under EURATOM, the European Atomic Energy Community.

"Whatever options are chosen for the energy mix, it is imperative that adequate investment is allocated for the development of new energy sources," says Borba.

Nuclear fusion reactions yield very large amounts of energy, 7 orders of magnitude greater than chemical reactions such as burning of fossil fuels. This immense advantage is overshadowed by the extreme conditions required to achieve nuclear fusion, characterized mainly by temperatures in excess of 100 million degrees Celsius. Fusion viability for energy production has yet to be demonstrated.

"This is why we have a worldwide coordinated research programme pursuing new technologies aiming at achieving the goal of fusion energy," notes Borba.

Many different organizations

In worldwide magnetic confinement fusion research, Europe can be described as the leader. First of all, it hosts the ITER project, the next-step fusion device under construction in the south of France in collaboration with China, Russia, India, Japan, South Korea and the United States. The Joint European Torus (JET), the largest fusion device currently in operation, is a European experiment located in the United Kingdom.

In Europe, two main organizations stand out in the fusion programme; the Fusion Development Agreement (EFDA) and F4E, "Fusion for Energy".

F4E was established in March 2007 and its offices are located in Barcelona, Spain. The main aim of F4E is to provide Europe's contribution to the ITER international fusion energy project. EFDA is an agreement between all European research laboratories associated with EURATOM and the European Commission. EFDA manages the collective use of JET on behalf of its European partners and plays an important role in the coordination of physics and technology related activities among the European laboratories. EFDA also promotes and supports training and manages international collaborations outside the ITER agreement.

"The first supercomputer dedicated to European fusion research, HPC-FF, was set up under EFDA," notes Borba.

EUFORIA, EU Fusion fOR Iter Applications, is a project funded by the European Union under the Seventh Framework Programme. It aims to provide a comprehensive framework and infrastructure for core and edge transport and turbulence simulation, linking grid and High Performance Computing (HPC) to the fusion modelling community.

The field of fusion energy covers a wide range of physics and technology areas, which demand different types of investments and levels of organization. It requires the interplay between basic research close to a university environment and very large science projects, and also a very high level of cooperation and coordination. Mobility of researchers is a key component in maximizing the synergy between the different organizations, and it is strongly supported at the European and international level.

Fusion energy is a challenging field of research

The extreme conditions required for fusion to occur pose a number of challenges in terms of both physics and technology. With regard to the former, the control of the fusion plasma and its stability is one of the main topics of research; while, according to Borba, "regarding the technological aspects, the development of suitable materials for armour and other functional or structural applications pose the biggest challenges."

In recent times, there has been significant progress in the development of a scientific basis for a magnetic confinement fusion reactor. In 1997, JET produced 16 MW of fusion power for a couple of seconds, capitalizing on similar successful experiments using Deuterium-Tritium fuel performed in 1991 and in the Tokamak Fusion Test Reactor (TFTR) in the Princeton Plasma Physics Laboratory in 1994.

The transport of energy in the very core of the plasma is now well understood in terms of ion temperature gradient instabilities, which generate plasma turbulence. This has been the result of extensive computer simulations and theoretical advances, together with detailed experiments performed at JET and other fusion devices.

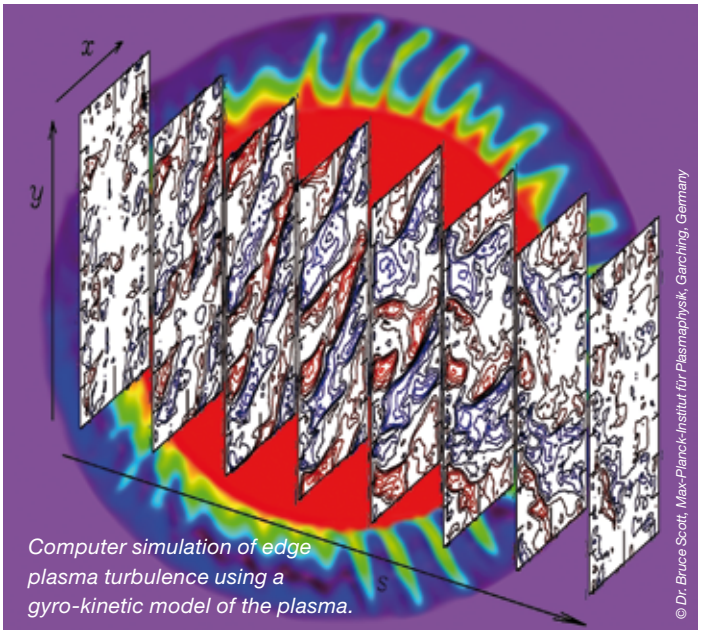
With regard to technological issues, an extensive qualification programme

was carried out to validate the design assumptions of all main ITER components, such as the superconducting magnets and high power handling plasma-facing components. The progress made gives increased confidence that the next-step device ITER will achieve its main objectives.

New opportunities from DEISA

The fusion community has benefited from over 10 million hours of computer resources under DEISA in the last couple of years, via the different organizations and projects. This has allowed significant progress to be made in the use of large-scale computer resources for fusion applications. DEISA facilitates access to a diverse set of computer architectures, which has created new opportunities for the fusion community. It was particularly valuable in the period leading up to the operation of the first dedicated high-performance computer for fusion applications (HPC-FF), by allowing some users to interact with different environments before the new computer was operational.

"After a period of adaptation, all projects benefited greatly from these opportunities. It is important to allow this cooperation to continue, in order to maximize the synergy between the different computer resources available for fusion research projects," Borba concludes. ■



Computer simulation of edge plasma turbulence using a gyro-kinetic model of the plasma.

For more information on fusion research projects supported by DEISA:

www.deisa.eu/science/deci/projects2009-2010/fullfgk3
www.deisa.eu/science/deci/projects2009-2010/ORBELEM
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Supercomputer simulations for different uses

In the field of fusion research, there have been supercomputer simulations of plasma turbulence, material properties, performance optimization of instruments and devices, etc.

One of the most important and challenging areas of research in plasma physics is the simulation of plasma turbulence, because it is responsible for most of the plasma energy losses. Due to the complexity of the phenomena involved, plasma turbulence can only be adequately described through the use of large-scale computer simulations.

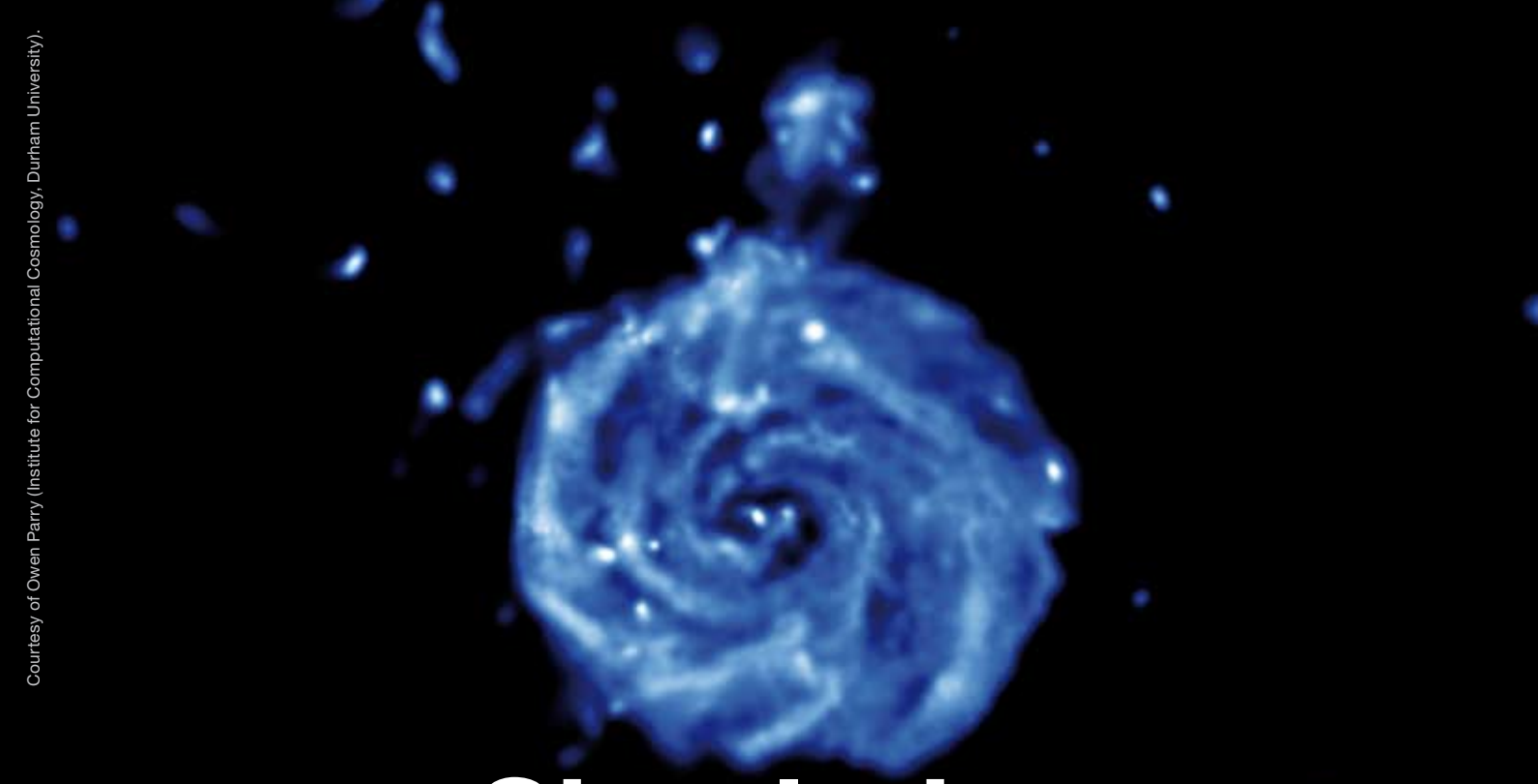
The timescales and physical scales of ion-driven turbulence and associated phenomena are somewhat easier to compute, because the ion mass is much larger than the electron mass. For this reason, thermal ion transport in the plasma core is now well understood and can be computed via these large-scale computer simulations, using gyro-averaged kinetic descriptions of the plasma ions and electrons.

However, electron-driven turbulence is more of a challenge, and this is where the increasing capacities of supercomputers, together with the continuing development of numerical schemes, will allow a more complete physical description of the Tokamak fusion plasma.

The testing of suitable fusion materials under neutron irradiation is very difficult and can only be performed for a limited set of samples. The qualification of the appropriate set of materials for a fusion plant will make extensive use of modelling of the material properties under irradiation. Such models are being constructed, but their establishment and validation, and, later, material development and testing, will require large-scale computer resources.

The integration of the various aspects related to performance optimization of different Tokamak designs requires a very large effort in integrated modelling and model validation. It is clear that some of the models will require large-scale computer resources.

In addition to the topic of plasma turbulence and related energy transport, large-scale computer resources will be used to examine the behaviour of fusion-born alpha particles, their various instabilities and their effect on plasma. Examples include the simulation of the heating and current drive methods and the study of plasma-wall interaction.



Courtesy of Owen Parry (Institute for Computational Cosmology, Durham University).

Simulating the formation of the milky way

Euan MacDonald

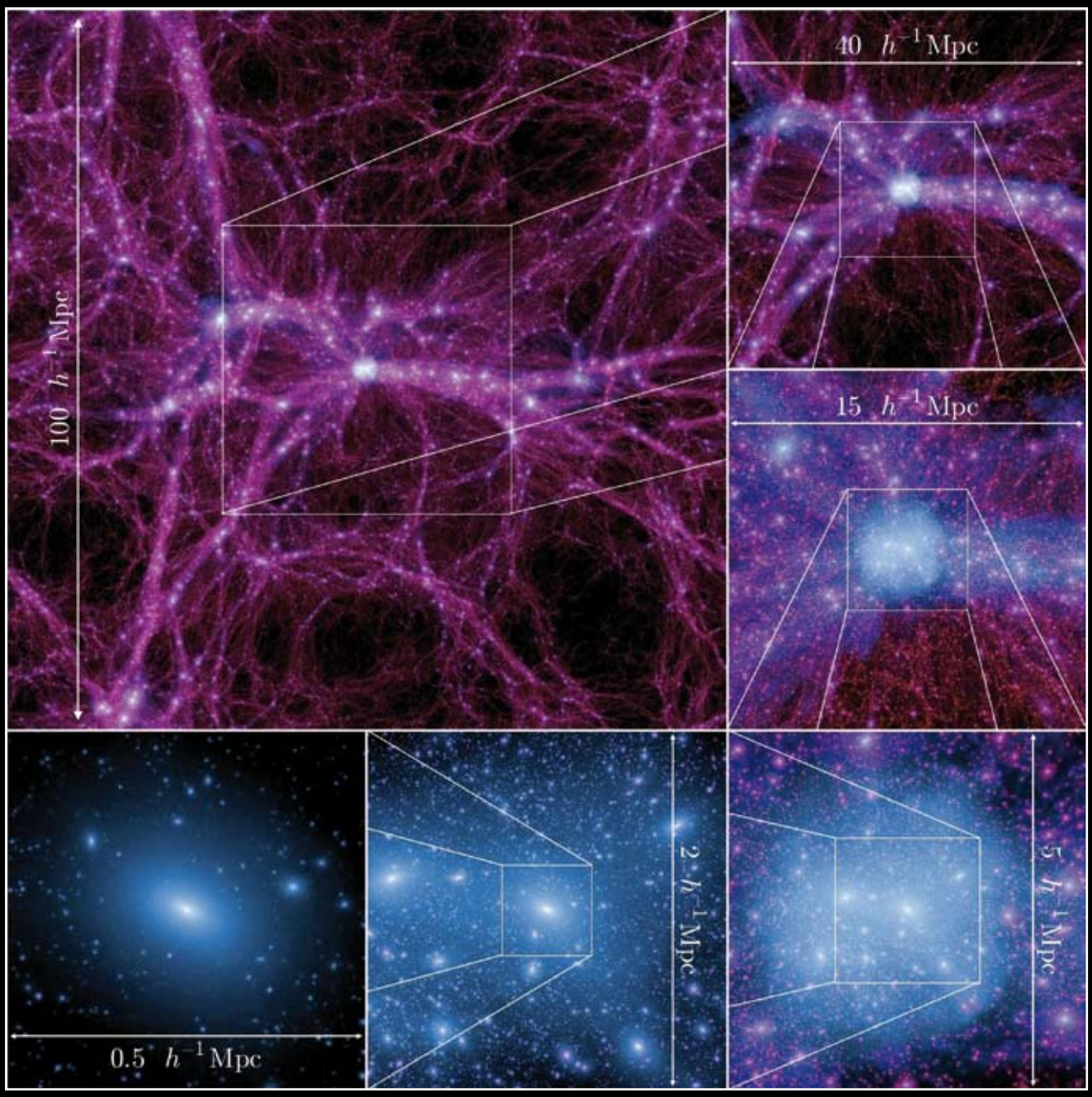
In May 2005, the DEISA Extreme Computing Initiative (DECI) was launched in order to enable a number of projects to be conducted that addressed some of the "grand challenges" in any area of science or technology. Few, however, have sought to confront a grander challenge than that of the AQUILA project, which brought together over 30 researchers from all over the world under the auspices of the Virgo Consortium for cosmological simulations: the supercomputer simulation of the formation of a realistic galaxy.

"Our universe seems a bizarre place," muses **Carlos Frenk**, Professor of Fundamental Physics at the University of Durham. "Thanks to recent advances in cosmology, which have revolutionised our view of the cosmos and opened up some of the most interesting questions in modern science, we now know that only some 4 % of it is made up of ordinary matter; 20 % is so-called "dark matter", and the remainder is formed by the recently-discovered "dark energy", of which almost nothing – apart from its existence – is known".

"Equally surprisingly, galaxies like our own Milky Way are thought to have arisen from quantum fluctuations generated immediately after the Big Bang. These notions, together with the view that our universe has a flat geometry, form the core of the current paradigm for the formation of galaxies, known as the cold dark matter (CDM) model. This model provides a hypothesis for the statistical properties of dark matter structures at early epochs when the universe was almost uniform".

Frenk, together with Professor **Simon White** of the Max Planck Institute for Astrophysics in Garching, Germany was the lead researcher on the AQUILA project, which sought to investigate the mysteries of galaxy formation through supercomputer simulations. The project, conducted by the Virgo Consortium for Cosmological Simulations (an international collaboration formed in 1996 that now includes over 30 researchers in the UK, Germany, the Netherlands, Canada, Japan, and

Picture (above) shows the face-on view of the gas distribution in one of the Aquila galaxies. The galaxy is a well-developed, warped spiral disk.



Courtesy of Mike Boylan-Kolchin (Max Planck Institute for Astrophysics).

A zoom of the large-scale structure of the cosmos, from the scale of superclusters to that of galaxies. This image shows the cosmic web of dark matter.

China), was the successor to the AQUARIUS project, the results of which were recently published in the prestigious scientific journal *Nature*.

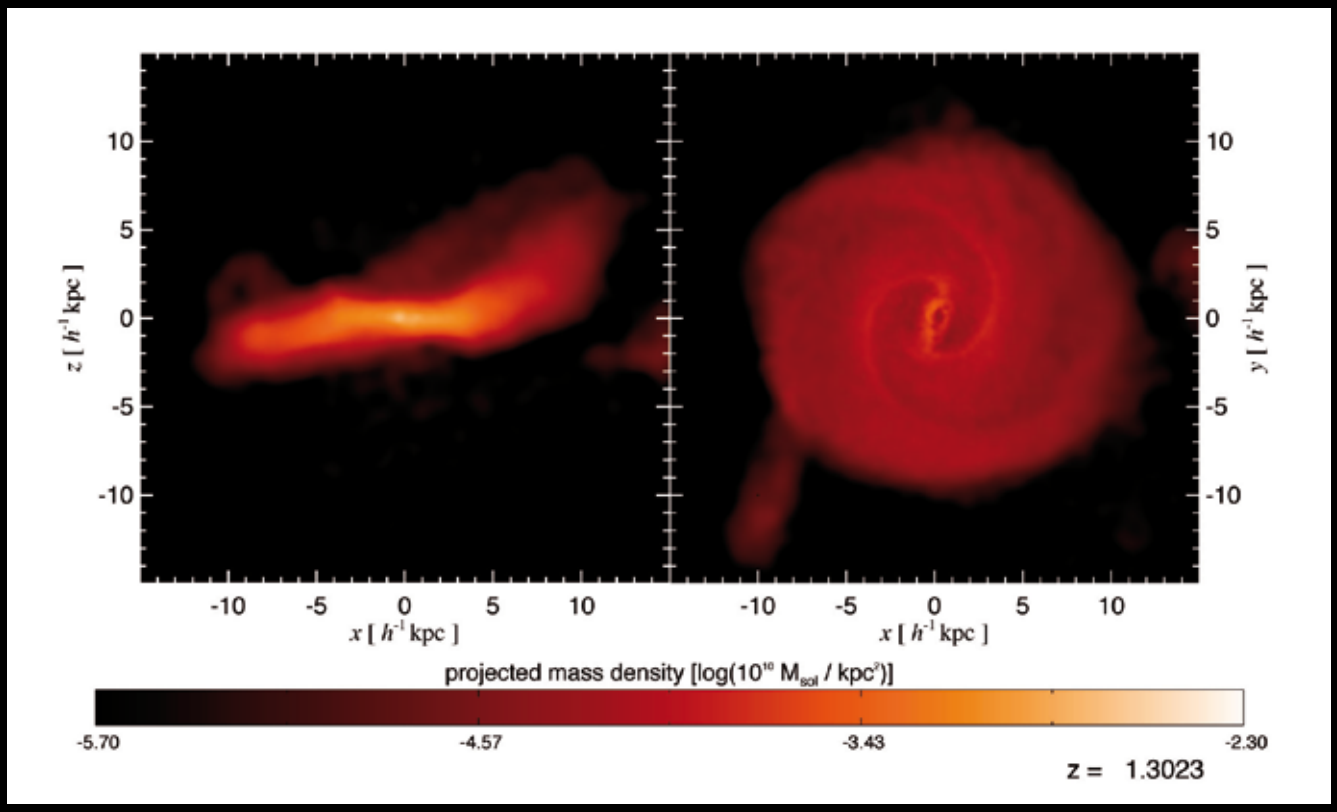
Simulating the formation of galaxies: more complex than you might think

"Galaxies are the basic building blocks of the universe," explains Frenk. "The CDM model provides the 'initial conditions' for their formation and we know the basic physics involved in their evolution. In principle then, calculating the formation of a galaxy like the Milky Way should merely be a computational problem".

"Unfortunately," he continues, "the reality is much more complex: nobody yet has managed to 'grow' a realistic galaxy in a computer. In spite of strenuous efforts over the past two decades, most simulated galaxies fail to form disks as thin and extended as those observed, and end up as large piles of stars that are unlike the galaxies that we observe around us. The reason is that even though the basic physics are relatively simple, the interaction of the many physical processes involved in galaxy formation is complex".

"Today, the increasingly sophisticated simulation algorithms and the expansion of computational capabilities have led to robust and increasingly detailed theoretical predictions that now make the CDM paradigm falsifiable by observation," Frenk notes. "Thus far, the paradigm has successfully passed tests based on a direct comparison of the distribution of matter on large scales (from 1 Mpc to the size of the observable universe) with a wide array of observations".

"The situation is, however, far less clear on small scales (a few kpc and below), where the CDM model is >>>



Courtesy of Markus Wadepuhl (Max Planck Institute for Astrophysics).

Edge-on and face-on views of the gas distribution in one of the Aquila galaxies. The galaxy is a well-developed, warped spiral disk.

challenged by a number of vexing problems. To give just one example, CDM halos are filled with rich substructure in the form of numerous dark matter 'subhalos', but the internal structure of these objects remained poorly represented by previous simulations. Moreover, the sheer abundance of these subhalos gives rise to a pressing problem: if, as currently hypothesised, these are the remnants of infalling galaxies, then one would expect hundreds to thousands of luminous satellite galaxies within the Milky Way, many more than the good dozen or so that can be observed. Whether or not this and other small-scale problems of CDM are potentially deadly for the theoretical paradigm is arguably one of today's most important questions in cosmology, one that can only be answered by improved simulation models that are able reliably to predict the structure on these small scales".

In the AQUILA project, then, Frenk and his team sought to confront these issues through conducting the largest, highest-resolution simulations ever attempted of the formation of Milky Way sized galaxies, fully embedded in their proper cosmological setting, using the most sophisticated hydrodynamical techniques that presently exist for the direct modelling of star formation and black hole accretion on galactic scales. Building on the work done in the AQUARIUS project, in which the largest ever simulations of the evolution of dark matter and the formation of the dark matter clumps in which galaxies form (so-called "galactic halos") were conducted, they added gas physics into the simulations, and also modelled the coupled evolution of dark matter and so-called baryonic matter (i.e. ordinary matter). The simulations were carried out independently by small teams within the Virgo collaboration while other leading groups around the world were also invited to participate.

The cutting edge: supercomputers and cosmology

"This project represented a bold and comprehensive approach to the simulation of galaxy formation, which had never before been attempted at such high resolution and with this level of faithfulness in the modelling of the relevant physics," he notes. "When the analysis is complete, we hope that at least some of the galaxies that emerge will resemble their counterparts in the real universe. In any event, the results of this project will represent the most complete and largest set of galaxy formation simulations ever performed".

He is also clear that advances in computational power, and access to supercomputing resources, have been crucial drivers of progress in this field. “Cosmology confronts some of the most fundamental questions in the whole of science many of which have preoccupied humankind since the beginning of civilization: How and when did our universe begin? What is it made of? How did it acquire its current appearance? In the past three hundred years we have developed a scientific methodology that allows us to tackle these questions in a rigorous way using a combination of theory, expressed through the language of mathematics, computation and empirical data. I regard myself as privileged to have had the opportunity to work in cosmology during the current golden era. All the indications are, however, that this era has barely begun”.

“DEISA will continue to play a vital role by stimulating international collaboration, making suitable facilities available to the best groups,” Frenk concludes. “Advances in this subject are tied in to advances in computing technology. Our current suite of simulations will redefine the state-of-the-art in the subject; we will require the next generation of computer technology to go beyond this, and to begin to prove in detail the process of galaxy formation”. And this, perhaps, is the grandest challenge of all. ■

For more information:
www.deisa.eu/science/deci/projects2007-2008/AQUILA

Carlos Frenk, Director of the Institute for Computational Cosmology at Durham University, and principal investigator on the AQUILA project.

DEISA’s role in AQUILA’s success

Carlos Frenk notes that, as the Virgo Consortium is an international collaboration, it was natural that they turned to an international infrastructure such as DEISA in order to carry out their project. The resources made available by DEISA were crucial, not only because they represented substantial amounts of computing power, but they also facilitated the transfer of data amongst the participating Virgo nodes. Researchers at different institutions across Europe used the infrastructure in a coordinated fashion.

760,000 standardised DEISA core hours were allocated to the project at the RZG supercomputing centre in Garching, Germany; ultimately, however, some 1,285,119 hours were actually used. The resources were used to carry out two series of simulations including the largest simulations of galaxy formation to date. One series was launched from Durham and the other from Garching. Both used sophisticated codes in which the complex astrophysics of galaxy formation were implemented using independently developed models built upon GADGET, a cosmological simulation code designed for massively parallel computers with distributed memory. A basic version of GADGET, which was developed by Volker Springel, one of the investigators on the project, is publicly available, and is presently the most widely used code in studies of cosmological structure formation. Roughly 400 publications using it are already in the refereed scientific literature.

Preventing heart attacks

Sanna Pyysalo

Bad cholesterol is a condition mainly affecting those in modern industrial countries. Using the supercomputing resources offered by DEISA, the LIPOS research project has explored the structure and functions of low density lipoproteins, whose excessive accumulation in coronary arteries can lead to the formation of cholesterol plaques.

Heart attacks and strokes are two of the most typical causes of death in industrial nations today. They result from atherosclerosis, where plaques form in a coronary artery. The first stage of this complex process is the accumulation of excess low density lipoproteins (LDLs), particles also known as "bad cholesterol", in the artery wall, which then undergo chemical changes.

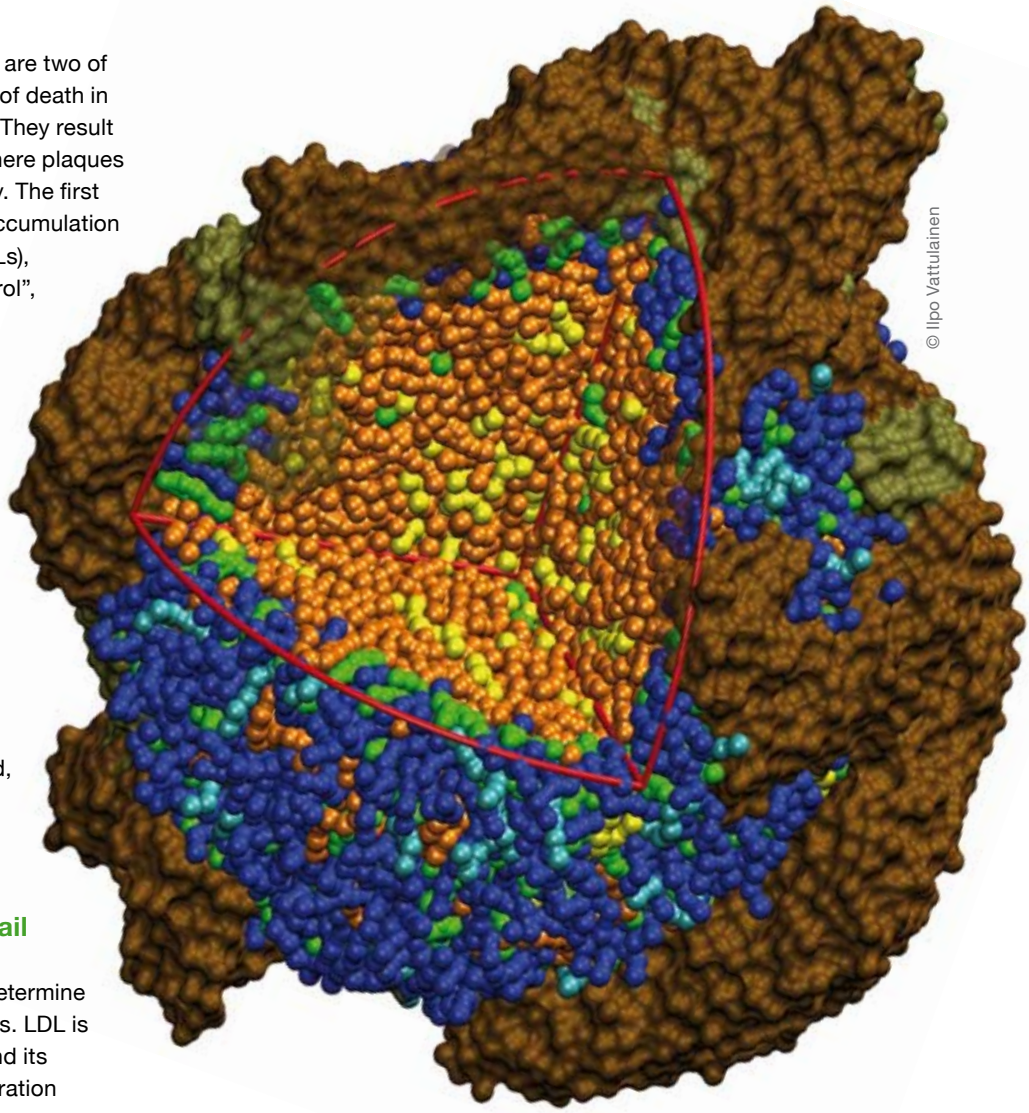
"To better understand how related diseases could be prevented, one first has to understand the structure and functions of LDL. This has been the essence of our research," says Professor **Ilpo Vattulainen**, the principal investigator in the LIPOS (Lipoprotein Structure and Dynamics) research project.

The work is being carried out by the Department of Physics at Tampere University of Technology in Finland, the Wihuri Research Institute in Finland, the University of Groningen in the Netherlands and the University of Western Ontario in Canada.

Research in almost atomic detail

The objective of the research was to determine the structure of low density lipoproteins. LDL is the particle transporting cholesterol and its esters to cells, so an elevated concentration of LDL correlates to an increased risk of certain diseases, such as atherosclerosis.

"There are substantial difficulties associated with understanding how cholesterol-related diseases emerge, or even the functions of

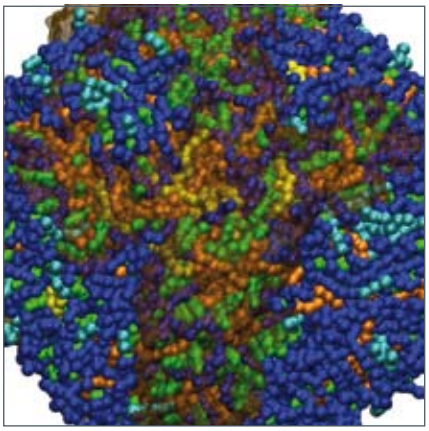


Equilibrated structure of a low density lipoprotein particle. A section of the particle has been cut out to make the internal structure visible. Different lipids are shown in different colors: blue and cyan for phospholipids, green for free cholesterol, orange for cholesterol esters, and yellow for triglycerides. The apoB–100 protein is shown in brown. Water and ions around the particle are not shown.

individual LDL particles. The functions of proteins depend on their structure and the structure of LDL is not well understood," explains Vattulainen.

This is largely due to their small size – only around 20 nm. Experimentally, it is particularly challenging to probe the structure of LDL and related phenomena over such small scales. However, atomistic and coarse-grained simulation techniques provide an excellent means of analysing molecular systems in almost atomic detail, hence complementing experiments.

"We paid particular attention to clarifying the role of lipids in the core particle of LDL, and their effect on the structure and dynamics of the protein sequence that surrounds it," Vattulainen notes.



© Ilpo Vattulainen

ApoB–100 displaces phospholipids and makes direct contact with the cholesterol ester/triglyceride core of the LDL particle. Colors are as in the left picture, except that the protein is shown as transparent.

Impressive results create new opportunities

The LIPOS research project began in the autumn of 2007, and following major surveys and background studies, the initial models for LDL particles were ready in spring 2008. Simulations using the initial models were started around May 2008 and were completed in the autumn of that year.

"The analysis is still partly in progress, but the first articles describing the main findings are already almost complete," Vattulainen says.

And what were the main findings of the research?

"It provided a great deal of insight into the distribution and dynamics of lipids inside LDL, and the effects of lipids on the structure of the protein sequence wrapped around LDL. In essence, we now know the structure of native LDL in almost atomic detail," Vattulainen explains.

The research and its results also create the opportunity for further work, in order to gain greater understanding of the overall function of LDL particles.

"The results allow us to initiate an intriguing sequence of further studies, looking at how LDL particles interact, for example, with certain enzymes, oxidative agents and sugars that are involved in the chemical alterations of LDL and the consequent formation of cholesterol plaques."

Pioneering studies with the help of DEISA

The LIPOS project has broken new ground in its field of science because the research method was truly unique.

"Previously, there have been no attempts at atomistic or coarse-grained simulations of LDL particles. In this respect, our study is pioneering as it is the first case in which LDL particles have been explored through simulations with full molecular detail," Vattulainen says.

An important factor in the success of the research project was the supercomputing resources made available through the DEISA framework.

"DEISA allowed us to carry out an extensive, state-of-the-art simulation project for a molecular entity that is biologically particularly relevant. Large-scale parallel simulations for a system of this kind would not have been possible without resources of this calibre."

The benefits of DEISA were, in Vattulainen's view, obvious.

"There are only a handful of places in Europe that provide access to supercomputing resources of this size. Networking in this manner provides major added value for Europe overall," Vattulainen comments. ■

"To better understand how related diseases could be prevented, one first has to understand the structure and functions of LDL," says Professor Ilpo Vattulainen, the principal investigator in the LIPOS (Lipoprotein Structure and Dynamics) research project.

Computations of the Lipos research project were performed at HECToR in Edinburgh, Scotland. There were 5 independent runs, which used up to 64 CPU cores each. 500 000 CPU hours were invested on the core of the production simulations.

To construct the initial models, MODELLER software was used on local computers. An open-source software package, GROMACS, was used for simulations (coded in C, parallelization via MPI).

Visualization and data analysis on local computers were done using GROMACS and VMD. GROMACS analysis tools were extended to allow flexible analysis of specific parts of the systems.

For more information:
www.deisa.eu/science/deci/projects2007-2008/Lipos

Understanding wall turbulence

Damien Lecarpentier

The DNS-BUMP project performed a Direct Numerical Simulation (DNS) of wall-bounded flows, in order to improve our knowledge of wall turbulence, a phenomenon that is of particular interest for aerodynamics. The database generated from the project will be used to develop and to validate turbulence models.

In fluid dynamics, flows are either characterized as laminar or turbulent. Laminar flows are regular and smooth, while turbulent flows have chaotic and unstable properties. Turbulent flows can be seen everywhere, from the whirls on the surface of the water in a river, to the air flow surrounding an airplane or a car. The transition from laminar to turbulent flow is a complex phenomenon. Turbulence itself remains a major issue for scientists, and a concern for many working in the automotive and aeronautics industries.

The DNS-BUMP project was conducted in 2006-2008 by a team of researchers from five different universities in France, Germany, Italy, Sweden, and the United Kingdom. It is directly linked to the objectives of the WALLTURB project, which brings together 16 partners, including 14 universities and 2 aeronautical companies (Dassault Aviation and Airbus UK) from 10 European countries. This latter project, which is funded by the European Commission under the 6th Framework Programme, began in 2005, with the goal of improving our understanding and modelling of turbulent fluid flows, and in particular of turbulent flows that occur near wall structures. The DNS-BUMP project aimed to contribute to this task by generating a database on "wall-bounded" turbulent flows.

Improving our understanding of wall turbulence

"Turbulence is a very challenging research domain in which only a few theoretical results have been achieved, despite the significant efforts that have been made in the last century," says **Jean-Philippe Laval**, researcher at the Laboratoire de Mécanique de Lille, France, and leader of the DNS-BUMP project. "Although some important discoveries were made in terms of ideal isotropic turbulence (i.e. turbulence which is uniform, whose properties do not depend on direction), today's major problems concern the understanding of more realistic turbulence processes involving boundaries (such as walls), which modify significantly the behavior of the turbulent flow."

The characteristics of near-wall turbulence are of particular importance for researchers and engineers working on fluid dynamics and aerodynamics. It is essential both from a theoretical and a modelling perspective.

"A better understanding of wall turbulence is of crucial importance if we are to develop better numerical models of turbulence more generally," says Laval. "Nowadays, many different numerical models of wall turbulence have been developed, but none of them is able to furnish accurate predictions in most of the industrial configurations in which we are interested. Numerical models are usually able to reproduce correctly the flow in the vicinity of a flat wall where there are no other external flows, but they usually fail to accurately predict flows over curved walls where there is a strong pressure gradient, meaning large changes in terms of external pressure."

"Adverse pressure gradients (which occur when the static pressure increases in the direction of the flow), are associated with a deceleration of the fluid flow, which can lead to a complex recirculation phenomenon," Laval explains. "This flow is of great interest in aeronautics as it is typical of the take-off configuration of an airfoil. An accurate description of the recirculation phenomenon is therefore very important in this configuration, but it is very difficult to model using numerical simulations."

Improving these models requires reliable data on turbulent flows. The aim of the DNS-BUMP project was precisely to help achieve this, by generating a database of wall-bounded turbulent flows under different air pressure conditions.

Generating a database of wall turbulent flows through direct numerical simulation

The approach undertaken by Laval's team is called direct numerical simulation (DNS). It is a type of

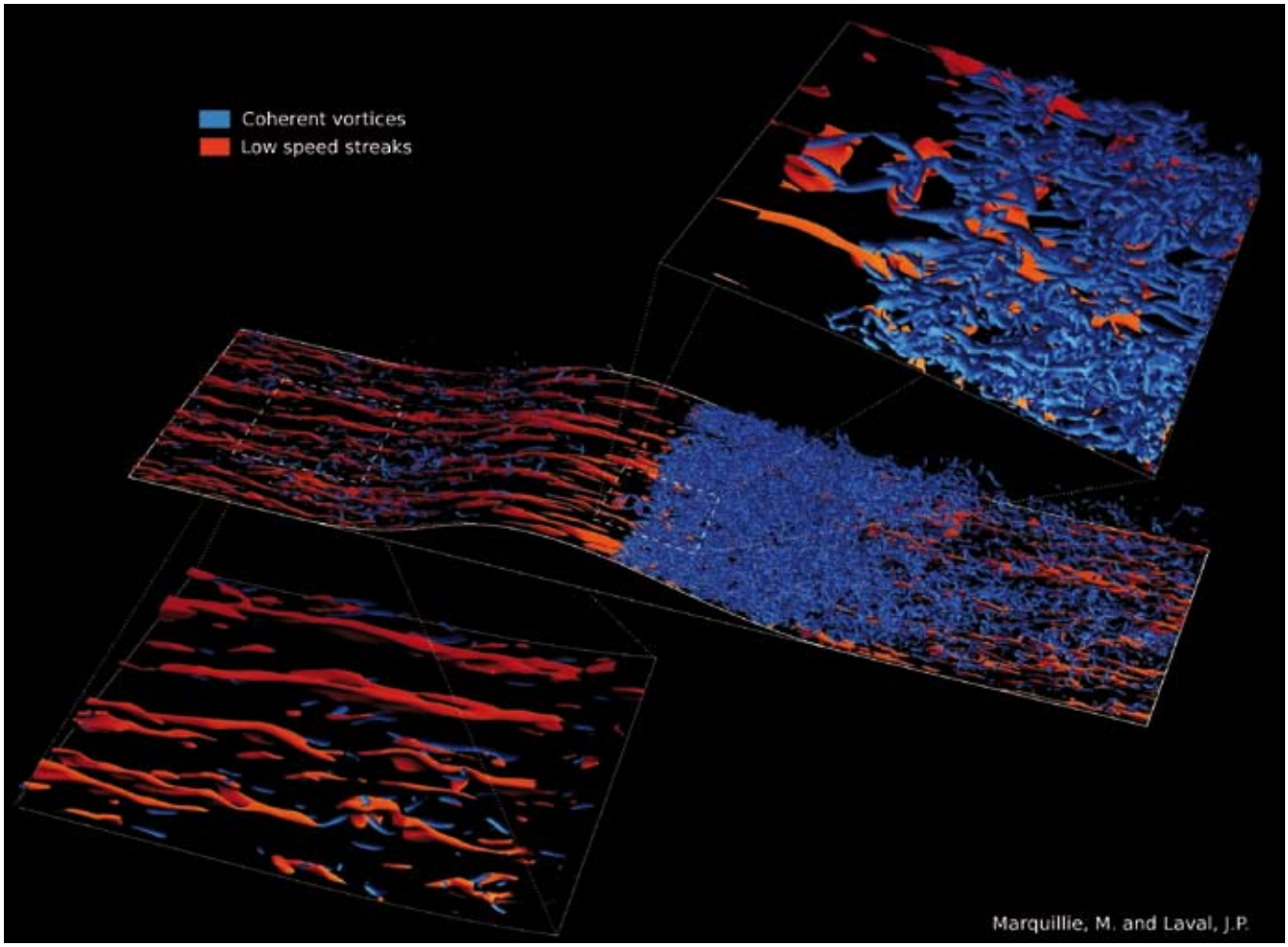
simulation very often used in computational fluid dynamics, in which the Navier–Stokes equations (used to describe the motion of fluid substances) are numerically solved without using any additional turbulence model. This means that the whole range of spatial and temporal scales of the turbulent flow must be resolved, which therefore requires a large amount of computing resources.

The issue of the complex behaviour of turbulent flows is very often addressed through statistical modelling. The Reynolds number (named after **Osborne Reynolds**, a pioneer in the field of fluid dynamics) gives a measure of the ratio of inertial forces to viscous forces for given flow conditions, and are used to characterize whether flow conditions lead to laminar or turbulent flows. Laminar flows occur at low Reynolds number (where viscous forces are dominant), while turbulent flows occur at high Reynolds number (with stronger inertial forces, responsible for flow fluctuations).

Direct numerical simulations are today limited to relatively low Reynolds number (low velocity and small scales) but are of significant interest as they can provide full time-resolved 3D information on the flow in question. Actual experiments, on the other hand, are usually only able to provide limited information, but can do so at higher Reynolds number (where the flow is characterized by more turbulence). The two methods are thus complementary. The aim of the DNS-BUMP project was to perform a DNS of a turbulent flow over a curved wall (a "bump") at the highest Reynolds number possible.

All in all, more than 8 Terabytes (TB) of raw data were recorded through the simulation by the research team, generating a very rich database that will, according to Laval, have multiple uses:

"The database generated from the DNS-BUMP project will be used within the WALLTURB project by many partners, in order to develop and to validate turbulence models. It can be used to extract turbulence statistics on the particular behavior of turbulent flows with pressure gradient, or as a reference simulation in order to evaluate the performance of numerical models with exactly the same configuration, which is difficult to achieve in experiments. More generally, the results will be very useful for many researchers working in the field of turbulence. The database generated by the DNS will be shared in the research community and will help to increase our understanding of wall turbulence and flow separation, and to improve turbulence models. These are important issues for the simulation of more complex and realistic turbulent flows. The first results of the project were presented in Lille, during an >>>



Visualisation of coherent vortices in blue and low speed flow regions (called streaks) in red on the lower wall of the simulation. Intense vortices are generated near the separation region of the turbulent boundary layer when the low speed streaks, well defined at the inlet of domain, are wiped out by the strong adverse pressure gradient.

Researcher Jean-Philippe Laval (on the right) leads the DNS-BUMP project. Matthieu Marquillie (on the left), Research Engineer at the Laboratoire de Mécanique de Lille, wrote the original code and optimized it for the DEISA project.

international workshop related to the WALLTURB project that gathered more than 100 wall turbulence specialists from all over the world. Our database met with great interest in the research community. In the future, the database will undoubtedly serve as a valuable reference tool, available to the entire community. Databases of good quality can remain useful in terms of providing test cases for more than a decade."

Post-processing of the data is the next step

Now that the data have been collected, some analytical work is still required: "We have collected enough data to compute most of the interesting statistics. Some statistics cannot currently be computed, as they would require additional computing power several orders of magnitude higher, which is obviously not possible at present. Our main efforts are now focused on post-processing of the data. Much of this has already been completed, and will be made available for the WALLTURB partners; however, the computation of some other statistics is still in progress. The next step of the project is, therefore, to complete the post-processing of the data, and to examine additional processing possibilities which could further increase our understanding of wall turbulence".

"Following this, our next goal will be to modify the numerical code, in order to make it ready for still larger simulations of such flows in years to come, when simulation at high Reynolds number becomes possible at a reasonable cost. This will require a complete reorganization of the code in order to enable it to run with several thousands of processors simultaneously, given that the architecture of new supercomputers includes an increasing number of processors. On the basis of the outcome of the current DNS project, we foresee a new project in which a challenging new DNS of a turbulent flow would be performed, in a slightly different configuration and at a much higher Reynolds number. However, a significant improvement over the current project would require a simulation with a Reynolds number increased by a factor of at least 5, which corresponds to – at least – two orders of magnitude in terms of computational power. The scale of such a project is at the very edge of what is physically possible with the computing power currently available within DEISA, but it will hopefully become feasible in the next 3 to 5 years." ■

For more information:
www.deisa.eu/science/deci/projects2007-2008/DNS-BUMP

wallturb.univ-lille1.fr

Taking advantage of the DEISA Extreme Computing Initiative (DECI) project, the DNS-BUMP research team sought to perform a DNS of a channel flow over a curved surface at a high Reynolds number (Re=600 at the inlet).

DNS is very demanding in terms of computational power. Given that the Reynolds number that is today within reach for simulations is still very low (compared to real-life situations), a very large DNS was of great interest, but only possible through a joint computing scheme such as the DEISA Extreme Computing Initiative, according to **Jean-Philippe Laval**.

For the 2006 and 2007 projects, the research team was allocated up to 160 000 CPU hours of NEC-SX8 at the High Performance Computing Center Stuttgart (HLRS), Germany. The first DECI project allowance of 100 000 CPU hours was used to start the DNS with 510 Million grid points, which required up to 400 GB of memory, and which was performed on 64 processors. However, half of the computational resources were used simply in order to generate a stable simulation, and the remaining time was not sufficient to collect enough data to compute useful statistics. Therefore, the team applied for extra computing time, which was granted in 2007, and was used to continue the simulation in exactly the same configuration, in order to improve the convergence of the statistics. All in all, more than 8 TB of raw data were recorded, generating a very rich database on turbulent flows.

Revealing the Sun's secrets

Sanna Pyysalo

Working with computer models, the SOLEX project, carried out within the DEISA framework, aims to investigate flows near the solar surface. The project began in September 2008, and was conducted by researchers from the Faculty of Mathematics at the University of Vienna, Austria, and the Max Planck Institute for Astrophysics, Germany.

The Sun is around 5 billion years old. Its extreme complexity as a multiscale phenomenon is still not entirely understood, but with the help of astrophysics, it has begun to reveal its secrets.

"Among the artifacts from the Babylonian civilization, archeologists have found many cuneiform script boards filled with calculations of astronomical phenomena. This was the beginning of the now-blossoming field of computational astronomy or astrophysics. Due to the tremendous increase in computational power and improvement of numerical methods, this branch of research is presently witnessing a truly golden age," notes Dr. **Herbert J. Muthsam** from the Faculty of Mathematics at the University of Vienna in Austria.

Dr. Muthsam is the principal investigator in the DEISA research project SOLEX (Solar Explorations – Surface Flows in Ultra-High Resolution). >>>

Dr. Herbert J. Muthsam from the Faculty of Mathematics at the University of Vienna in Austria is the principal investigator in the DEISA research project SOLEX. The research group is working on computer models to investigate flows near the solar surface.

The research group is working on computer models to investigate flows near the solar surface. The research is being done in cooperation with the Faculty of Mathematics at the University of Vienna and the Max Planck Institute for Astrophysics in Germany.

"Even though our Sun provides us with a flood of light, there are many phenomena that are inaccessible to direct observation. The interior is, of course, hidden from us, and there are limitations to the size of the details that we can observe on the surface."

The innermost two-thirds of the Sun are relatively quiet, a rotating sphere. Near the center, energy is set free through nuclear fusion. This energy is then transported outwards by radiation. In the outermost third of the solar body, the energy transport mechanism changes. No longer is energy transported by radiation, but by convection.

"Hot material streams upwards in large cells, transporting energy. On top of the bulk convection zone sits the granulation layer. This is the focus of our investigations in this project," Muthsam explains.

Granulation consists of relatively small cells of upwardly streaming hot material. As the material approaches the surface, it radiates energy out into space; as it does so, the material becomes cooler, and sinks down again.

"In contrast to the bulk convection zone, the granulation layer is accessible to direct observation – we actually see it when looking at the Sun," Muthsam adds.

ANTARES code as a microscope

In order to study such phenomena as the solar surface, the SOLEX project team has developed the ANTARES (ANTARES standing for A Numerical Tool for Astrophysical RESearch) code.

"In doing so, we have sought to implement the best possible numerical methods, in order to achieve the sharpest possible picture for any given computational effort. In addition, we have equipped ANTARES with the possibility to zoom into especially interesting features in order to obtain extra resolution," Muthsam continues.

ANTARES can, therefore, be used as a "microscope", in order to model a small portion of the Sun in the greatest detail feasible.

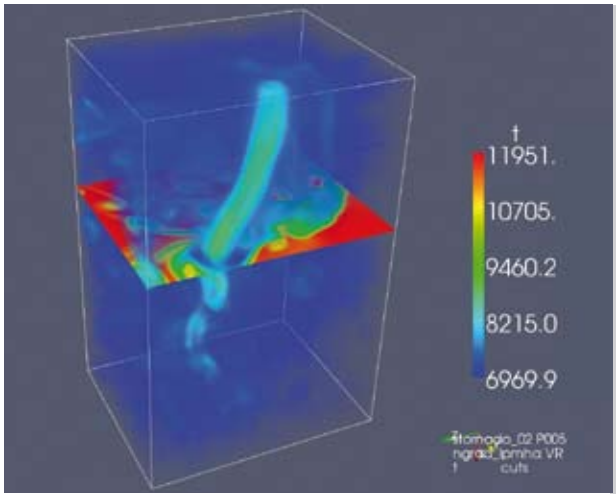
According to Muthsam, several other projects are exploring the same subject. These include, on the observational side, the Swedish Vacuum Telescope, which is delivering large amount of data, the recent Hinode satellite, and the Sunrise mission, a balloon telescope due to be launched this year and set to deliver unprecedented resolution.

But why is it important to go into such fine detail? Dr. Muthsam offers at least two reasons for this. The first concerns the mounting body of evidence that the Sun has not just one dynamo as previously supposed (the one that causes sunspots to appear in 11-year cycles, thereby causing solar storms and also influencing satellites and terrestrial power lines) but also second, situated near the solar surface.

"If so, it is probable that this dynamo operates on very small scales. Hence the interest in these scales."

The second reason is that, above the solar surface (which has a temperature of 6000 kelvins), there is a corona at a temperature of one million kelvins. The question is how the plasma in the corona is being heated. There are two plausible mechanisms for this, magnetohydrodynamic waves and sound waves.

"It is still not clear which one is correct, or exactly how it works," explains Muthsam. "Our goal within the SOLEX project was therefore to look into a region of normal solar granulation at high resolution and to figure out what physical phenomena are appearing."

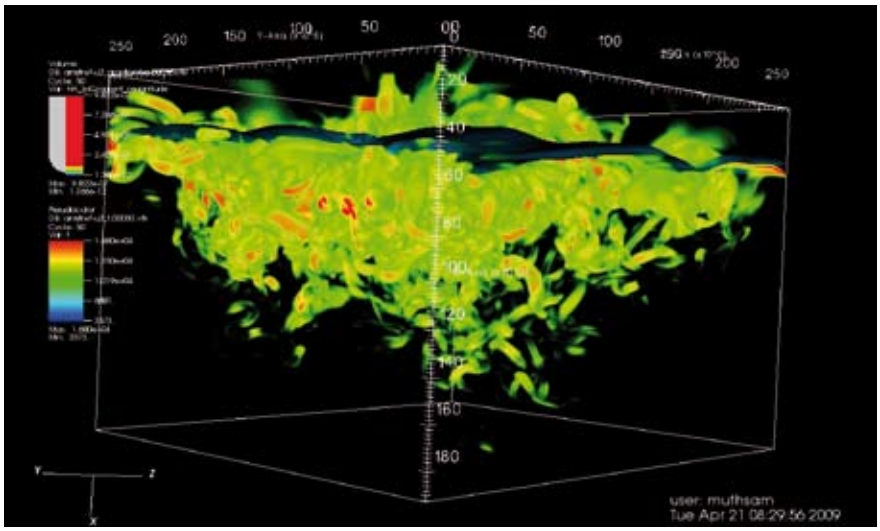


Tornado reaching up to the solar surface. The horizontal cut shows the temperatures in this slice (blue: cool, red: hot). The blue areas mark regions of vigorous downflows, whereas in the red areas material is streaming upwards.

Tornadoes in the photosphere

The main goal achieved within the DEISA framework was to simulate conditions for normal solar granulation. This is the successor to a computer run that modelled exploding granules, which are considerably larger than their normal counterparts.

"The present run had markedly higher resolution than its predecessor. We now have a spacing of grid points of 10 km in the horizontal. The first



These are regions mostly below the visible solar surface. The orange colours mark regions of downflowing material which are highly turbulent, whereas the upflows in between are more laminar.

question was whether, in normal granulation, we would see the same phenomena that we found with exploding granules, in particular a tornado-like movement as material rises from the inner layers to the photosphere – the solar surface layer which we can observe from Earth."

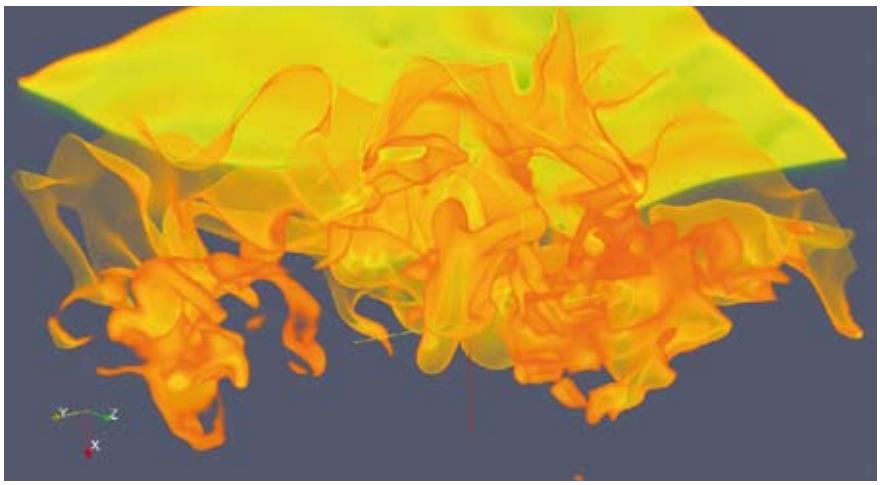
Present calculations do indeed show that tornadoes also appear in normal granules, which cover most of the solar surface. The diameter of tornadoes is typically 100 km or less. They are spinning rapidly and thus are relatively evacuated inside, where the pressure is only about one half as much as in the ambient medium.

Unique combination of research features

The calculations have yielded much information, which the research group is presently analysing.

"With these high resolution runs we can, for example, study the generation of sound waves. This question is of importance for the heating of the corona. Many other properties of these highly turbulent flows will be investigated based on these simulations and the task will take quite some time to come," Muthsam notes.

The roots of the ANTARES code stretch back many years.



A visualization of the complicated structure of the convection zone. In fact, many intertwined vortex tubes are visible. From above one can see into the Sun approximately down to the blue surface, which is visible in the upper part of the image.

All the computations carried out within the SOLEX research project were performed on the Huygens machine at SARA, in Amsterdam, and the data were saved at RZG, Garching. The research used up to 256 CPU cores. A total of 190 000 CPU hours and up to 800 GB memory were used. ANTARES was coded in Fortran90. Parallelization was done via MPI. Visualization and data analysis were performed on local computers, with the open-source software Paraview and Visit. Special filters were written for Paraview in order to adapt it to the specific needs of the analysis.

"In recent times, the pace and scope of development have increased because funding is more adequate and the number of researchers involved has increased. So the extraordinary resources that we have obtained through DEISA have significantly improved our research project."

The significance of the SOLEX project lies in its uniqueness. The research group has inserted two features into the ANTARES code in order to maximize informational output for a given computational effort: high resolution numerical schemes and the option for grid refinement.

"This combination does not exist anywhere else in this research area," Muthsam emphasizes.

The development of the research methodology is ongoing.

"We are continually upgrading the ANTARES code with ever-better numerics, but also broadening the domain of applicability in stellar physics. The project as a whole is therefore open-ended and will surely last for a very considerable time-span," he concludes. ■

For more information:
www.deisa.eu/science/deci/projects2007-2008/SOLEX

Turbulence and gravity in star formation

Damien Lecarpentier

The mechanisms leading to the formation of stars are still poorly understood. Using DEISA's computational resources, a German project team performed simulations of two of the most important physical processes involved in the phenomenon – turbulence and gravity – which will help to improve our understanding of the star formation process. The GRAVTURB project was conducted in 2008 by three researchers from the Universities of Heidelberg and Würzburg.

Star formation is one of the most important phenomena occurring in the universe, yet the mechanisms that lead to it remain poorly understood. “This is because star formation takes a very long time, relative to the life span of a human individual,” explains **Christoph Federrath**, researcher at the Institute for Theoretical Astrophysics, Heidelberg, and leader of the GRAVTURB project. “Take, for example, the case of the Orion Nebula (the closest region of massive star formation to Earth, situated south of Orion’s belt): there, the process can take around two million years! It is, therefore, simply impossible to directly observe the whole phenomenon that leads to the formation of stars.”

In order to overcome this problem, astrophysicists usually combine direct observations of different star-forming regions, at different evolutionary stages, and numerical modelling. Computer simulations play an increasingly important role in astrophysics, and can contribute to improving our understanding of star formation. In the GRAVTURB project, such simulations have allowed the team to investigate the combined effects of gravity and turbulence (i.e. gravoturbulence) on the process leading to the transformation of dense gas into stars.

Integrating turbulence and self-gravity in simulations

The properties and manner of evolution of a star are closely related to its mass: stars of different masses (i.e. low-mass and high-mass stars) are thought to form as a result of different mechanisms. The determination of the statistical distribution of mass in newly formed stars – the stellar initial mass function – is one of the central keys to improving our understanding of star formation.

The main objective of the GRAVTURB project was to accurately model the mass distribution of stellar objects forming in the turbulent interstellar medium (i.e. the matter mostly made of gas that exists between the stars within a galaxy), including self-gravity.

Self-gravity is the gravitational attraction caused by the gas itself, and acting upon itself, causing dense gas clouds to collapse under their own weight. This phenomenon is known to be a major factor in the process leading to star formation, particularly in its later stages.

“Turbulence and self-gravity are the two most important physical processes in star formation. Supersonic turbulence (i.e. random and chaotic gas motions moving faster than the speed of sound waves travelling through the clouds) creates density enhancements in the interstellar medium, which form the seeds of the gravitational collapse of dense gas into stars. Supersonic turbulence tends to compress the gas locally into dense cores. These cores, in turn, can collapse due to their self-gravity to form single stars or stellar systems”, Federrath explains.

“Our previous simulations did not include the effects of self-gravity. However, we know that self-gravity is the physical mechanism that eventually leads to the collapse of the dense gas seeded by turbulent motions. In the GRAVTURB project, the effects of self-gravity were integrated into our simulations.”

Simulating the formation, accretion and resulting mass distributions of collapsed objects in high resolution

An accurate study of star formation processes requires supercomputing capacities capable of providing high-resolution numerical simulations. “The star formation process covers roughly six orders of magnitude in length scale, ranging from an entire molecular cloud down to the scales of individual stellar objects, which is enormous,” according to Federrath. “Even by using the most powerful modern supercomputers, we are still unable to cover the full range of length scales involved within a single calculation.”

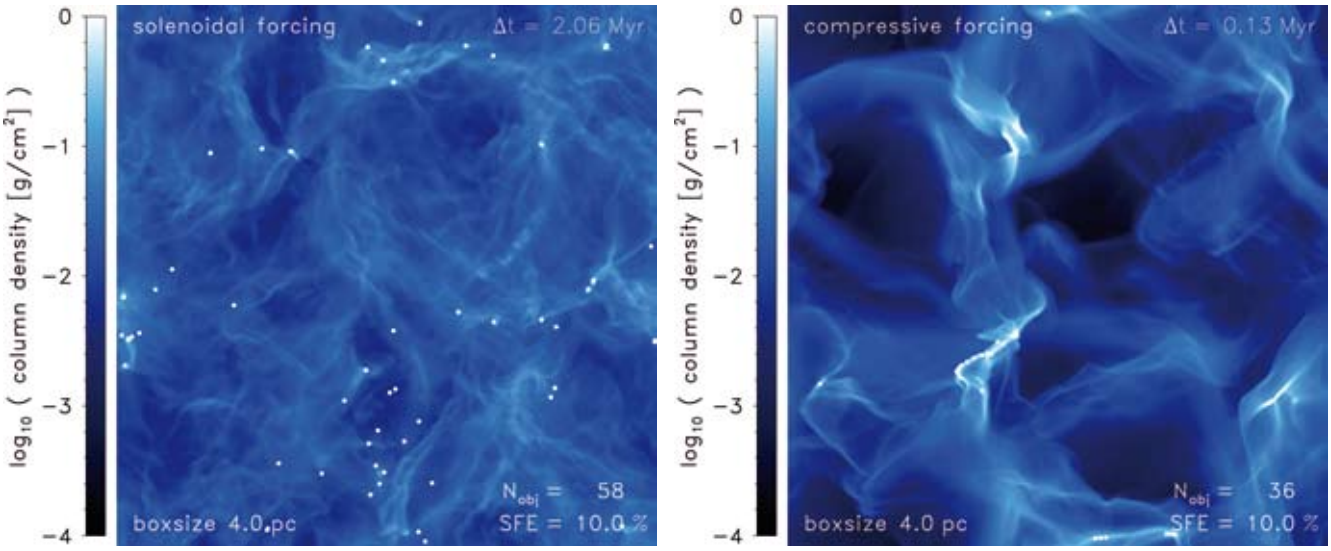
Hence the utility of the DEISA infrastructure for astrophysicists. “DEISA provides access to Europe’s best supercomputing facilities enabling us to study star formation processes in detail,” Federrath notes. “In the GRAVTURB project, a complex system of equations describing the spatial and temporal evolution of the gas had to be solved in three dimensions. This required powerful massively parallel supercomputers.”

Thanks to DEISA’s computing resources, the project team was able to reach an unprecedented level of detail in their simulations. “Within the DECI framework, we were able to study the formation, accretion (i.e. growth) and resulting mass distributions of collapsed objects in high-resolution numerical simulations of driven supersonic turbulence,” says Federrath.

The team was also able to investigate the influence of two extreme kinds of turbulence forcing – a mechanism by which turbulent gas motions are excited – on the formation of stars: “solenoidal” forcing, which mainly excites rotational gas motions (vortices), and “compressive” forcing, where the gas is directly compressed in colliding gas streams.

“We found that compressive turbulence forcing turns gas into collapsed and accreting objects on timescales at least one order of magnitude faster than solenoidal forcing. This result has important implications for analytical models of >>>

Christoph Federrath is Researcher at the Institute for Theoretical Astrophysics, Heidelberg, and the leader of the GRAVTURB project.



Spatial distribution of gravoturbulent gas for solenoidal turbulence forcing (left) and compressive turbulence forcing (right). The interplay of supersonic turbulence and gravity creates a complex network of gas compressions in shocks, where cores and stars (white dots) most likely form. In the case of solenoidal forcing it takes roughly 2.06 million years for significant star formation with a star formation efficiency of 10 percent. In contrast, compressive forcing produces stars at a much higher rate, such that the same star formation efficiency is already reached after 0.13 million years.

the star formation rate (i.e. the rate at which gas is turned into stars) based on the density statistics of supersonic turbulence. In particular, our results show that the ratio of solenoidal to compressive modes of the turbulence must be taken into account in a consistent theory of turbulence-regulated star formation."

Realistic simulation of star formation in clouds is the ultimate goal

The GRAVTURB project enabled the German team to develop and test the code modules necessary both for the present work and for future studies, which will also include the effects of magnetic fields on star formation.

Currently, the team is working on a follow-up project at the Leibniz Supercomputer Centre (LRZ) in Munich. "The DEISA framework allowed us to study the mass distribution of dense cores. In the follow-up study, we aim to resolve the accretion disks that form around individual stars. This will allow us to probe the mass distribution of stars themselves, rather than the dense cores alone," says Federrath.

"Future numerical simulations will also include detailed modelling of the thermal physics involved by solving the equations for the formation and destruction of chemical species (i.e. atoms, molecules, ions, etc.) in the interstellar medium," he adds. "This will allow us to predict the spatial distribution of these chemical species, which we can then compare with observational maps of nearby star-forming regions. For this purpose, we have recently applied for computing time from Deisa. These simulations will include a simplified chemical network allowing us to predict the spatial distribution of observed chemical species. The ultimate goal is to have a sufficiently realistic simulation (including all of the necessary physical processes) of the formation and evolution of stars in clouds, which we can then compare directly to observational data obtained with modern telescopes in order to test different star formation scenarios." ■

For more information:
www.deisa.eu/science/deci/projects2007-2008/GRAVTURB

The simulations in the GRAVTURB project were performed on the SGI Altix at the Leibniz Supercomputer Centre (LRZ), Germany, and on the IBM Power6 system Huygens at the SARA Computing and Networking Services in the Netherlands. A total of 550 000 CPU hours were allocated to the project. The amount of CPU hours was split equally in order to run parallel simulations at LRZ and SARA. One simulation used a purely solenoidal divergence-free turbulence forcing, while the second used a purely compressive curl-free turbulence forcing, both including self-gravity. The whole star formation process covers roughly six orders of magnitude in length scale, from the size of a typical molecular cloud (10 pc = 3.1×10^{14} km) down to a few astronomical units (1 AU = 1.5×10^{8} km, which is the distance from the Sun to the Earth). This required the performance of adaptive mesh refinement simulations, covering part of this vast range of length scales.

Bioglasses have been used in bone and tooth prostheses since the 1970s. However, the ways in which they interact with living tissue is still not well understood at a molecular level. In order to address this issue, the BIOGLASS project was initiated in 2007 by Professor Piero Ugliengo and Doctor Marta Corno from the University of Turin in Italy, in close collaboration with a team from the University of Modena, using DEISA resources to simulate the structural and vibrational features of different bioglasses at a quantum-mechanical level.

Advancing bone implants

Euan MacDonald

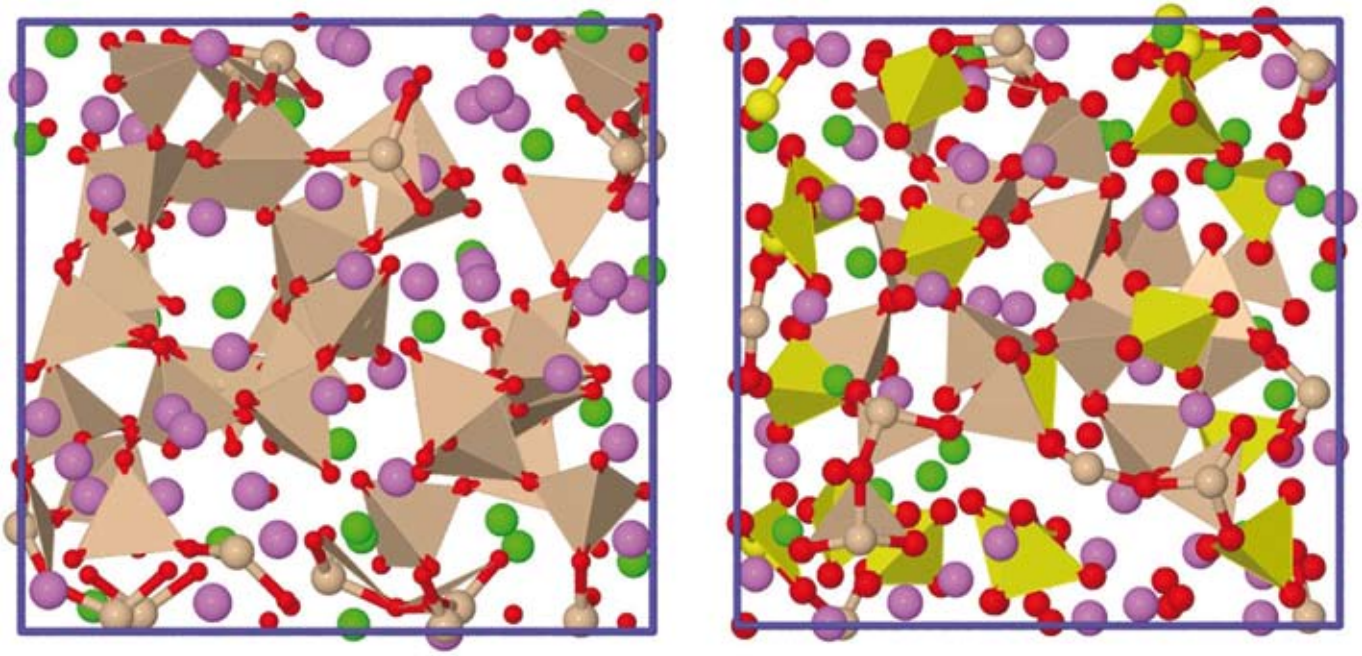
Bioactive glasses – or "bioglasses" – were developed in the late 1960s, when Professor **Larry Hench** and his team of researchers at the University of Florida discovered that certain silicate glass compositions were able to form strong bonds to bone when implanted in rats' femurs. Given that metallic or synthetic polymer materials are rejected by the human body, this was an important medical advance in terms of bone implants and prostheses.

"Over time, research has moved on from the study of inert biomaterials to focus on those that are capable of actually stimulating tissue regeneration and growth," notes **Piero Ugliengo**, Professor at the University of Turin and the lead researcher on the BIOGLASS project. "However, despite the improvement of various specific properties of bioglasses by the addition of 'doping atoms' to the original composition, the fundamental mechanism governing the interaction between the inorganic material and the human body – known as the 'Hench Mechanism' – is still not well understood at a molecular level".

One crucial point in this process is the formation on the bioglass surface of an hydroxyapatite-like layer (the calcium phosphate of which the bones of mammals are largely formed), which in turn is recognized by the living cells leading to bond formation between the prosthesis and the tissue. This issue has been the subject of ongoing, interdisciplinary collaboration between various research centres throughout Italy during the last six years, involving both experimental work and computer simulations. The BIOGLASS project, undertaken using DEISA resources in collaboration with Professor **Cristina Menziani** and Dr. **Alfonso Pedone** from the University of Modena, has taken the simulations of the quantum mechanics (QM) of bioglasses and hydroxyapatite to the next level.

Modelling the quantum-mechanics of bioglasses: A daunting task

"The objective of the BIOGLASS project was to analyze structural and vibrational features of different bioglass models, with variable content of phosphorous in their unit cells, using computer simulations at a quantum-mechanical >>>



Unit cell content of the B3LYP optimized structures of P0 (0 % phosphorus, on the left) and P9 (9.5 % phosphorus, on the right) bioglasses models. Silicon–phosphorous frameworks are here represented as tetrahedra (yellow ones for phosphorus atoms); calcium ions as green spheres; and sodium ions as violet spheres.

level of theory," according to Dr. **Marta Corno**, who worked closely with Ugliengo on the project. "Phosphorus conditions the release rate of silica into the body, and this plays a vital role in the integration of the bioactive material with living tissue. However, bioglasses are, by nature, amorphous materials, which makes their quantum mechanical simulation a daunting task".

Usually, bioglasses are simulated by adopting a very large unit cell, envisaging enough structural disorder to accurately represent the actual material and applying periodic boundary conditions to the calculation to avoid spurious surface effects. However, although this strategy works well for classical molecular simulation, it rapidly becomes prohibitively expensive when applied to a quantum mechanical (QM) model, in which, unlike the classical molecular mechanics (MM) approach, all electrons and nuclei are treated explicitly. Doing so requires the choice of a means of approximating the energy generated by the interactions between electrons and nuclei. These approximations – referred to as "hybrid functionals" – play a key role in density functional theory, on which the project was based; in this case, the hybrid B3LYP functional, which has been proven to give excellent results in this area, was used. The challenge, then, was to adopt a cell-size that was small enough to be feasible using B3LYP, yet retaining enough structural disorder to closely imitate the real material.

"To tackle the problem we adopted a multi-scale strategy, combining classical techniques with quantum mechanics methods," notes Corno. "The researchers at the University of Modena have many years of experience in this field, and have developed a strategy for simulating amorphous glasses. Firstly, a specific composition is fixed and the corresponding number of atoms is located in the unit cell of the model, according to the experimental density; then a classical molecular dynamics simulation is run, starting at high temperature so that a melt-like status for the bioglass is obtained. The third step is the progressive cooling of the system, so that the melt solidifies into a highly disordered bioglass. Lastly, classic techniques of energy minimization are carried out on the most representative structures, in order to generate the proper relaxed structure for full quantum-mechanical periodic calculations. By merging computational techniques in this way, we were able to strike a balance between the large cell units of molecular dynamics and the requirements of quantum simulations".

In order to test the validity of the strategy, the researchers generated models of 45S5 Bioglass composition with 78 atoms in the unit cell following the above procedure, and carefully compared the resulting structures optimized using the QM and MM approaches. Given that QM methods are more accurate than those of MM, any large differences between structures optimized at the two levels would indicate a flaw in the adopted force-field. Fortunately, the comparison revealed a high degree of similarity between the two structures, demonstrating the credibility of the procedure and of the adopted force field. The analysis was then extended to four different bioglass models, each studied at variable

phosphorus composition, in order to uncover the precise nature of the phosphate groups within the unit cell – a fact that has important implications for the dissolution properties of bioglass when in contact with body fluids.

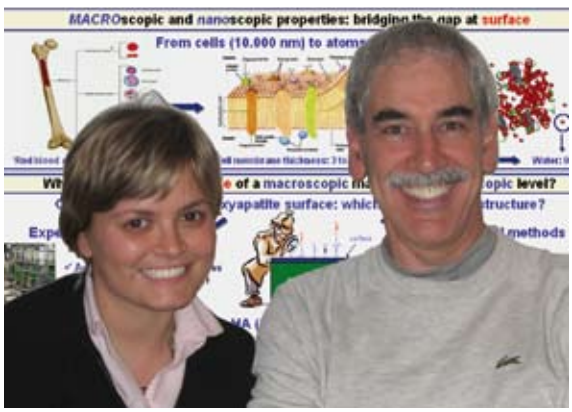
Simulating bioglasses could lead to important advances in medical science

The quantum-level simulation of bioglasses using DEISA resources has generated a number of impressive results. According to Ugliengo, "integrating the quantum mechanics approach allowed us to represent the electronic features of the bioglass, which had been entirely missing from classical simulations, providing important insights on the nature of modifying cations and the bridging oxygen atoms of the silica framework".

"It is worth stressing that this was the first full quantum-mechanical calculation of the vibrational spectrum carried out with the hybrid B3LYP functional, which is one of the most accurate. This enabled us to make a detailed assignment of the vibrational modes. Besides being important in its own right, this advance can facilitate enormously the work of spectroscopists in assigning the spectral features of an experimental spectrum recorded for a real bioglass".

Bioglasses have a wide range of important applications, and, as life expectancies increase, so does the need for implants capable of replacing repairing damaged bone tissues. "In particular, recent work has shown the high potential of bioactive glasses for 3rd-generation tissue-engineering applications, where a highly porous, biodegradable scaffold combined with tissue cells hosts the *in vitro* growth of immature bone like material, then implanted *in vivo* where the tissue-engineered construct adapts to the living environment and stable mature bone is formed. Although most of these achievements have been on the experimental side, classical and quantum mechanical simulations, like those of the BIOGLASS project, can be extremely useful in helping experimentalists design better materials," Ugliengo explains.

"The project has allowed us not only to gain insight on the vibrational features of bioglasses as a function of phosphorous content, but also to identify new optimized bulk structures that could be used as a starting point for designing new surfaces; the next step is to move from the quantum mechanical simulation of the bulk to that of the surface interface between the bioglass and the body tissues. We will be applying again to the DEISA initiative in the near future in order to be able to continue our work in this field". ■



The BIOGLASS project was initiated in 2007 by Professor Piero Ugliengo and Doctor Marta Corno from the University of Turin in Italy, in close collaboration with a team from the University of Modena. It used Deisa resources to simulate the structural and vibrational features of different bioglasses at a quantum-mechanical level.

For more information:
www.deisa.eu/science/deci/projects2007-2008/BIOGLASS

Supercomputing resources essential to quantum-level simulations of bioglasses

According to Ugliengo, DEISA resources were essential in achieving the targets of the BIOGLASS project, for several reasons. Most importantly, because very large unit cells were adopted, a large number of CPUs (at least 128, or better 256 cores) were needed to complete the tasks in the allotted time. The necessary calculations were made possible by a highly sophisticated programme called CRYSTAL06, developed by a group headed by Professor Roberto Dovesi at the University of Turin, which is able to solve the Schrödinger equation for molecules, polymers, 2D slabs and 3D crystals on an equal footing. CRYSTAL06 was able to exploit the supercomputing resources available within the DEISA initiative by running in a massive parallel fashion using both standard highly optimized BLAS libraries and distributed memory. This is extremely important for treating systems of the size of the bioglasses because the diagonalization of the huge Fock matrix is carried out in a well-balanced and distributed way on all the available CPUs.

All calculations were run using either the IBM BCX/5120 supercomputer provided by CINECA supercomputing center of Bologna, or at the Marenostrum as provided by the Barcelona Super-Computing Center, both nodes of DEISA. The best compromise between waiting time and efficiency was achieved by using 128 CPU cores for each run lasting 24 elapsed hours; the CRYSTAL06 code has been extremely well engineered on both systems. In effect, DEISA enabled the researchers to carry out a project that was more ambitious by far than anything that would have been possible using only in-house resources.

Improving Cloud Modelling

Damien Lecarpentier

The Stochastic Subgrid-Scale Cloud (SSSC) project, directed by Heikki Järvinen and Petri Räisänen, researchers at the Finnish Meteorological Institute (FMI), experimented with a new approach to cloud modelling which enables a better representation of the crucial interaction process between clouds and radiation in climate models.

Climate modelling has become a crucial tool for research on climate and global change. Correct representation of clouds in climate models is a question of great importance, given the potentially high impact of clouds upon climate change.

"The impact of clouds upon climate change is a very complex issue," **Heikki Järvinen** explains. "On one hand, clouds trap emitted infrared radiation and thus tend to reduce the top-of-the-atmosphere infrared radiation. On the other hand, they reflect solar radiation. The net effect, so-called 'cloud radiative forcing' is – at present – negative, i.e. in an undisturbed climate clouds tend to have a cooling effect on the planet."

"Changes in the global climate will, however, undoubtedly also impact upon the ways in which clouds and temperature interact, known as 'cloud feedback'," Järvinen adds. "Whether the net effect of this impact is to change that feedback from negative to positive will depend, amongst other things, upon whether the cloud amount or water content, or their vertical distribution with altitude, change significantly."

While an adequate representation of clouds in climate modelling is crucial, many important processes that occur in the atmosphere, such as the interaction of clouds with the radiation emitted by the Earth-atmosphere system, are still unresolved by current computer-driven models.

"Atmospheric General Circulation Models (GCMs) – which model the atmosphere – are the basic modelling tools used in climate research and climate simulation. However, the representation of clouds and their interaction with radiation remains a major issue, due to the coarse spatial resolution of this particular model: a grid cell typically covers an area of 200 km by 200 km in the horizontal. This implies that many cloud features important for radiation cannot be explicitly resolved. This is quite problematic as these interaction processes are essential to the Earth's radiation budget which, in turn, largely determines the Earth's climate."

"There is, therefore, a strong need to improve the representation of clouds in climate models, and one could even say that a biased cloud scheme can ruin a climate simulation resulting from an otherwise accurate climate model."

Stochastic cloud modelling in a coupled climate model

"In climate models, clouds are usually computed using grid-box average quantities, such as grid-box mean temperature and humidity. In our study, cloud formation is described as a stochastic process. It mimics the chain of events as they occur in nature but is inherently random. The need to preserve the grid-box mean quantities, however, represents a powerful constraint on the process."

"Our study is based on several recent developments – from our own work, and that of other scientists – that enable us to address cloud subgrid-scale variability in climate models. The Tompkins cloud scheme (a statistical cloud scheme developed by **Adrian Tompkins** for data assimilation) allows us, for example, to derive the magnitude of subgrid-scale variations in cloud water amount in a physically consistent fashion. The Monte Carlo Independent Column Approximation (McICA) (a recently developed method for computing domain-average radiative fluxes) and the stochastic cloud generator enable a flexible description of subgrid-scale cloud structure in GCM radiation calculations."

"The SSSC project represents the first test of these approaches in long integrations within a coupled atmosphere-ocean GCM," Järvinen points out.

"The first tests with the stochastic subgrid-scale cloud modelling have been successful. In these tests, the atmospheric GCM used the observed sea surface temperature and sea-ice cover, which implies a forcing of the atmospheric simulation towards the observed evolution of the climate. In the SSSC project, the atmospheric GCM was coupled with an oceanic GCM and these were run in a coupled mode. In this case, there is no forcing towards the observed climate evolution, excepting perhaps the observed atmospheric CO_2 concentration. A coupled atmosphere–ocean GCM was particularly required for our study, in order to avoid use of fixed sea surface temperature of an atmosphere-only GCM, which would have limited the validity of the simulations."

"In a nutshell, our study aimed at exploring the use of an advanced treatment of subgrid-scale cloud radiation effects in climate models, by using a coupled atmospheric–ocean model. Its scientific objectives were twofold: first, to test and demonstrate the viability of the stochastic approach for the subgrid-scale cloud and radiative transfer parametrizations; and second, to use this approach to improve the representation of cloud–radiation interaction in GCMs."

Computational resources

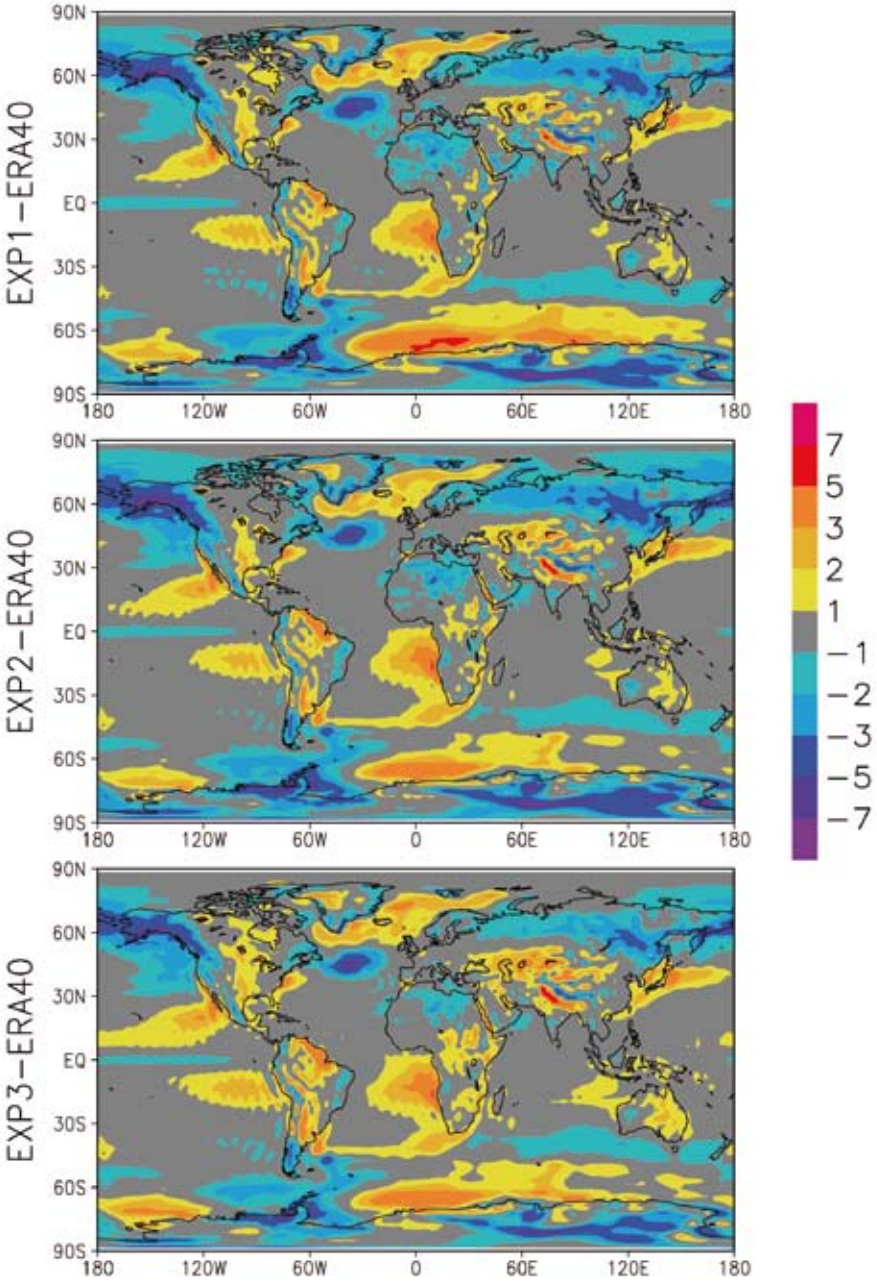
In order to carry out this study, a large amount of computational resources was required. Researchers used DEISA resources within the DECI framework and experiments were conducted in 2008 on the NEC SX-8 at the High Performance Computing Center Stuttgart (HLRS) Germany, where the Finnish team coupled the general atmospheric circulation model ECHAM5 to the general ocean circulation model MPIOM, two models that were developed by the Max Planck Institute for Meteorology (MPI-M) in Hamburg, Germany.

"This model setup is very time-consuming for any computer and, in practice, it would have been impossible for us, using the resources available to us at our Institute in Finland alone, to conduct this experiment to the extent made possible by the DEISA quota," Järvinen acknowledges. >>>

"Three 240-year long experiments were carried out with three specific model configurations. The first experiment involved the standard version of the ECHAM5–MPIOM coupled atmosphere–ocean GCM; the second used a version employing the Tompkins cloud scheme; and the third a version employing the Tompkins cloud scheme together with McICA radiation calculations and the stochastic cloud generator."

"On the NEC SX-8 processors, each run took between 3 and 4 hours per simulated year Unexpected problems regarding the parallelization of the coupled model across several 8-processor nodes precluded the use of a larger number of processors, but the experiments were completed successfully nevertheless," says Järvinen.

According to Researcher Heikki Järvinen, the new cloud modelling method can be safely included into the coupled climate models. Järvinen works at the Finnish Meteorological Institute.



Comparison of simulated time-mean near-surface air temperature in kelvins to the ERA40 reanalysis data produced by the European Centre for Medium Range Weather Forecasts. Figure EXP1 is computed with standard version of the coupled model. In figure EXP2 and the Tompkins cloud scheme is included. In figure EXP3 the Tompkins cloud scheme is included and subgrid-scale cloud information utilized in radiation calculations through the stochastic cloud generator and Monte Carlo Independent Column Approximation.

Unexpected results

The results, however, proved to be quite unanticipated for the research team: "Perhaps surprisingly, the modifications tested here had overall a relatively small effect on simulated climate. Given that this new cloud modelling method represented quite a significant change compared to the standard model, we had anticipated that it would have a larger impact. Nothing major was detected, however, and this was rather unexpected."

These unexpected results did not, however, mean that the experiment was worthless; quite to the contrary: "While this might seem like an unexciting result, it is actually an important indicator of the feasibility of the proposed stochastic approach in state-of-the-art climate models," Järvinen points out. "It shows, in particular, that the new cloud modelling method can be safely included into the coupled climate models, and that its benefits can begin to be exploited. The new approach improves substantially the internal physical consistency of the model, and allows also us to produce a stable model climate. It is therefore a viable option for application in multi-century climate simulations."

"We are now equipped with convincing evidence of the applicability of our approach within GCM implementations. Hopefully this work will contribute towards improving the models that will be used in the 5th assessment report of the Intergovernmental Panel on Climate Change (IPCC)." ■

For more information:
www.deisa.eu/science/deci/projects2005-2006/SSSC

Earthquake scenarios for Europe

Sanna Pyysalo

Seismic hazards and ground motion amplitudes will be better estimated in the future thanks to the EuQuake project. Its research results were achieved using supercomputing resources offered by DEISA. The project started in June 2008 and ended in August 2009.

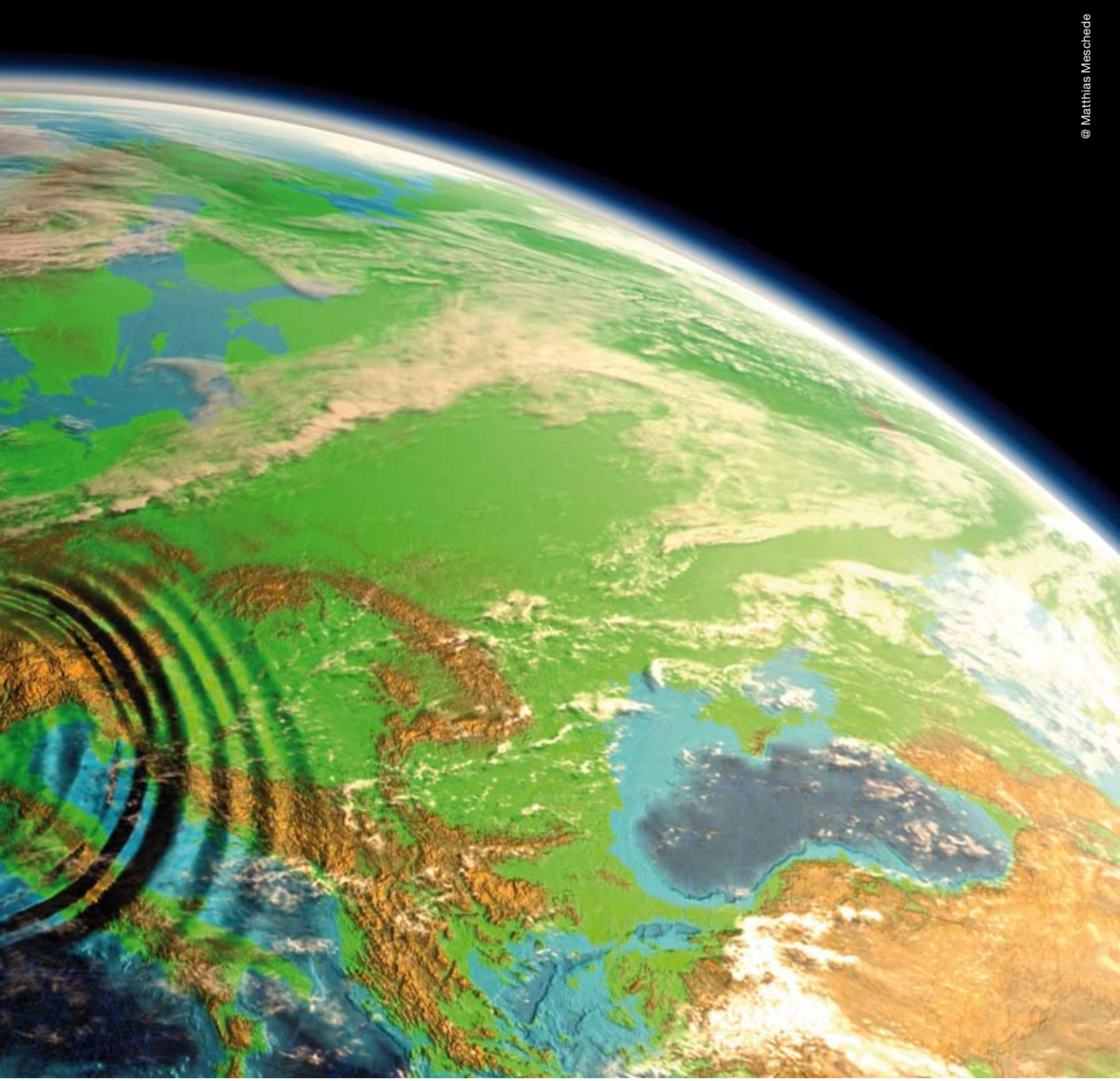
Seismic waves generated by earthquakes carry a wealth of information on the Earth's interior structure and the behaviour of the earthquake's source. The aim of the EuQuake project, carried out by the Section of Geophysics of the Department of Earth and Environmental Sciences at the Ludwig Maximilian University of Munich, Germany, was to calculate theoretical seismograms for given three-dimensional velocity models and earthquake sources. The research group was led by Dr. **Martin Käser** and used new numerical algorithms and high-performance computing (HPC) to achieve this goal. The project was largely funded by the Emmy Noether Programme of the German Science Foundation. Numerical simulation algorithms are the central tool for modelling and explaining field observations at seismological stations on the European continent. By minimizing the difference between synthetic and observed seismograms it is also possible to recover information on the physical properties of the subsurface structure below Europe.

"Improved understanding in this field will allow us to better estimate seismic hazard, ground motion amplitudes and the consequences of ground shaking after earthquake events, for example via real-time earthquake parameter determination in early-warning systems," says Dr. Käser.

Many steps towards the goal

The main goal of the EuQuake project was to create a simulation software tool to be run on large supercomputers in order to produce accurate synthetic seismic data sets for earthquake scenarios on the European continent.

In the first part of the project, the technical prerequisites for large-scale simulations had to be met, and the necessary input data provided.



© Matthias Meschede

Schematic visualization of the propagation of earthquake waves at the Earth's surface where the faster P and S body waves have travelled further than the Love and Rayleigh surface waves that produce much higher amplitudes.

"Next, wave field calculations were carried out for past earthquakes for which observations are available. In the future, it is envisaged that these calculations will be performed on a semi-automatic basis, as soon as an earthquake occurs," Käser explains.

After the simulation, the waveforms are stored a format compatible with observational data in order to allow the application of the same processing tools to both empirical and synthetic results.

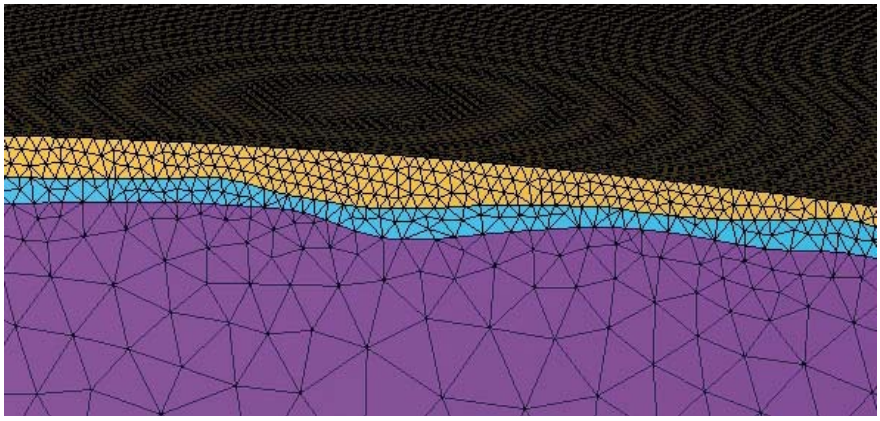
Models of the Earth´s crust are necessary

The main finding of the EuQuake project was that the crustal structure of the Earth has an enormous influence on arrival times of earthquakes and on seismic wave forms in particular, even though the layers it consists of are remarkably thin when compared to the dimensions of the European continent and the wavelengths of the propagated waves.

"We were able to show that we are still dependent, to a high degree, on the simplification of crustal models in order to represent the crust in numerical simulations. The automatic generation of accurate 3-D simulation setups for the ´on-demand´ computing of large synthetic data sets is only in its infancy," notes Käser.

Furthermore, the research group found that a quantitative measure for the frequency-dependent effects of the fine-scale structure of the crust is crucial to successful simulation setups.

"Only with such a systematically evaluated error analysis can we create appropriate discretized models and >>>



Color-coded discretization of the Earth's crust and upper mantel (purple) using an unstructured tetrahedral mesh. The geometrical flexibility of the mesh allows for the correct incorporation of major discontinuities such as the interface between the upper (yellow) and lower (blue) crust and the Moho-discontinuity.

For more information:
www.deisa.eu/science/deci/projects2007-2008/EuQuake

give a quantitative quality measure to our synthetic seismograms."

Significant results for earthquake research

Numerical and computational methodologies have dramatically improved in the past few years. Nevertheless, due to the complicated nature of elastic wavefields and the long propagation distances of the waves, these calculations are computationally extremely expensive.

"Our research was unique, because we tried to consider with high levels of accuracy the geophysical and geometrical properties of the Earth's crust – the first 5-60 kilometres just below the Earth's surface," Käser says.

This is particularly challenging because the top layer consists of highly heterogeneous geological material both vertically and laterally, is of variable thickness and has the dominant influence on the shape, strength and arrival time of the seismic signals and, therefore, on ground shaking.

The EuQuake project was very significant for international research into earthquakes.

"It clearly showed that there is still a lot of work to be done towards the validation of the new European crustal models that are continuously being put forward. Much research effort is being put into the integration of more and more geophysical data into the creation of new seismic velocity models."

However, most modern simulation technologies still seem unable to take the resolution of these models fully into account, especially in the vertical direction. This means that accurate seismic wave propagation simulations after earthquake events are still limited to rough approximations of the crustal velocity models on a continental scale. Therefore, the ability to reliably predict ground motion in any given scenario is currently not dependent on the availability of missing information or the resolution of the velocity models, but rather on the validation of these models and the corresponding discovery of their weaknesses or errors.

"EuQuake has shown that we only can overcome these problems by investing in even more efficient and accurate simulation technology, which will require close and long-term collaboration between seismologists, computational geoscientists, numerical mathematicians, software engineers and computer experts from the most powerful HPC sites worldwide," Käser states.

DEISA´s help was essential

Developments in the field of seismology in recent years have highlighted the need for massively 3-D simulation technology in order to understand and explain the information from an ever-increasing stream of seismic observations.

"Despite the obvious societal relevance of the subject matter, Earth science is too small a community to be able to create its own supercomputer hardware infrastructure. Therefore, we as computational seismologists are absolutely dependent on the HPC infrastructure of DEISA, with its distributed resources on huge parallel supercomputing systems," emphasizes Käser.

In other words, studies like those of the EuQuake project would simply be impossible without DEISA.

"This is why we believe that DEISA should play an important role in establishing a new working model for our CPU-intensive applications in the Earth sciences. We intend to embed the work started during the EuQuake project within further EU-wide initiatives and, in particular, to make efforts to establish an e-infrastructure for Earth sciences on an international scale." ■

Computations for the EuQuake project were performed on HLRB II in Garching, Germany, MareNostrum in Barcelona, Spain, and Huygens in Amsterdam, The Netherlands. There were several test and production runs, which used from 128 to 2048 CPU cores per simulation. A total of approximately 600 000 CPU hours were invested in these simulations. To construct the discretized models, commercial software packages like ANSYS ICEM CFD and GAMBIT were used on local computers. The simulations were carried out by the in-house developed solver "SeisSol" for seismic wave propagation problems, coded in Fortran90 using MPI for parallelization. Output visualization and data analysis were performed on local computers using MATLAB, PARAVIEW, and BLENDER.

Revealing the mysteries of galaxy formation

During the past decade, the study of the origins and evolution of the Universe has become a research discipline in its own right thanks to advances in both observational and computing technology. Rosa Domínguez-Tenreiro and her research group have been able to study structure formation and evolution in the Universe by means of computer simulations.

Tiina Raivo

"We try to answer the outstanding questions such as why galaxies exist, why they come in different shapes and sizes and what drives their evolution. It is worth noting that, because light takes time to travel from the point at which it is emitted to the point at which it is collected in a telescope, light coming from distant galaxies was emitted when the Universe was younger than today; thus distant galaxies will appear younger to us than do close ones," says **Rosa Domínguez-Tenreiro**. This allows astronomers to actually glimpse the Universe at different ages: galaxies relatively close to us provide a snapshot of the present-day Universe, whereas those much further away reflect the Universe at a stage when it was still young.

The GALFOBS (Galaxy Formation at Different Epochs and in Different Environments: Comparison with Observational Data) project is concerned with the study, in various environments and during different cosmological epochs, of the generic statistical properties of galaxies. It looks both at specific details particular to individual galaxies and at their grouping properties. The project started in December 2007. During spring and summer of 2008 enabling work was done, and the codes were adapted to the HLRB-II machine at the Leibniz Supercomputer Centre (Leibniz Rechenzentrum, LRZ) in Munich, Germany. It was not until October 2008 that the main production runs started.

"One of the main challenges for astronomers and cosmologists is to understand how galaxies have formed and evolved from tiny density perturbations shortly after the Big Bang, until they acquired the properties of the adult galaxies we observe today," Domínguez-Tenreiro explains.

The dramatic improvements in observational astronomy, as reflected in the ever-growing size of telescopes, the significant development of data management as well as the advent of new computational techniques and algorithms mean that the present decade offers unparalleled opportunities for the advancement of scientific knowledge in this particular field. >>>

The GALFOBS project team. From left to right: Arturo Serna, Francisco Martínez-Serrano, Rosa Domínguez-Tenreiro, José Oñorbe, Paola Alpresa, and Alexander Knebe. Jorge Naranjo and David Vicente, from the Barcelona Supercomputing Center, were absent. The picture was taken at the Universidad Autonoma de Madrid, Science Faculty.

"We can now meet these challenges by studying galaxy formation and evolution in a cosmological context by means of hydrodynamical simulations; simulations that not only combine high spatial and temporal resolution while simultaneously utilizing sufficiently large computational volumes, but also seek to model the relevant physical processes taking place on sub-resolution scales," notes Domínguez-Tenreiro. "While simulations in the previous decade were only capable of modelling the actions of gravity, we are nowadays capable of following the formation and evolution of 'virtual' galaxies in our computer simulations that can then be directly compared to their observational counterparts. This provides us with an advanced understanding of the Universe and allows us to further test the physical theories and models underlying the simulations," she continues.

A new hydrodynamical code designed

"To conduct the GALFOBS project, the simulations had to be run with extremely high resolution (i.e. including small-scale details) and, at the same time, in volumes large enough to represent the whole Universe and, moreover, with suitable sub-resolution modelling."

The Universe itself is believed to be of infinite size; this, however, cannot be modelled in a computer. In fact, the range of scales that can be simulated and modelled is technically limited by the computing power available. The larger the volume and the higher the resolution of small-scale details, the more technical difficulties in terms of CPU time, computer memory, etc., occur. Therefore, compromises between "computational volume" and "accuracy of the calculations" must be struck. The GALFOBS team has overcome this problem by using a specific hydrodynamical simulation code called P-DEVA that has been designed and implemented to very challenging specifications.

In particular, the probabilistic implementation of chemical enrichment used in P-DEVA has enormous potential, but it requires high-resolution simulations in large volumes using a large number of particles. This requires running simulations at the cutting edge of today's computing capabilities, making full use of all that the latest technology can provide: "We need very powerful computers, an efficient system for the storage of outputs, a fast communication network for their transfer, and technical support for the refinement of codes and their porting to systems with different architectures. For us, features such as these could only be accessed through the DEISA infrastructure, the use of which was absolutely necessary to the success of our project," says Domínguez-Tenreiro.

"A second phase of the project is now in progress. Its outcome will be the spectral energy distributions and images in different wavebands of the galaxies produced in the simulations. This will then be compared to the observational data, either on individual galaxies or samples of them, to test the suitability of the physical hypotheses upon which our work is based. These comparisons will create new possibilities for collaboration with astronomers involved in observational projects, and perhaps even lead to new technological developments."

Pioneering research on complex cosmological simulations

"GALFOBS was our first DECI project. We were in real need of an extension of the CPU time at our disposal. Our previous facilities did not allow us to run such big simulations. This was the first "Grand Challenge" simulation including an elaborated, self-consistent implementation of metal enrichment, fully metal-dependent cooling and chemical stellar feedback that was ever run within a fully self-consistent cosmological framework," Domínguez-Tenreiro explains.

"Moreover, this was the first time that such a complex cosmological simulation was performed up to the present age of the Universe (13.7 billion years after the Big Bang). In this regard, the galaxies or samples of galaxies identified at this age can be compared to actual, close galaxies, whose properties are better characterized than more distant ones. Once it has been shown that these virtual galaxies have properties consistent with observed local galaxies, we can then feel

confident that comparing the snapshots of their mass assembly and star formation history (from simulations) with data on more distant galaxies does indeed make sense. For this reason, successfully running such a complex simulation up to the present epoch is a very important milestone in the field. Of course, this was not an easy task because the calculation of galaxy evolution takes a huge amount of CPU time." says Domínguez-Tenreiro.

"The plan for the future involves more detailed simulations, with more detailed sub-resolution physics models, and higher resolution in particular, in comparable volumes. This will, in principle, be more expensive than the previous runs, but given the acceleration in computing technology and the room still available for improvements in code scalability if appropriate adjustments to the code are performed, we expect this objective to be achievable in the next few years. DEISA supercomputers are, in the current state of affairs, the only way we have to access large enough shared-memory machines on which we can run our codes and achieve scientifically significant results. Without DEISA, this project and those we are planning in the future would simply be unfeasible," Domínguez-Tenreiro concludes. ■

More information:
www.deisa.eu/science/deci/projects2007–2008/GALFOBS

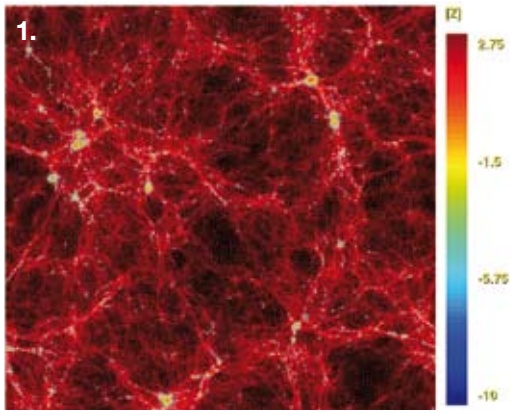


Figure 1 shows the gas and stellar densities of a 40 × 40 × 8 (Megaparsec)³ slice 1,78 billion years after the Big Bang (13% of the current age of the Universe). Note that the cosmic web stands out, with brighter regions indicating overdense areas, and darker regions representing underdense or almost void regions. The element content (i.e. the logarithm of the metallicity in units of the solar one) has been superimposed onto this image, according to the color scale given to the right of the figure.

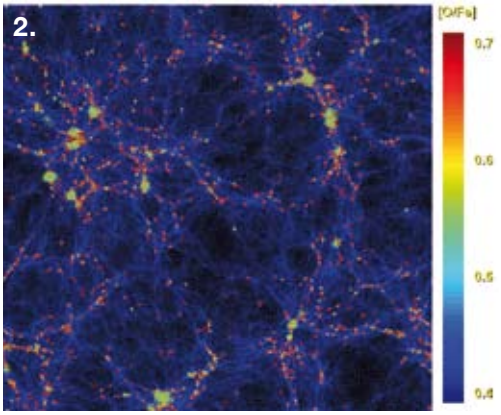


Figure 2 shows the same slice, this time with the oxygen-to-iron ratio superimposed, according to the colour scale on the right. This ratio has a very important astrophysical meaning, as oxygen is thought to have formed from massive star explosions, shortly after these stars form (short timescale stellar nucleosynthesis process), while iron is mainly produced in less massive, binary supernovae explosions, a long time after the less massive stars form (large timescale stellar nucleosynthesis process). It can be seen in this figure that, at these early stages, this ratio is super-solar.

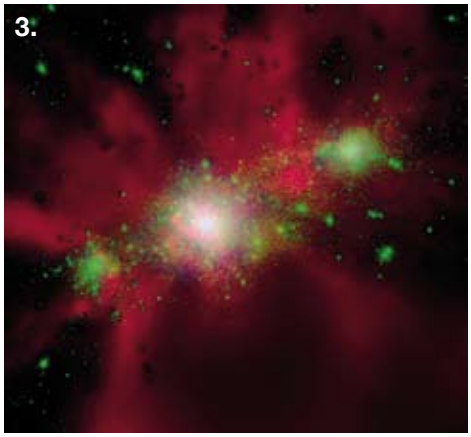


Figure 3 shows a projection of a 8 × 8 × 8 (Megaparsec)³ cube in a dense region, when the Universe was 2/3 of its current age. Three galaxy groups seen in this figure happen to be close to each other, and aligned along a cosmic filament. Hot gas is drawn from magenta to almost white as its temperature increases. Dark matter is shown in green. Cold gas and stars are shown in blue, but they are hardly seen as they are inside the dark matter substructures.

The first exciting results from the GALFOBS project are realistic samples of massive local galaxies. The dynamical and structural properties of these galaxies, as well as their stellar age distribution, have proved to be in very good agreement with large observational samples of massive local galaxies. They have also obtained disk galaxies with properties consistent with observations such as the relatively high disk-to-total ratios, the thin stellar disks, and with the Tully–Fisher and the luminosity–size relations. In addition, the GALFOBS project has enabled the researchers to delve deeper into group identification and their properties at different cosmological times, developing algorithms that mimic observational and physical criteria. Lastly, the stellar mass function at different cosmological epochs has also been studied. Indeed, as the GALFOBS project has brought some simulations up to the current Universe age, they have been able to obtain the stellar mass function at the current cosmological epoch. This is the first time that this has been achieved for a simulation of this quality, and it is an important step forward as this function is a fundamental constraint of different galaxy formation models. "These results are important in and of themselves, as in many respects this is the first time that they have been obtained. Moreover, they have opened up new possibilities for collaboration with observational astronomers," explains Domínguez-Tenreiro.

Controversy over spin glasses laid to rest

Tiina Raivo

Victor Martin-Mayor and Peter Young head research groups that are studying the phase transition for a particular type of spin glasses, called Heisenberg spin glasses. The controversy over the behaviour of this particular type of spin glasses lasted over 20 years until finally settled by the work of these research groups.

Spin glasses are magnetic alloys that have one salient feature: their properties are never stable over time. When you cool a spin glass below its critical temperature, its properties will continue to change for years. This "aging" phenomenon is not peculiar to spin glasses alone: many other systems of great industrial relevance, such as polymers and structural glasses, also suffer from it. Nevertheless, spin glasses are regarded by scientists as a particularly simple model system for the study of aging.

"We are concerned with the change of ordering properties of the atomic magnets for a particular type of spin glasses, namely Heisenberg spin glasses, at their critical temperature. In order to explore the ordering changes we need to analyse low-enough temperatures. In order to get significant results, our simulated systems need to be large enough. That's why the full name of our project is Heisenberg Spin Glasses: Large Lattices at Low Temperatures," says **Víctor Martin-Mayor**.

In Heisenberg spin-glasses (named after **Werner Heisenberg**, one of the greatest physicists ever who did pioneering work in quantum mechanics), the atomic magnets can be visualized as "arrows" of fixed length, or as points in the surface of a sphere. In "normal" spin glasses (called Ising spin glasses), the magnetic moments can point only to the north pole or to the south pole of this sphere. In Heisenberg spin glasses, on the other hand, they can point anywhere. Some materials are better described as Ising-like, while others are Heisenberg-like. Experiments show that the two types of materials behave rather differently.

The HSG (Heisenberg Spin Glasses) project started in fall 2007, after Martin-Mayor, a researcher at the Complutense University of Madrid *(Universidad Complutense de Madrid)* in Spain, and his group had published the results of their research on Heisenberg spin glasses. These results were soon added to by the research conducted by **Peter Young** and his student **L.W. Lee** at the University of California in the USA. It was clear that neither of the two sets of results were conclusive, but all involved felt that a full understanding was within reach. Instead of competing the researchers decided to collaborate. "The 2007 DECI call for proposals was opened just at the ideal moment for us. We had a well-framed problem, and knew how to solve it. We just needed the computational resources and DECI was ready to provide them," recalls Martin-Mayor.

Martin-Mayor, Young and their research groups are interested in the nature of the phase transition for Heisenberg spin glasses. The changes from liquid to vapour, for example when boiling water, or from liquid to ice when freezing water, are phase transitions. The general feature of these two phenomena is a change of order at the microscopic level. When water is heated until it reaches the boiling point, the water molecules start a fast, random motion. This changes if the water is kept cooling until it freezes: at 0 °C water molecules order into a crystalline structure.

"Phase transitions are a kind of microscopic revolution that happens at a critical temperature. Above the critical temperature, molecules or atoms are significantly more disordered than below it. Phase transitions are ubiquitous in the physics of condensed matter. They receive a lot of attention from scientists, since many interesting things happen close to the critical temperature, while the system properties are relatively constant at other temperatures. Furthermore, sudden changes in material properties triggered by small changes in temperature can be used by engineers. For instance, information is imprinted in a hard disk by ordering the microscopic magnets the disk is made of," explains Martin-Mayor. >>>

Researcher Víctor Martin-Mayor at the front door of the Physics Department of the Complutense University of Madrid, Spain.

Significant number of CPU hours used for simulations

Research into spin glasses is computer-intensive in two ways. "To start with, we are considering disordered magnetic alloys. At a microscopic level, two samples of the very same spin glass material are not identical. These differences can be quite significant as far as the ordering magnetic pattern is concerned. In order to get significant results, we need to simulate hundreds or even thousands of samples," says Martin-Mayor.

"In terms of scientific results, we have obtained conclusive evidence of a spin glass transition in Heisenberg spin glasses. Furthermore, we have demonstrated that there is a single phase transition in the system, even if two quite different types of ordering arise. The controversy over the behaviour of this particular type of spin glasses has lasted for some 23 years now, and we think that it has basically been settled by our work. As originally conceived, the project has been successfully concluded. DEISA gave us enough momentum to complete our research. Our results were reported in a research paper that was written in May 2009, and have already appeared in the journal *Physical Review B,*" he continues.

Future developments

In the future, Martin-Mayor intends to extend the research program in two ways: "First, Heisenberg spin glasses are, in a sense, an ideal limit. Real materials always have some traces of anisotropic interactions. In order to integrate our theoretical work with experiments, we need to understand in detail the effect of these residual interactions. Second, we have gathered information on the equilibrium spin glass phase, which is clearly relevant to the nonequilibrium experimental work. I think that, since we have already cleared up the phase diagram, it would be of great interest to undertake new simulations of very large systems in order to investigate their aging behaviour."

"In addressing the nonequilibrium, speed is an issue. Nowadays, we roughly need 1 microsecond to update a single spin. To get close to experimental conditions, we would need to simulate a large number of spins (1 million or so), performing on each some 10 000 million updates. This is roughly equivalent to 300 years on a single CPU. In order to approach that goal, parallel computations are clearly needed. We need to get many CPUs collaborating in the simulation on a single sample, in order to significantly speed up the computation. Technically, this is considerably more demanding than our previous work in DEISA, where each CPU worked on an independent copy of the system," explains Martin-Mayor.

"We do basic research. We seek to advance knowledge on glasses and are convinced that this knowledge will be of practical usefulness in the future, but it is not easy to guess when and where. If I had to make a bet, my money would be in computer science. Computers are being used to solve many problems, where many mutually contradicting goals need to be balanced. The theory of spin glasses has already proven useful to the analysis of difficult optimization problems, and my feeling is that some powerful tools will be made available to engineers in the future as a result," explains Martin-Mayor.

Computing

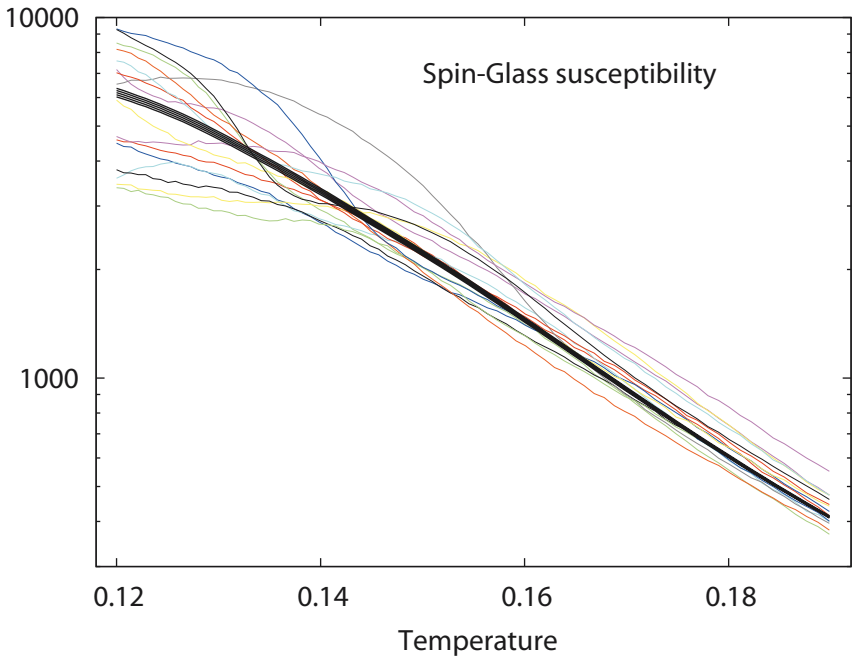
The computing time needed in order to obtain significant results even for a single sample can be prohibitive, especially if the system is large or the temperature is low. Physicists have invented a clever way to combat dynamical slowing down, by allowing the temperature of the sample to be a dynamical variable: sometimes it is high, sometimes it is low. This is traditionally done by simulating on the same CPU as many copies of the systems as values can take its temperature. Pairs of copies exchange their temperature periodically,

according to certain rules. “This was just too slow for us, since the total CPU time has to be divided between the many copies of the system,” notes Martin-Mayor.

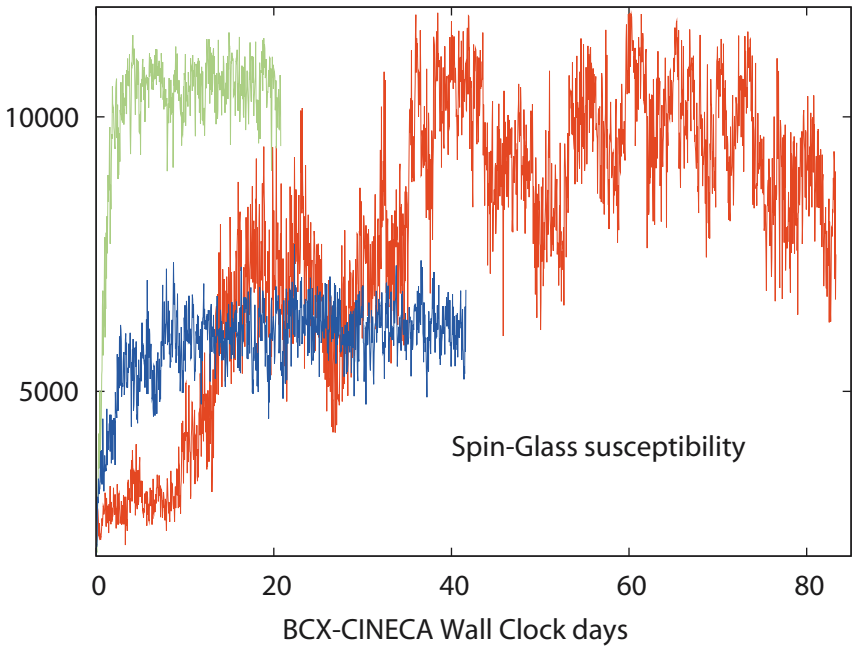
According to Martin-Mayor, the obvious solution was to have a large number of processors (79 plus a central controlling processor) working on different copies of the same sample. The processors needed to be synchronized very often to exchange their temperatures and, less often, to check dynamically the magnetic properties. “To our knowledge, this had not been attempted before, and for good reason. We needed a large number of well communicated CPUs in order to simulate a single sample, but then we needed to simulate hundreds of samples. These kind of computational resources are not easily available for scientists in our area. The DECI call for proposals that would give us access to DEISA resources was an opportunity that we simply could not miss.”

“Thanks to DEISA, we have made an important step forward in the understanding of this particular phase transition. We were granted 1 million CPU hours in the CINECA supercomputing centre, in Bologna, Italy. We got enough computers to put our research to work. Even if quite large, the thermalization time turned out to be feasible with our parallel computation. We got some 40 samples from CINECA, from a final total of 164. The work was then completed with an extra allocation of some 4.7 million CPU hours in the *Red Española de Supercomputacion*, a network of supercomputing centres in Spain. Our experience with DEISA was crucial in getting such generous time allocations, as we could demonstrate to the Access Commission that our research was working in reality,” Martin-Mayor concludes. ■

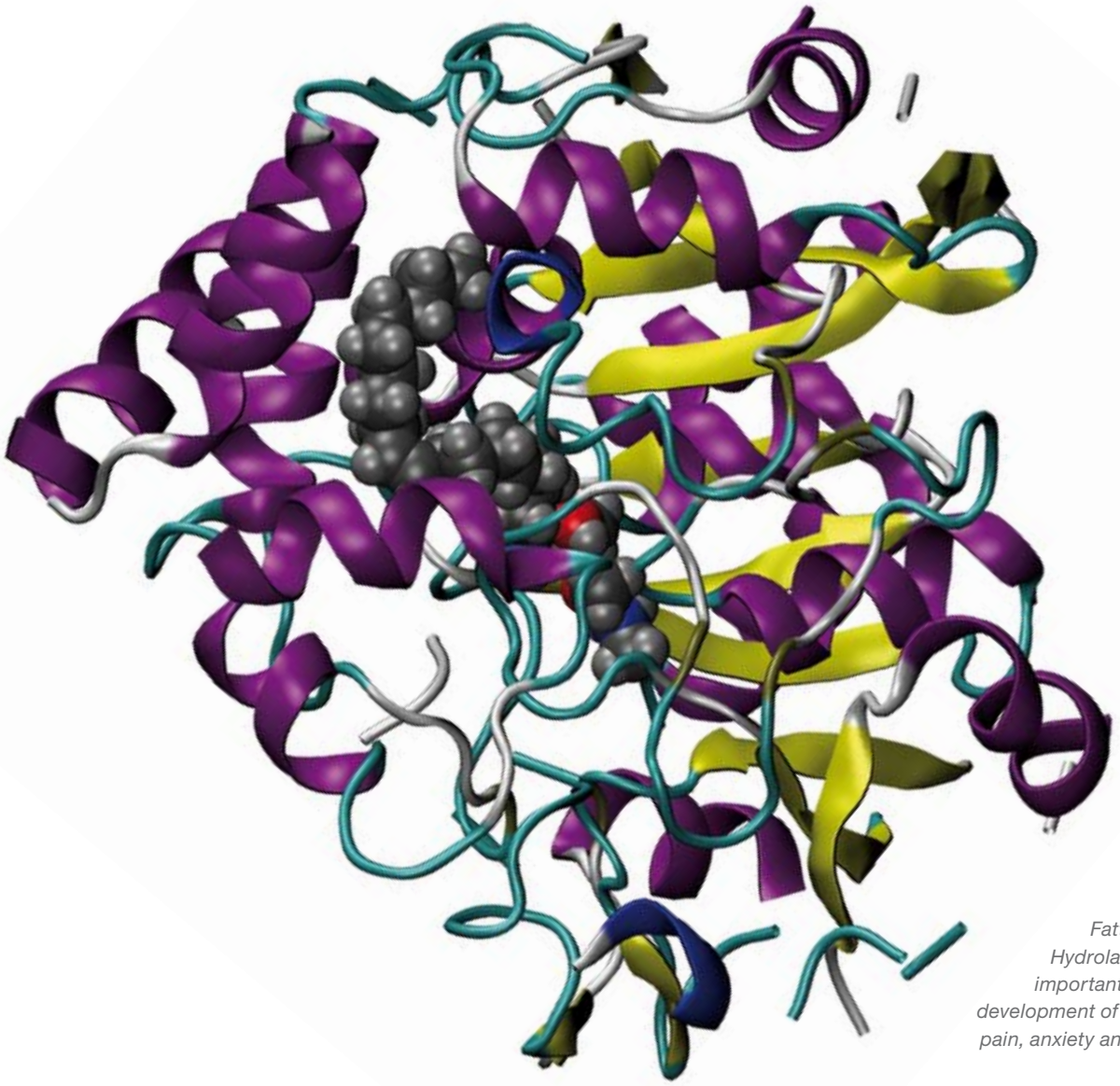
More information:
www.deisa.eu/science/deci/projects2007-2008/HSG



The temperature dependency of the spin glass magnetic susceptibility for some 10 samples to compare with the average behaviour. A Logarithmic scale is needed to represent the extreme sample-to-sample variability.



Real simulation data on the time evolution of the spin glass susceptibility. The horizontal axis in the plot is wall clock time. For some samples, it was necessary to have 80 CPUs working for almost 90 days before the results were stable with time.



Fatty Acid Amide Hydrolase (FAAH), an important target for the development of drugs to treat pain, anxiety and depression.

Modelling enzymes:

Euan MacDonald

Biological enzymes are large molecules within cells that function as catalysts, speeding up the chemical reactions that make life itself possible. Understanding these, then, is crucial to a better comprehension of the biomolecular world; however, until recently, the vast computational resources required to accurately simulate enzymes at a molecular level simply didn't exist. Seeking to exploit the resources made available within the DEISA framework, a team of researchers from the University of Bristol in the UK and the Wroclaw University of Technology in Poland set out to simulate the catalytic functions of one such enzyme in unprecedented detail.

the catalysts of life

"Enzymes are outstandingly efficient natural catalysts," begins Doctor **Adrian Mulholland**, of the University of Bristol in the UK. "More specifically, they are large biological molecules that are used in cells to speed up the chemical reactions that are necessary for life. Understanding how they work would provide fundamental insight into the chemistry of life, allowing us not to only appreciate the beauty of the biomolecular world, but also to harness their power to create new medicines, new biomaterials and new biocatalysts".

Mulholland is the lead researcher of the TotalEnz project, which also involves his University of Bristol colleagues **Christopher Woods** and **Narin Lawan**, and **W. Andrzej Sokalski** and **Borys Szefczyk** from the Wroclaw University of Technology, Poland. The project developed from the groups' long-standing interest in trying to understand the action of enzymes using computer simulation, making use of new software and algorithms that have made it possible to perform such simulations with unprecedented detail using high performance computing resources.

Modelling enzymes: new possibilities, new challenges

"The aim of the project was to investigate the catalytic mechanism of the archetypal enzyme chorismate mutase," notes Mulholland, "in order to try to understand how it is able to speed up its natural chemical reaction (the transformation of a small molecule called chorismate into another small molecule called prephenate)."

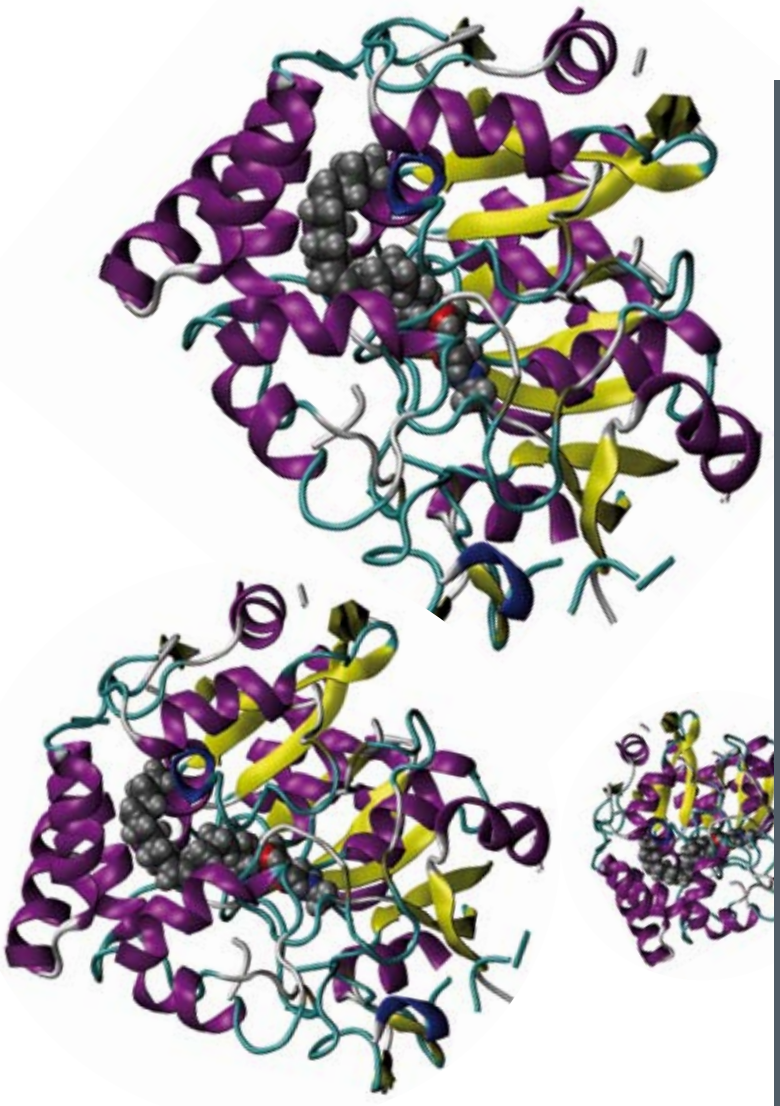
"Recent developments now allow the accurate, first principles calculation of free energy barriers of enzyme catalysed reactions; moreover, we ourselves have developed new software and algorithms that allow us to model the reaction in unprecedented detail. Our goal was to bring together the possibilities created by these new algorithms and software with the extreme computing resources available under the DEISA framework in order to analyse the contribution of each part of the enzyme to its catalytic power. The aim was to run large numbers of simulations of the enzyme-catalysed reaction for different mutants (variants) of chorismate mutase, thereby building up a catalytic map that would show us how changes to the enzyme changed its catalytic power."

"High performance computing resources are vital for the modelling of biomolecules and biomolecular processes. These simulations are, however, incredibly challenging, requiring high levels of detail (e.g. using quantum mechanics to model the reorganization of electrons in a chemical reaction) but are also of an immense size (e.g. modelling the motions of tens- or hundreds of thousands of atoms over long timescales)."

If, however, the challenges involved were daunting, the potential benefits to be reaped from the successful completion of the project are at least equal in scale. "Greater knowledge of how an enzyme works, and how its catalytic power can be tailored by making changes to the enzyme will allow for the development of novel enzymes that could be used for biosynthesis of fine chemicals. This knowledge will also be useful in researching new medicinal drugs, as many drugs act by disrupting enzymes, or by chemically reacting with them. Enzyme modelling can thus not only aid in the development of new drugs, but also in understanding the ways in which changes in an enzyme (mutation) can help in the development of drugs that are less susceptible to the disease developing resistance."

Research that seeks to combine the very cutting edge of two distinct scientific fields rarely runs entirely smoothly, without having to contend with unforeseen obstacles; and, as Mulholland discusses, the TotalEnz project was no different in this regard.

"The success of this project was – and remains – absolutely dependent upon access to significant computational resources; far beyond anything that was available locally. The simulations of the chemical reaction required the >>>



Dr. Adrian Mulholland is the lead researcher of the TotalEnz project. The project developed from the long-standing interest in trying to understand the action of enzymes using computer simulation, making use of new software and algorithms that have made it possible to perform such simulations with unprecedented detail using high performance computing resources.

application of novel software and algorithms and these required us to use the supercomputer in a novel way.

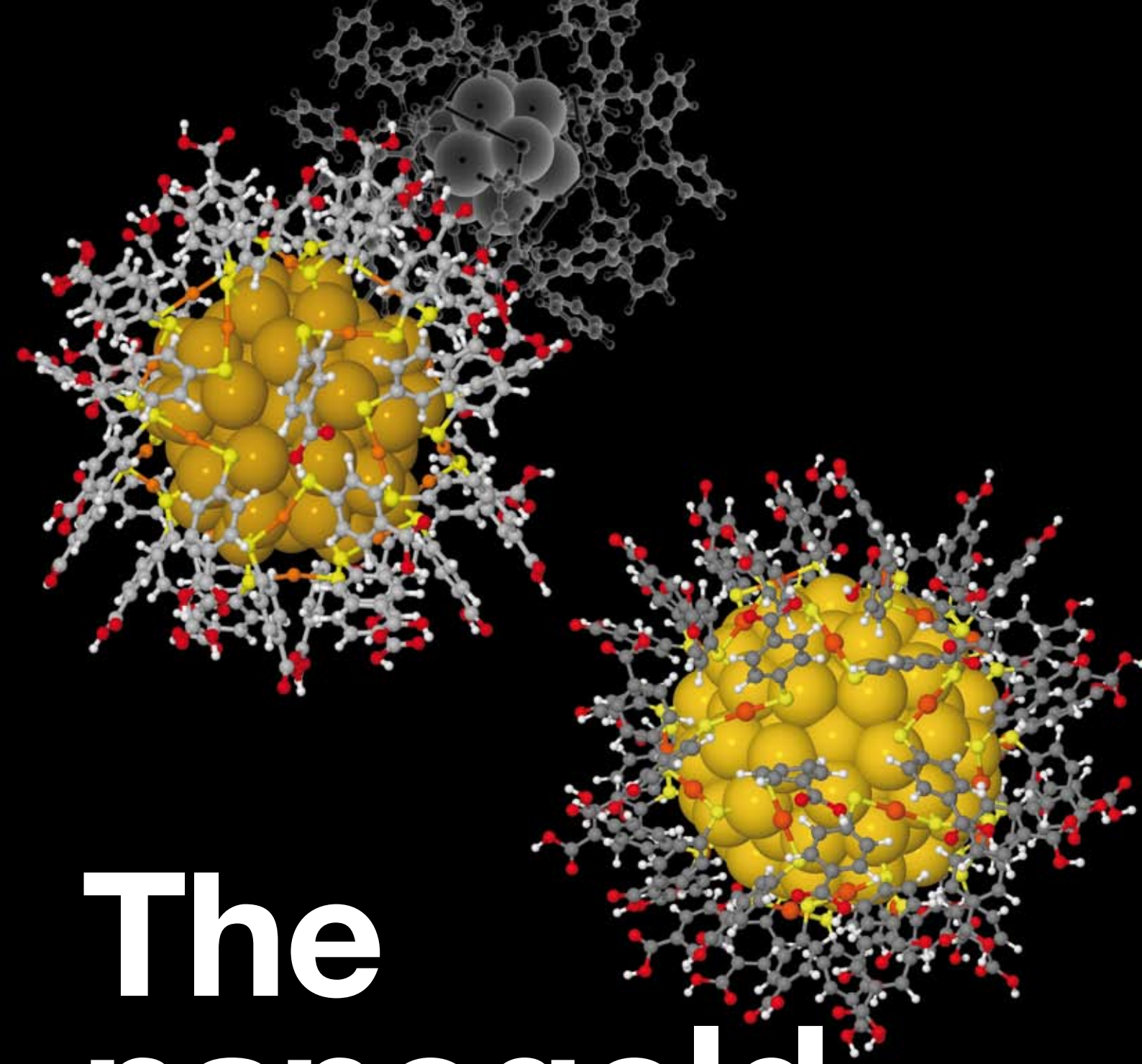
"We were able to use some of our computer time to run the initial simulations of chorismate mutase, with some interesting and encouraging results," concludes Mulholland. "More importantly, however, we were able to overcome the obstacles that arose, and to get our software up and running – this means that we are now in a position to begin running the full simulation. Indeed, we have, with encouragement from DEISA, submitted a new application – for TotalEnz2 – which would enable us to fully simulate not just chorismate mutase, but also fatty acide amide reductase (an enzyme that is a target for drug design), in 2010. Beyond that, our plan is to investigate a wider range of enzymes so that we may be able to investigate patterns in catalytic ability."

Further Technological Advances Required

Even if TotalEnz2 is successfully completed as envisaged in 2010, Mulholland is in no doubt as to the scale of the challenges that remain for his group, as they seek to continue combining computational science with the study of biological catalysts.

"Current supercomputers are not yet sufficient, and simulations still don't quite have the detail, size or timescale that is really necessary to understand complex biochemical phenomena. Advances in computer hardware, algorithms and software are therefore necessary to allow us to model biomolecular machines (i.e. the flow of ions through a trans-membrane ion pump) with the same accuracy that we currently model man-made machines. The ability to model and predict biomolecular processes is key to the development of bioengineering and biomanufacturing, two fields that have the promise to lead to a bioindustrial revolution." ■

More information:
www.deisa.eu/science/deci/projects2007-2008/TotalEnz



The nanogold rush

Mika Remes

Gold is valuable even in fragments of a millionth of a millimeter. Gold particles measured in nanometers are being studied intensively at the Nanoscience Center in Jyväskylä, Finland. A research group led by Professor Hannu Häkkinen is investigating special superatom structures associated with gold nanoparticles, and compounds based on these superatoms that have promising applications ranging from new materials to destroying cancer cells. >>>

In the 17th century, alchemists worked furiously in their laboratories to find a method to prepare gold. In a way, modern nanoscientists work the opposite way; by investigating the properties of gold at the atomic level and by reformulating gold they hope to create something completely new.

But gold does not render its secrets easily even at the nanoscale. Researchers have revealed the properties of gold atom clusters only during the past couple of years. Professor **Hannu Häkkinen** and his research group working at the Nanoscience Center of the University of Jyväskylä have played a key role in this investigation. Häkkinen's group was the first in the world to use computational models to elucidate properties of tiny gold atom clusters.

Attracted to America

In order to understand the importance of this computation result we must first join Häkkinen on a time journey to the United States of the 1990s. That is where Häkkinen started his eventful journey to become a nanogold hunter.

"In 1991 I defended my doctoral thesis on computational physics at the University of Jyväskylä's Department of Physics. After the dissertation work I felt ready to go out into the world. The following year I was accepted as a post-doc researcher in the famous Georgia Institute of Technology at Atlanta to perform research on metal nanoparticles, their structures and electronic properties," Häkkinen explains.

In 1994 he returned to the University of Jyväskylä to work as senior assistant at the Department of Physics. In 1997 he was nominated as an adjunct professor, after which he was again tempted to seek research work in the United States.

While attending a job interview Häkkinen dropped in to see his old employer and acquaintances in Atlanta. To his surprise, he was offered a senior researcher position in his previous research group. He was happy to accept the offer and in 1998 he returned to Georgia Institute of Technology.

From one nanoboom to another

The late 1990s was a time of breakthrough for nanosciences in the United States. That was when research into the atomic structures and catalytic properties of gold particles at the nanometer scale was initiated.

Through empirical research, physicists had discovered that very small gold particles worked as mysteriously effective catalysts at low temperatures. The presence of gold particles caused oxidation reactions even in below-room temperature conditions. This was strange, because gold is known for being a chemically or catalytically inactive element when in its normal form.

"Theoretically and computationally this was a totally new field of research. At the time we did not even know the stable structures of the gold particles, let alone what happens to molecules on the surface layer. The chemical properties of clusters comprising a few tens or hundreds of gold atoms were totally different from the macroscopic properties of gold."

During the five years he spent in Atlanta, Häkkinen focused especially on gold particles, in which the core of gold was protected by a molecular layer of organic sulfur and carbon.

"Their chemical preparation in a solution from gold salts became known in the mid 1990s although the atomic structure still remained unknown. These solution-derived particles were prepared in Atlanta by Professor **Robert Whetten**'s research group. As for myself, I set about modeling the atomic structures of these particles, which also became one of my main research areas while working in the research group of Professor **Uzi Landman**," says Häkkinen.

Häkkinen's second term in the United States came to an end in 2003, when he was offered the interesting opportunity to work at the Nanoscience Center founded in Jyväskylä.

"Jyväskylä provided a unique opportunity to combine chemistry, physics, and computational sciences. That was a good base to continue the research, building on the experience collected in the United States."

Professor Hannu Häkkinen's group was the first in the world to use numerical computation and succeed in elucidating properties of tiny gold atom clusters.

Long-awaited breakthrough

The breakthrough in solving the structure of chemically protected gold nanoparticles occurred as late as in 2007. The Nobel Prize-winning chemist, **Roger Kornberg** and his research group at Stanford University were the first in the world to succeed in determining the atomic structure of a particle that consisted of 102 gold atoms and 44 organic thiolate molecules.

It turned out to be quite special. The core of the atomic cluster contains only gold atoms, but some gold atoms remain outside the core cluster forming a protective cover together with thiolate molecules.

These gold–thiolate units stabilize the nanoparticle's electronic shell structure so that the metal electrons in the gold core are organized in the structure characteristic of noble gas atoms.

Hence, the gold nanoparticle becomes a type of large-sized, noble gas "superatom". Since this type of protected particle is extremely stable, it can be used as, for example, a component in new nanomaterials, which, in turn, opens extremely interesting application possibilities in different fields of science.

”Kornberg managed to prepare such a pure solution that it allowed growing a discrete crystal that contained only one type of gold nanoparticles. The researchers were able to analyze its atomic structure empirically by X-ray crystallography.”

Heavy computing

Robert Whetten from Atlanta gave Häkkinen, now back in Jyväskylä, a hint about Kornberg’s breakthrough even before it was published in *Science* in October 2007.

”After my Atlanta years, in Jyväskylä we had developed efficient methods for modeling the structure and behavior of gold nanoparticles. The structure determined by Kornberg resembled the structure we had predicted through numerical computation and published already in 2006. I asked Kornberg to provide his research results for us in advance and promised that we would clarify why gold nanoparticles appear in this form by using numerical computation,” says Häkkinen.

After having received Kornberg’s results Häkkinen’s group worked furiously for six weeks with the computations. They had a tight deadline to meet. On the publication of Kornberg’s results in the *Science* journal, they would be available to everyone, and Häkkinen’s group would lose their head start advantage.

The solving of the particle’s electronic structure was continued by exploiting the supercomputer resources of CSC in Finland, PDC in Sweden, and at Jülich in Germany. Häkkinen reckons the computations took ten CPU years of supercomputing time.

”It was the most massive computational challenge I have ever been involved with. We had a tight schedule, because we had promised to deliver the results to Kornberg before his article in *Science* was published. When we started, we did not know how long the work would take, and whether the software and parallel computing environments would perform without errors. We had to modify the programming during computation. However, we succeeded and produced reliable results on time. The results were confirmed by using two different codes of the electron structure. It would not have been possible without sufficient computational experience, good computing resources, and motivated researchers,” says Häkkinen.

Predictions that work

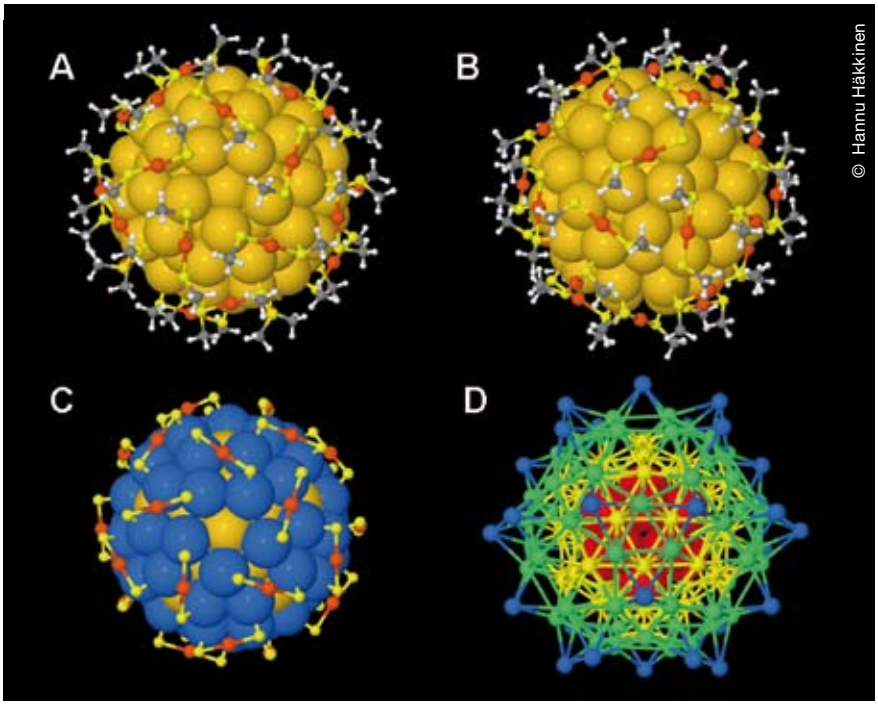
The success of the computation work has been very beneficial for Häkkinen’s group.

”Nano-scale gold particles have raised intense international interest and competition between research groups. Our work provided us with a head start in numerical modeling and theoretical explanation of particles and functional nanosystems composed of them.”

Using numerical calculations, Häkkinen’s group has also determined the structures of the smaller superatoms consisting of 11, 13, and 39 gold atoms. Their surface layers have contained either phosphorus–thiolate or phosphorus–chloride components.

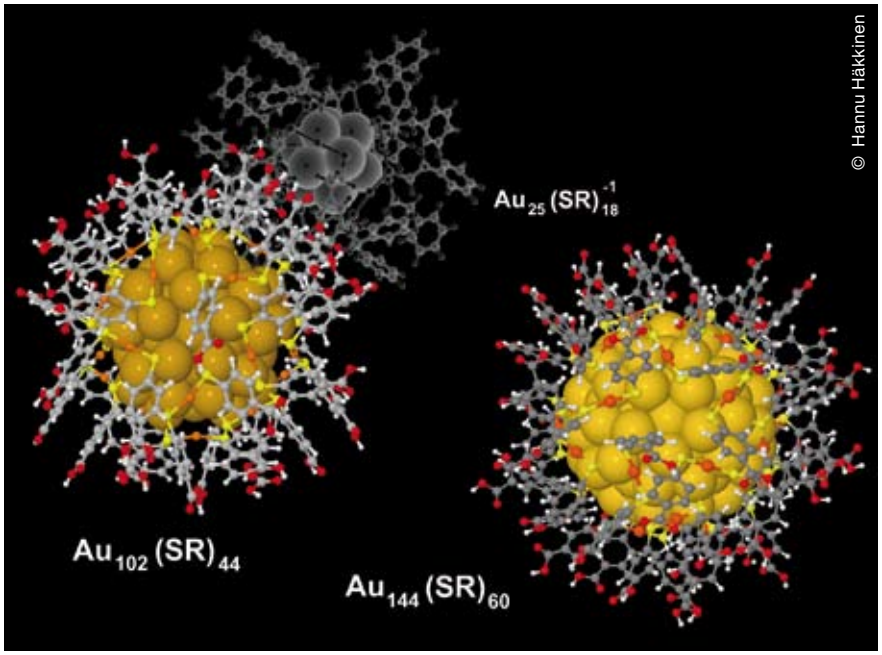
”Already in 2006 we predicted that gold plays a dual role in gold–thiolate clusters: some gold atoms are in the core, while some are covalently bound to the thiolate coating. Thanks to these results Kornberg was willing to provide us with his test results in advance, hence allowing us to determine the structure through numerical calculation,” says Häkkinen.

At the same time as performing the computations on the particles that contain 102 gold atoms, Häkkinen with his group also predicted the atomic structure of a smaller gold particle that consists of only 25 gold atoms protected by thiolate ligands.



A chemically stable particle consisting of 144 gold atoms and 60 thiolate molecules. In images A and B the entire particle is shown from two different angles. Image C shows the gold core surface (blue) and the sulfur–gold–sulfur units (yellow–orange–yellow) protecting it. Image D shows the bedded structure of the particle consisting of all 144 gold atoms (different atomic layers depicted in different colors).

”This structure was detected a few months later at the University of North Carolina in the USA. Our most recent structural prediction concerns a particle that contains roughly 144 atoms. The beautiful image we had visualized of the particle was published as the cover photo of the chemistry journal that published our manuscript. >>>



A visual image of the nanometric-scale atom structures of chemically protected nanoparticles. The yellow gold core is covered by a layer of thiolate molecules (SR) and gold atoms (orange) providing chemical protection. The thiolate molecules consist of sulfur (yellow), carbon (gray), oxygen (red), and hydrogen (white).

Our results and predictions are now highly regarded within the international scientific community," says Häkkinen.

Fascinating applications

After the computation work on determining the atomic structures and stabilities of gold particles had been completed, Häkkinen's group has started to look for chemical application possibilities for gold nanoparticles and to clarify what kind of materials systems they could be used in.

"We want to use numerical computing to determine whether these particles can be combined into a chain or linked together through organic molecular chains to form two- or three-dimensional structures, and to find out the properties of such structures," says Häkkinen.

There are numerous application possibilities for the properties of gold nanoparticles in, for example, nanoelectronics, chemistry, and medicine. One of the most interesting ideas is to use gold nanoparticles to destroy cancer cells, because they become extremely absorbent at the infrared spectral range.

"Scientists abroad have already tested the idea of having gold nanoparticles attach themselves onto cancer cells and heating the particles with an infrared laser. The metallic core becomes so hot that it may kill a cancer cell next to it. It is an interesting possibility, although it is too early to say whether the idea can be developed into a risk-free and functional therapy for human use."

Within his own group Häkkinen concentrates on basic research into nanoparticle properties.

"With gold nanoparticles, we are struggling with the core of the nanoscale microworld. We also need more and more of multi-scale modeling and for that we must develop efficient programs. Thus, plenty of work still remains. Once we know the details well enough, we can concentrate on applications. That work we gladly pass on to the engineers," Häkkinen concludes. ■

More information:
www.deisa.eu/science/deci/projects2007-2008/NANOGOLD

CSC and DEISA made the massive work possible

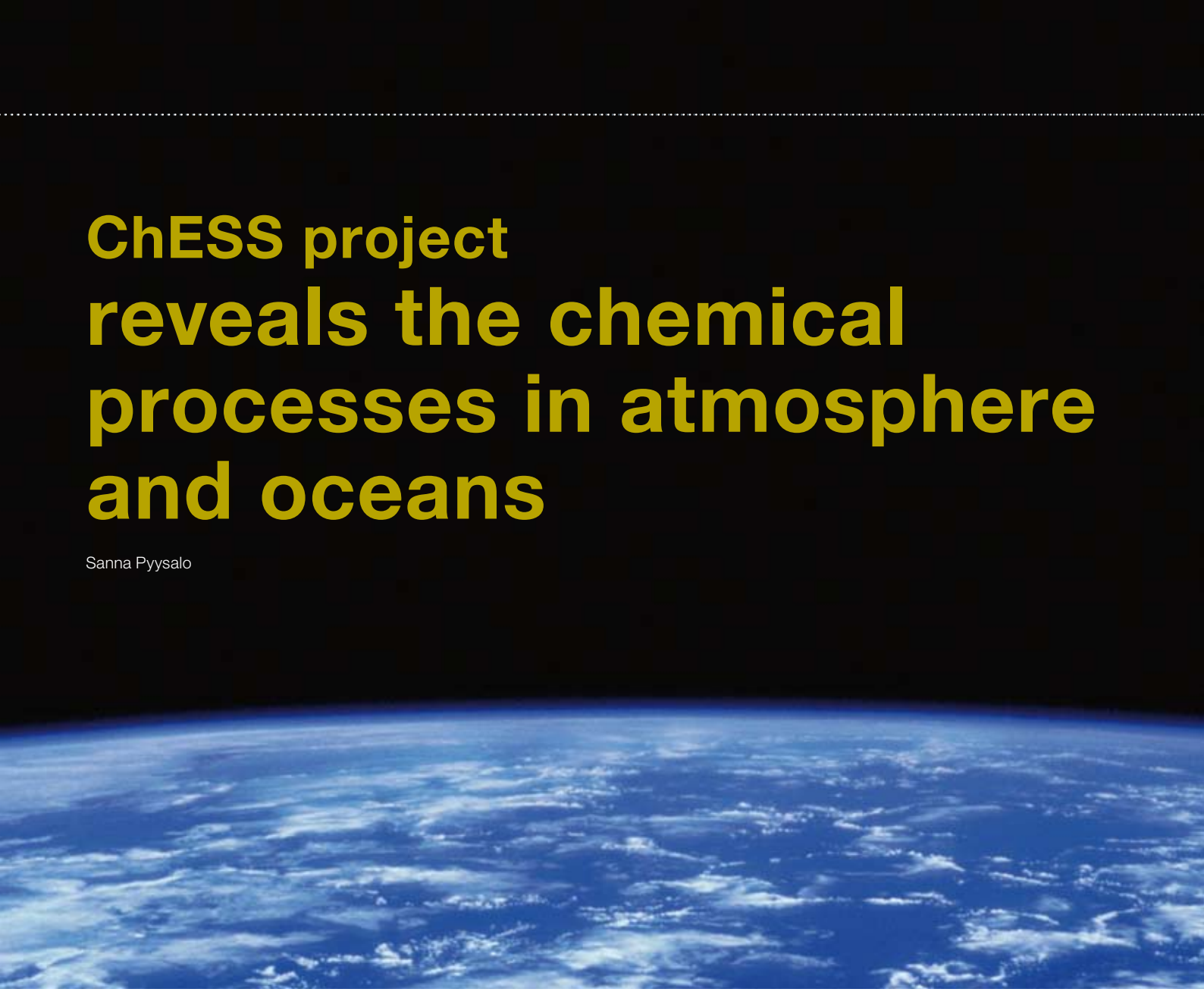
During six weeks in early autumn 2007, a research group led by Professor **Hannu Häkkinen** used the supercomputing resources of three countries for numerical computing to confirm the stability of the atomic and electronic structure of a particle consisting of 102 gold atoms. The particle had been empirically discovered by **Roger Kornberg** in the United States. The research was funded by the Academy of Finland.

The computing resources granted by CSC and DEISA were utilized in the project. In Finland the computations were performed on CSC's Cray and HP computers, in Germany on the IBM cluster located in Jülich, and in Sweden on the supercomputer of PDC.

The main tools were the massively parallel open source codes GPAW and CP2K based on density functional theory. The electronic structure of the gold atom was taken into account at the scalar relativistic level with valence value 11.

During the computing project, post-doc researchers **Michael Walter** and **Olga Lopez-Acevedo** from Häkkinen's group participated actively in the development of the GPAW software in this project funded by the Finnish Funding Agency for Technology and Innovation (TEKES), collaborating with groups from CSC, Tampere University of Technology, Helsinki University of Technology, and the Technical University of Denmark from Copenhagen.

In addition to Häkkinen, the following researchers participated in the numerical computation of the structure of gold nanoparticles: senior researchers **Jaakko Akola**, **Pentti Frondelius**, **Olga Lopez-Acevedo**, **Michael Walter**, and **Karoliina Honkala** from the University of Jyväskylä, and Professor **Henrik Grönbeck** from Chalmers University of Technology in Gothenburg.



ChESS project reveals the chemical processes in atmosphere and oceans

Sanna Pyysalo

The ChESS project is investigating the role of chemical processes in Earth System Models. The main goal is to study the role of chemical transformations for the constituent cycles in the climate system. The research is being carried out at the Max Planck Institute for Chemistry and the Institute for Atmospheric Physics of the German Aerospace Center (DLR).

Earth System Models (ESMs) seek to simulate all aspects – physical, chemical and biological – of the Earth system in and above the land surface and in the ocean. In other words, the interacting domains (atmosphere, hydrosphere, cryosphere) of the environment are simulated in conjunction to study the nature of feedbacks between the different domains and processes and how they influence the properties of the whole system.

A challenging task, in particular, is to represent the constituent cycles of chemically active species, since a wide range of temporal and spatial scales and a large number of species are involved.

The ChESS project (Coupling the Chemistry in Earth System Models on multiple Scales) sought to investigate the chemical processes in ESMs on various scales, from the global to the local scale, in order to improve these models; indeed atmospheric chemistry and ocean biogeochemistry are important players in the terrestrial climate system.

”The issue is that the chemical processes involve a wide range of spatial scales. Those are scales which provide a form for discussing relative lengths, areas, distances and sizes. The ChESS project is trying to bridge these scales by implementing a modeling system with consistent process formulations on all scales”, says the principal investigator Dr. **Patrick Jöckel** from the Max Planck Institute for Chemistry (now at German Aerospace Center, DLR).

The main goal of the research project is to investigate the role of chemical transformations for the constituent cycles in the climate system and thereby for the climate variability. A further goal is to investigate the impact of climate change on the chemical composition of the atmosphere and ocean. >>>

Developing the Earth System Model

The research of the ChESS project is based on the ECHAM/MESSy Atmospheric Chemistry (EMAC) model. In ChESS, this model is extended by *two more components.

First, the project couples a *dynamic ocean model (MPIOM) and a representation of the oceanic biogeochemistry (HAMOCC).

”This allows a direct ´chemical coupling´ between the ocean and the atmosphere, since fluxes of constituents between atmosphere and ocean can directly be calculated and do no longer rely on pre-scribed boundary conditions”, explains Dr. Jöckel.

Secondly, the project couples a regional model (COSMO). Several instances of COSMO can be nested into the global EMAC model. The required dynamical and chemical boundary conditions at the COSMO domain boundaries are provided by the EMAC model or by the next coarser COSMO model. Due to the modular structure of the Modular Earth Submodel System (MESSy) the chemistry representation is consistent on all scales.

”Both couplings are ´on-line´, meaning that the various components exchange their data during run-time via the message passing interface. The obvious advantages of the on-line approach are a higher possible coupling frequency, a better run-time performance, and most importantly, the possibility to assess feedbacks between different domains and components”, says Dr. Jöckel.

Coupling the physical atmosphere-ocean system

The ocean coupling project began in 2007 and is still ongoing.

”Currently, we are in the phase of evaluating the coupling of the physical atmosphere–ocean system”, explains Dr. Jöckel.

The nesting of the regional model is funded by the MACCHIATO project of the DFG, a German research funding organization. The project started in January 2008 and is ongoing until December 2010.

”Now we are evaluating the implementation of the physical coupling. Evaluation of the nesting with chemistry will follow soon.”

In both research cases, the first results are a proof of concept.

”In coupling of the ocean, we could show that our implementation of direct coupling was faster than the classical coupler approach and had the advantage of allowing higher coupling frequencies. The physically coupled system is stable and able to reproduce previous results of other model systems. The evaluation is ongoing and the first publications are in preparation”, tells Dr. Jöckel.

The implementation of the on-line nesting of the regional model into the global model is technically complete, and the system is now being evaluated.

Dr. Jöckel points out that so far most climate models have been either only physically coupled atmosphere–ocean systems or chemistry climate models (CCMs) without an interactive ocean component.

”The extension of the EMAC CCM by a dynamic and biogeochemical ocean component provides a unique comprehensive ESM for the investigation of constituent cycles in the climate system. The on-line nesting of a regional model into a global model with consistent exchange of dynamical and chemical boundary conditions is unique. No such model system yet exists”, says Dr. Jöckel.

Useful tools for the future

There are many fields in which the research results can be utilized in the future.

For example, the system can be applied for hind-casts of the climate system providing additional information on the chemical composition of ocean and atmosphere. With this, the reconstruction of the climate history can be supported.

”The research is also useful in climate projections with fully interactive constituent cycles between the ocean and the atmosphere, including a direct downscaling for specific regions on the globe”, says Dr. Jöckel.

The results also enable detailed process studies due to the new zooming option. High resolution model results can be better compared to observations from measurement campaigns than results from the coarser global model grid.

”It is also planned to extend the coupling of the regional model by a two-way nesting, so that the smaller scales will also exert a feedback onto the larger scales. Last but not least, we want to couple an interactive surface/land-biosphere model”, Dr. Jöckel adds.

DEISA played an important role in the ChESS project.

”The development of such a comprehensive modeling system requires numerous test simulations and therefore requires a lot of additional computational resources. The flexibility of the DEISA grid with additional resource allocation is a big advantage”.

Moreover, the DEISA high-performance grid-file system greatly improved the efficiency of the data exchange between the researchers involved. Independent of where the simulations were performed, the resulting data could be archived and further analyzed at the respective home site.

”The technical support from DEISA was very good, fast and efficient”. ■

Computations with EMAC in the framework of the ChESS project were performed on Hygens at SARA.

Several short test simulations required for the technical development were performed, but also some preliminary long term simulations.

17222 SBUs were spent on testing the nested global–regional model setup with 32, 256 and 512 CPUs.

571172 SBUs on 96 CPUs have been invested for simulations (totaling approximately 1500 simulation years) with the physical atmosphere–ocean system for pre-industrial and industrial conditions, and 11724 SBUs for the first steps with the physically and chemically coupled atmosphere–ocean setup. The analysis of the results was mainly performed at the RZG using the DEISA_DATA file system.

***Figure 1** shows the global (annual) average surface temperature (or skin temperature) in Kelvin over time. The black line is for pre-industrial conditions, the red line shows the result of a transient simulation, i.e., the transition from pre-industrial to today conditions.*

***Figure 2** shows the same quantity. The black line is again for pre-industrial conditions and the red-line for an annual increase of atmopsheric CO2 of 1%/year up to present day condistions (in the 70ies), and constant after that.*

***Figure 3** shows the result of our model (black line) compared to some other models that participated in the IPCC, more specific the AR4 scenario was used. Here, not the absolute temperature, but the anomaly (i.e. the deviation) from the 1960-1990 mean is shown (also in Kelvin).*

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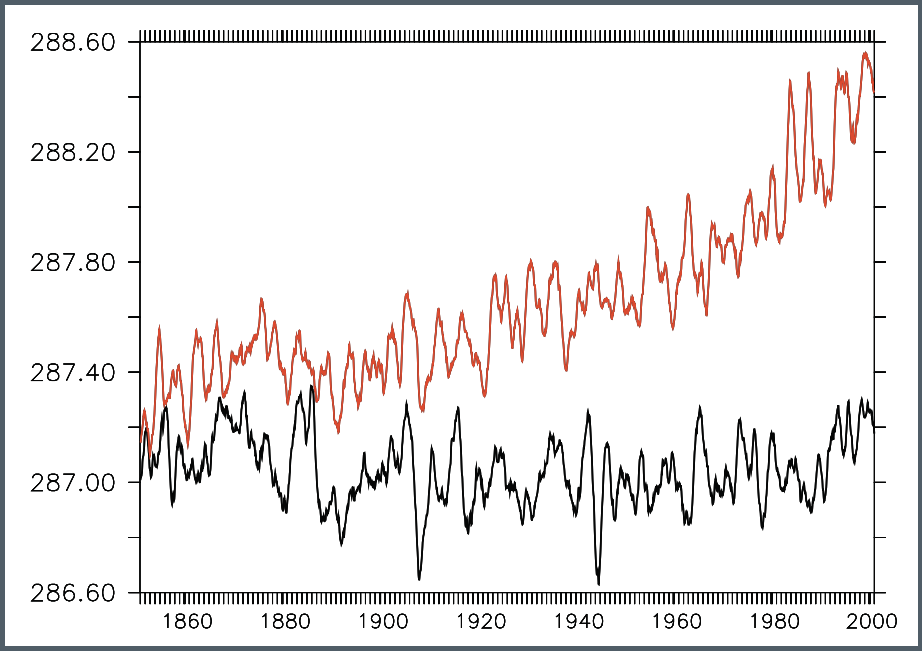

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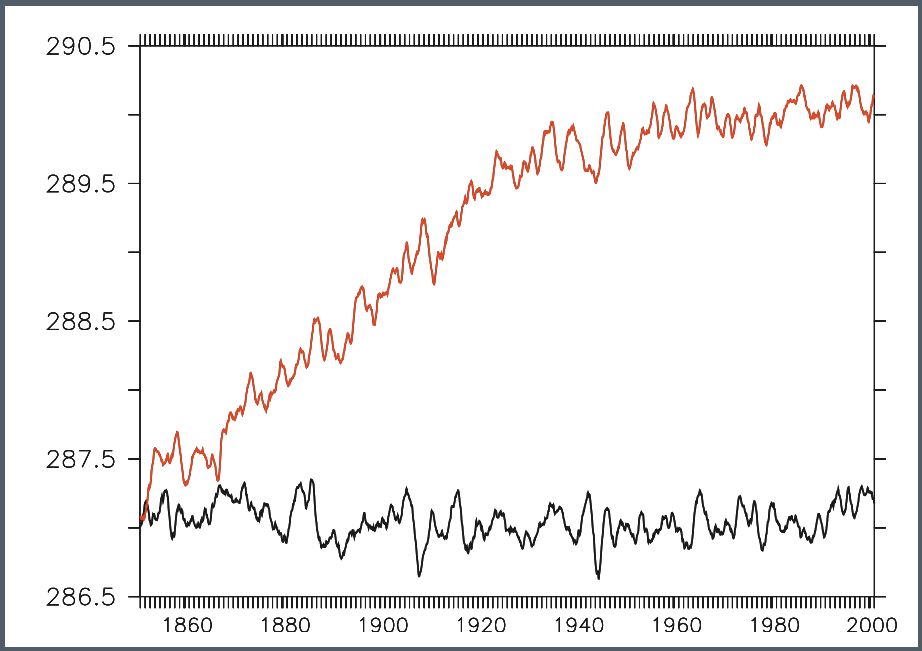

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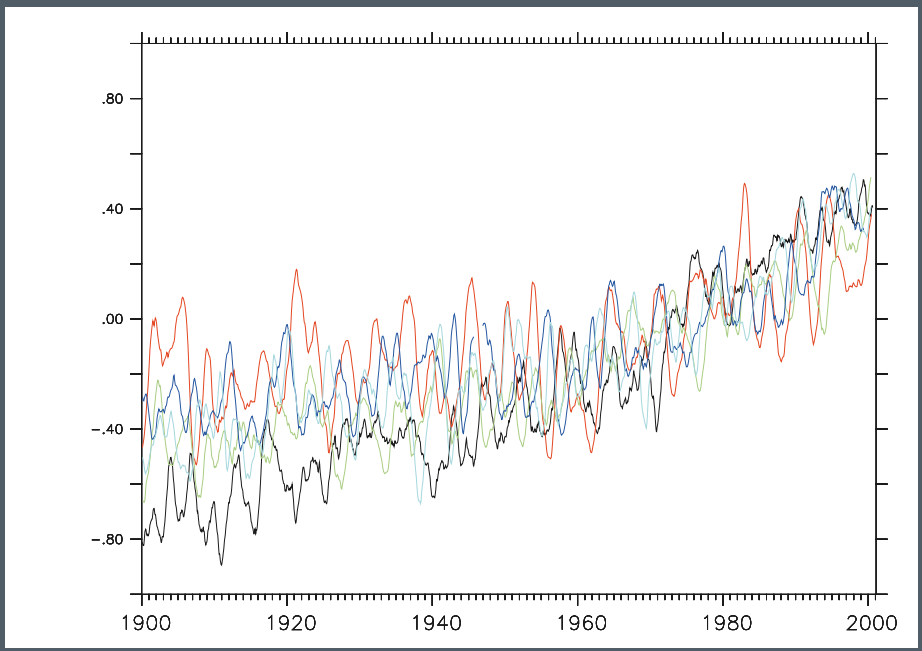

Distributed
European
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DEISA

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The purpose of this research infrastructure is to enable scientific discovery across a broad spectrum of science and technology, by enhancing and reinforcing European capabilities in the area of high performance computing. National supercomputing platforms have been strongly integrated to provide transparent access to a pool of European computing resources for scientific end users and user communities. The joint and coordinated operation of this environment is tailored to provide enhanced computing power and resources for leading computational scientists, and to enable new, groundbreaking research activities in science and technology.

DEISA operates as a virtual European supercomputing centre. Human competences are also pooled, to provide first class, substantial added value services to computa-

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