DEISA

DEISA DIGEST 2011

Extreme computing in Europe

CONTENTS

DEISA DIGEST
www.deisa.eu

ISBN 978-952-5520-40-8

Editor-in-Chief
Ari Turunen, CSC

Editorial Board
Hermann Lederer, RZG
Ari Turunen, CSC

Copy editors
Hermann Lederer, RZG

Editors
Tiina Autio, Vehrä
Sanna Pyysalo, Teonsana Ltd.
Nina Morgan, Teonsana Ltd.
Pirjo Rötkönen, Teonsana Ltd.

Graphic Design and layout
Up-to-Point Ltd.

Cover picture
Supernova Ia explosion
SN-DET-hires project

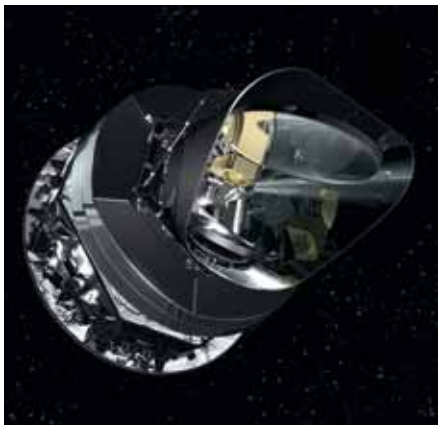
Printed by
Redfina Ltd.

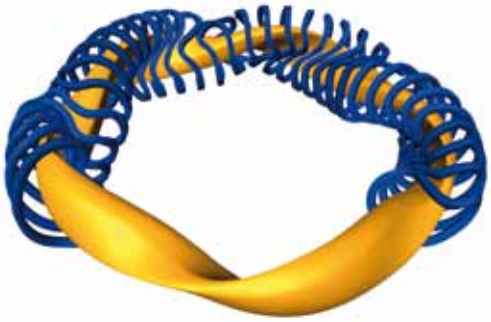
DEISA is a consortium of leading national supercomputing centres that operates a production quality, distributed super-computing environment at continental scale.

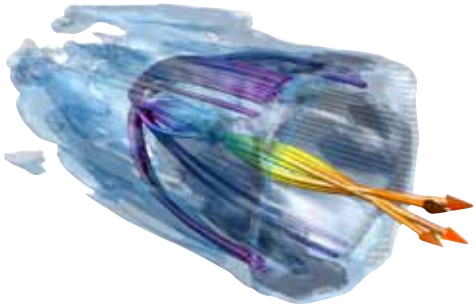
The purpose of this research infrastructure is to enable scientific discovery across a broad spectrum of science and technology, by enhancing and reinforcing European capabilities in the area of high performance computing. National supercomputing platforms have been strongly integrated to provide transparent 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.

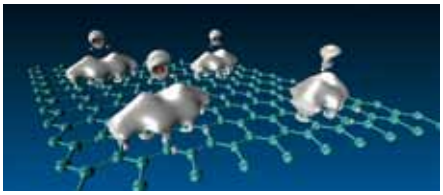
Distributed European Infrastructure for Supercomputing Applications

e-infrastructure









EDITORIAL

DEISA: Six years of Extreme Computing

Hermann Lederer, (Deisa external relations and dissemination) RZG, Germany.

DEISA (Distributed European Infrastructure for Supercomputing Applications) is a consortium of leading national Supercomputing Centres in Europe.

The DEISA Consortium has deployed and operated an European Supercomputing infrastructure on top of national HPC services.

DECI – the DEISA Extreme Computing Initiative – was introduced in 2005 to enhance the impact of the DEISA infrastructure for the advancement of science in Europe. DECI has proven to be an extremely useful instrument in several ways, and DECI has taken over an effective role as attractor for the computationally most challenging science projects in Europe. About 180 European research institutes and universities have already benefited from DECI. DECI has been a catalyzing instrument to enhance the fraction of collaborative, multi-national projects. It has also stimulated the creation and establishment of new science communities.

DECI has succeeded in attracting leading researchers to participate in DEISA with challenging projects. DEISA has contributed to the popularity of HPC simulations to address important problems in science and technology. The world's top research projects now see DEISA not only as an excellent infrastructure for HPC simulations, but also as a source of prestige due to the intense competition for DECI/DEISA projects.

More than 450 challenging projects from major areas of computational sciences were hosted for scientist teams from 37 countries, including researchers from the Americas, Asia and Australia. Expert teams for application and infrastructure services are providing support for a persistent European HPC infrastructure.

In addition to DECI, direct support for whole science communities with a critical mass in their fields of science and with a broad basis in several European countries was initiated and established. Communities from Life Sciences, Climate Research, Astronomy and Fusion Energy Research showed an ongoing demand for DEISA resources related to HPC cycles, application support, and access to different state-of-the-art supercomputer architectures.

Through the dual support strategy, DECI and support for Virtual Science Communities, European multi-national scientific collaborations have been further strengthened.

DEISA has enabled European computational scientists to obtain access to the most powerful national computing resources in Europe regardless of their country of origin or work, and also smaller countries are able to participate in cutting-edge research through internationally competitive computational science.

Insight into the differences between usage of national and European resources and facilities gained by DECI also facilitates the understanding of requirements of users of European leadership-class supercomputers installed by PRACE.

This DEISA Digest 2011 magazine focuses on recent key results of the DEISA Extreme Computing Initiative and Extreme Computing projects from Science Communities in Life and Space sciences, covering major science areas ranging from Astronomy to Earth Sciences, to Engineering, to Life and Materials Sciences, and to Plasma Physics.

The reader can gain insights, for example, into how a model of the human body is developed by the *Virtual Physiological Human project*, how the history of the early Universe is discovered and how lighthouses of the Universe are simulated, how drugs against HIV are under development by studies of viral RNA, how turbulent combustion processes can be simulated and optimized under realistic conditions, how the efficiency of aircraft wings can be enhanced, how catalysts work, how data storage capacities can be improved, how climate models can be improved, or how progress can be made in nanotechnology by the study of water-carbon-interactions at the molecular level.

This DEISA Digest is the third such magazine on extreme computing projects in DEISA. Further extreme computing projects have been described in the DEISA Digests 2008 and 2010.

After the formal end of the DEISA-2 project on April 30, 2011, DECI will be continued under the umbrella of PRACE, the "Partnership for Advanced Computing in Europe", which is not only deploying leadership-class Tier-0 supercomputers in Europe, but also planning to continue essential DEISA services at Tier-1 level of national supercomputers through a respective Tier-1 related EU FP7 grant called PRACE 2IP as of mid 2011. ■

Acknowledgement

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

Discovering the history of the early universe

Sanna Pyysalo

LFI-PLANCK is a project to study the cosmic microwave background radiation caused by the Big Bang, using the Planck satellite. By doing so, scientists can discover the structure of the early universe. Planck is a multinational project and uses DEISA´s supercomputing resources for data simulation.

The Planck is a satellite that surveys the whole sky in the microwave area, in nine different wavelengths. It was launched into space in May 2009.

The LFI-PLANCK project allows scientists to look at the early universe. This they can do with the Planck satellite, funded by the European Space Agency ESA and launched in May 2009. The satellite surveys the whole sky in the microwave area, in nine different wavelengths.

The Big Bang created large amounts of microwaves and the microwaves that Planck measures are mainly cosmic microwave background radiation (CMB).

"CMB has travelled through the universe throughout most of its history. The universe is now 13,700 million years old, but the CMB was formed when the universe was only 380,000 years old. It means that we are now looking very far away and also very far back in time, before any galaxies had formed. By doing so, we can find out the structure of the early cosmos," explains **Hannu Kurki-Suonio**, a lecturer in cosmology and relativity at the Department of Physics at the University of Helsinki, Finland.

Planck is the third satellite that has been designed for this research. The first, launched in the 1980s, discovered that CMB can be studied to explore the structure of the universe.

Planck is a multinational project that involves about 100 different research institutes and projects and about 500 researchers from about ten European countries plus the USA and Canada.

More wavelengths, better resolution

The Planck satellite has major advantages compared to previous satellites. First of all, it measures the sky on many different wavelengths, including shorter ones of less than a millimeter.

"This is important since we can separate what is CMB and what parts of the radiation come from astrophysical objects, galaxies, quasars and interstellar dust," Hannu Kurki-Suonio says.

The second advantage is that Planck has better resolution. Now it is possible to see details in the sky that are three times smaller than earlier.

The third advantage has to do with sensitivity.

"The signal being measured is very weak. We want to observe small changes in the brightness and polarization of CMB to be able to find out the structure," Kurki-Suonio points out.

In order to be as sensitive as possible, the instrument has to be cooled to a very low temperature. Otherwise thermal noise will interfere with the findings. Planck is the first satellite that has an active cooling system.

"The instruments for detecting the highest frequency have been cooled to a temperature that is only one tenth of a degree from absolute zero."

The only disadvantage of the cooling system is that it will not last forever. It will stop working at the end of 2011 and then the high frequency instruments will start to warm up.

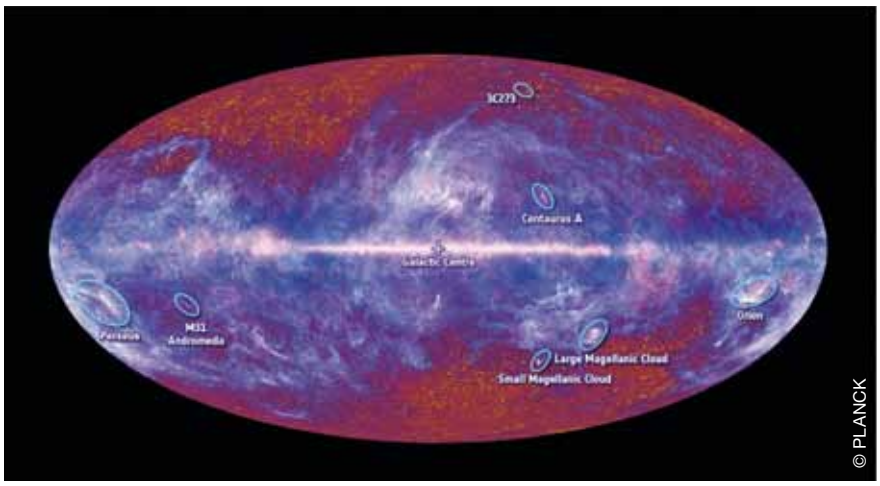
"We can still continue the research with low frequency instruments. Eventually the project will end because CMB doesn't change over time."

Useful for astronomy and cosmology

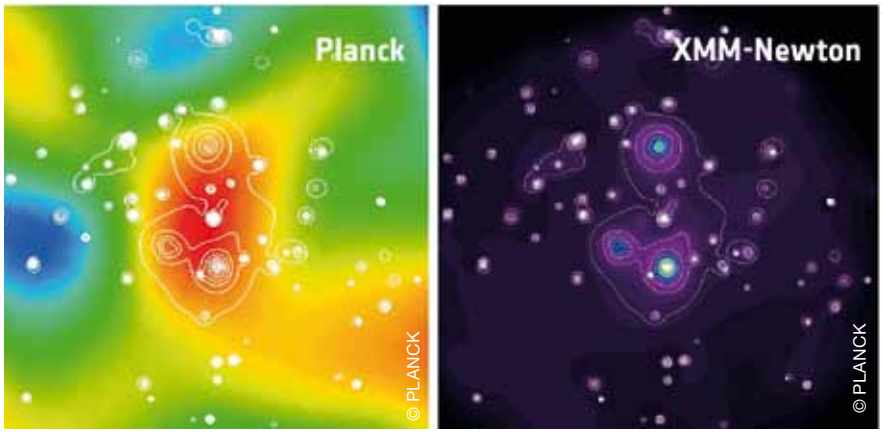
There are two research consortiums within Planck, the high and low frequency instrument. It is the low frequency instrument, LFI-PLANCK, that has applied for DEISA ´s supercomputing resources.

"In order to do the actual data analysis, we have to analyze the simulated data and compare it to the real data. For the simulations we need DEISA´s super-computing resources," Kurki-Suonio explains.

The Planck satellite has served both astronomers and cosmologists. The first results concern galaxies. The results from studying cosmic background radiation will be published at the end of 2012.



Emission from gas and dust in the plane of the Milky Way dominates this multi-colour all-sky image of the microwave sky, synthesized using data spanning the full frequency range of Planck, which covers the electromagnetic spectrum from 30 to 857 GHz. Other galactic features recognizable in the image are the Galactic Centre and the giant molecular clouds of Perseus and Orion, both of which are extremely active regions of star formation.



This image shows the newly discovered supercluster of galaxies detected by Planck (with the Sunyaev-Zel'dovich Effect) and XMM-Newton (in X-ray emission). This is the first supercluster to be discovered through its Sunyaev-Zel'dovich Effect.

International cooperation with the DEISA resources

LFI-PLANCK is a truly international project. Italian researchers work on the same issues as their Finnish colleagues. **Paolo Natoli** from Italy is the co-leader of one of the main projects and has worked for Planck since before its approval as an ESA mission in 1996.

"I participate in the data analysis effort for Planck. My field of expertise is the anisotropies of cosmic microwave background radiation and their use to constrain theoretical models of our universe," Natoli tells.

He describes Planck as a genuine Swiss watch; it works flawlessly. The DEISA resources have also proven very effective and useful.

In order to analyze the data of a high precision satellite like Planck, one needs to create many virtual replicas of the data gathering and reduction processes.

"These replicas are called Monte Carlo simulations. They are essential in propagating our knowledge of the instrument down the final, scientific results. This is where DEISA comes into the picture."

The DEISA network and resources are used mainly for production of massive Monte Carlo simulations. Several supercomputing centers are participating in this effort and all the European centers are linked to DEISA. >


© PLANCK

The universe is now 13,700 million years old, but the cosmic microwave backgroud radiation was formed when the universe was only 380,000 years old. "It means that we are now looking very far away and also very far back in time, before any galaxies had formed. By doing so, we can find out the structure of the early cosmos," explains Hannu Kurki-Suonio.

"We also have significant participation from NERSC/DOE in the United States, which is not part of DEISA. Since the production of Monte Carlo simulation is very central to the exploitation of Planck data, it is no exaggeration to say that DEISA is playing a very important role in Planck," Natoli says.

"Since the production of Monte Carlo simulation is very central to the exploitation of Planck data, it is no exaggeration to say that DEISA is playing a very important role in Planck,"

Non-gaussianity under research

Another group of scientists from Spain is working work on the issue of non-gaussianity. The co-coordinator of the Non-Gaussianity Working Group is **Enrique Martinez-Gonzalez**, vice director at the Institute of Physics of Cantabria.

Gonzalez was the responsible scientist for the delivery of part of the detectors of the LFI instrument and he is also one of the two coordinators of the Isotropy and Statistics of the CMB project.

"These activities aim at testing the standard inflationary model, which predicts that the temperature anisotropies follow a Gaussian distribution. Any deviation from the Gaussian distribution would invalidate the simplest standard inflationary model and thus would favor other alternative scenarios, like non-standard inflation or the existence of cosmic defects," Martinez-Gonzalez says.

He describes DEISA as working very well.

"DEISA resources have been very useful for the analyses we have performed so far. On the one hand they have helped us in the assessment of the functioning of the LFI and its impact on the data, and on the other hand they have already allowed us to perform some preliminary analyses on the Gaussianity of CMB."

DEISA is consequently very important for carrying out the CPU-intensive tests the scientists need to perform with the large amounts of data being received from the satellite.

"These tests are crucial for the understanding of the performance of the instrument and for the correct interpretation of the data," Martinez-Gonzalez says. ■

DEISA Resources:

Monte Carlo simulation of Planck data and analysis of this simulated data is performed at CSC – IT Center for Science in Finland and at CINECA, Italy.

These simulations are typically run every three months corresponding to the flight data accumulated and analyzed so far. The noise and signal parts of the data are simulated separately. One realization (simulation and analysis to the sky map level) of the full data for all 22 radiometers of the Planck Low Frequency Instrument takes about 30 minutes for noise and 1 hour for signal, using 1 024 cores on at CSC.

For the signal, the typical number of Monte Carlo cycles is 100, taking about 100 000 CPU hours.

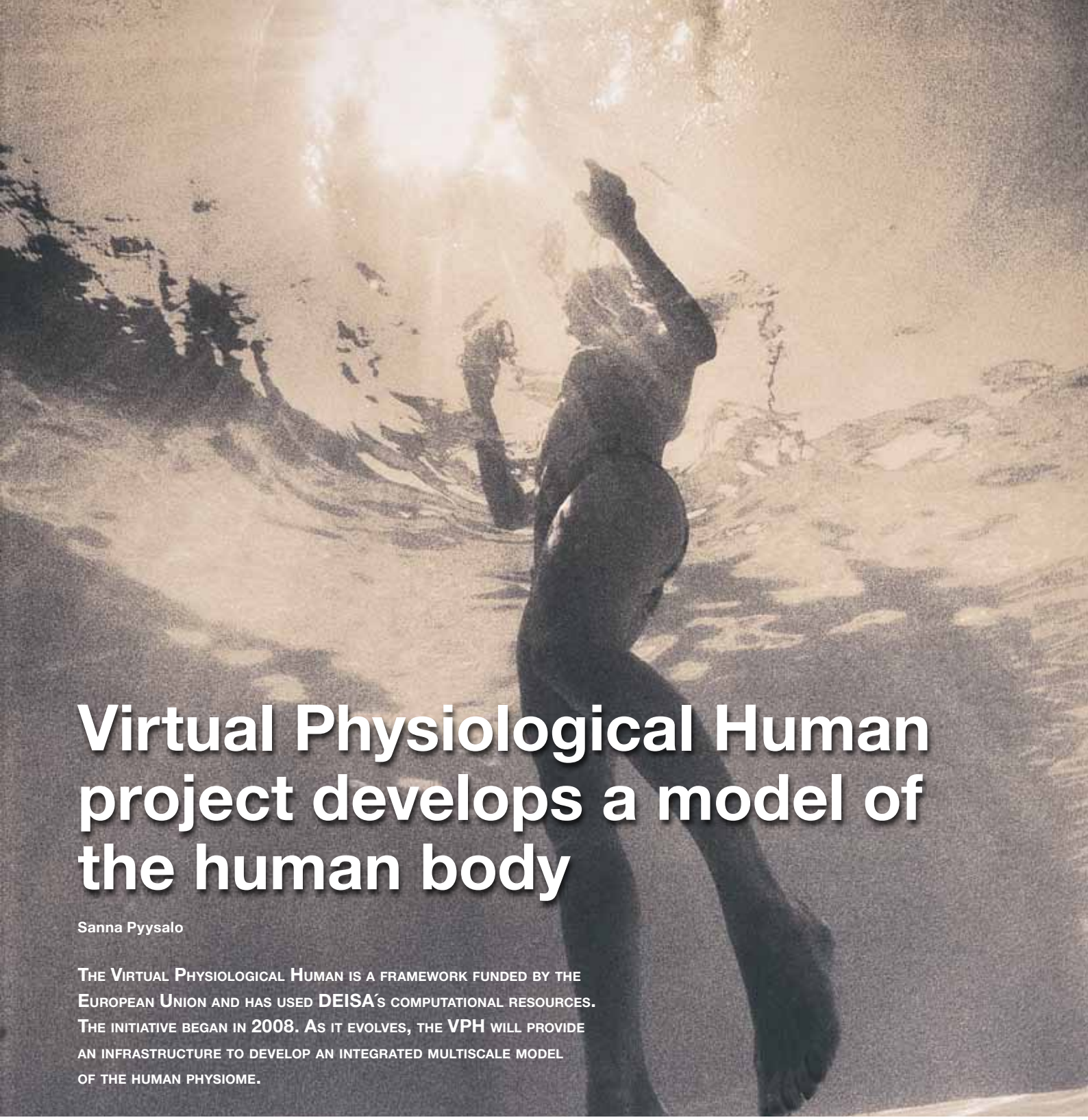
For noise, the typical number of MC cycles varies from 100 to 1000, taking between 50 000 and 500 000 CPU hours.

In 2009 and 2010, a total of about 3 600 000 (standardized) CPU hours

were used on the CSC-It Center for Science Cray XT5 and the CINECA SP6 machines.

The simulations are performed using Level-S software assembled by the Max Planck Institute for Astrophysics Planck Analysis Centre (MPAC).

The analysis to sky map level is done with the Madam software developed within the Planck project. This is coded in Fortran-90, parallelized via OpenMP and MPI. Visualization and further steps of the data analysis are done on local computers and Hippu at CSC using IDL and HEALPix.



Virtual Physiological Human project develops a model of the human body

Sanna Pyysalo

The Virtual Physiological Human is a framework funded by the European Union and has used DEISA´s computational resources. The initiative began in 2008. As it evolves, the VPH will provide an infrastructure to develop an integrated multiscale model of the human physiome.

The Virtual Physiological Human (VPH) is a methodological and technological framework that, as it evolves, will enable collaborative investigation of the human body as a single complex system. It is a framework that will facilitate personalized, predictive and integrative medicine.

”The VPH provides the European research infrastructure with a tool that will allow biomedical researchers to complement their conventional reductionist approach with what we call an integrative approach, where biological processes are described from a systems point of view,” tells **Stefan Zasada**, a researcher from the Virtual Psychological Human Network of Excellence (VPH NoE).

VPH NoE aims to connect the various VPH projects within the 7th Framework Programme of the European Commission. It consists of a group of universities, institutions and organizations that is leading the coordination and connection of diverse activities within the VPH Initiative.

The motivation behind the VPH is to provide the infrastructure that enables scientists and clinicians to collaborate in the development of an integrated multiscale model of the human physiome. An integrated physiome model can be used to investigate problems that have hitherto been impossible to examine.

The framework is formed by large collections of anatomical, physiological and pathological data stored in digital format and by predictive simulations developed from these collections. VPH models aim to integrate physiological >

processes across different length and time scales. These models make possible the combination of patient-specific data with population-based representations.

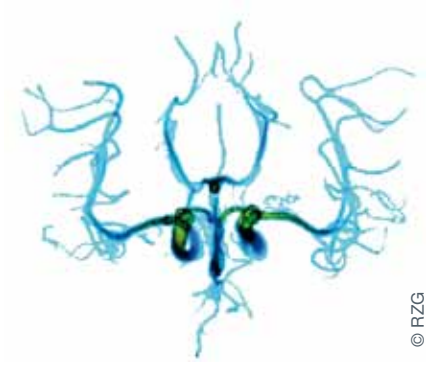
”As such, VPH researchers require access to large amounts of computational power, provided at different scales, from local campus-based clusters, through to resources provided at an EU level by EGEE/EGI and DEISA and PRACE, the Partnership for Advanced Computing,” Zasada says.

15 ongoing research projects

Through the DEISA Virtual Community support,the VPH initiative is supported as a whole,rather than a single project. Currently there are 15 VPH research projects looking at a range of medical computing scenarios, from cancer treatment evaluation to heart modeling. There is also a Network of Excellent project that manages the DEISA allocation for all VPH-I projects.

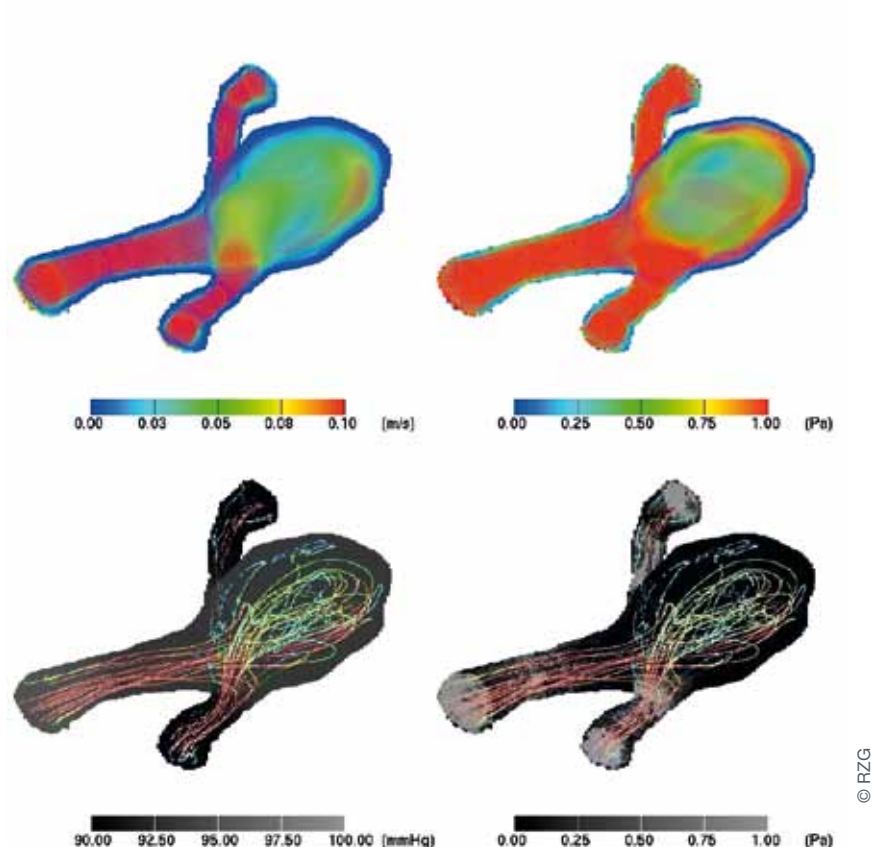
The initiative began in 2008 and is ongoing. A recent round of funding has led to a number of new VPH projects due to start in 2011.

”Since this community represents a range of projects, the results are very diverse, and can’t easily be summarized. The main point is that the VPH Initiative is working towards personalized medical simulation,” explains Stefan Zasada.



© RZG

An example of a real-time in situ rendering of a cranial haemodynamics simulation run using the HemeLB brain blood flow simulation code using the VPH Virtual Community DEISA allocation. The colours in the neurovasculature represent the velocity of the blood flow field, with high velocities depicted in green through to lower velocities in blue.



© RZG

A visualization of an aneurysm. (Top left: volume rendered velocity; top right: volume-rendered von Mises stress; bottom left: external pressure and streaklines; bottom right: external von Mises stress and streaklines).

The VPH has great significance in the field of medical research. The projects in the VPH Initiative are seeking to develop personalized multi-scale computational models of the human physiome. They could ultimately be used by a clinician to, for example, investigate courses of treatment virtually, and determine their efficacy, before they are actually used on a patient.

The results of the Virtual Physiological Human project will be used in many ways in the future.

”Potentially, the results will revolutionize the whole of clinical treatment, by providing doctors with tools that they did not earlier have,” Stefan Zasada says.

The project will actively continue into the future.

”As mentioned, several new projects are due to start, and more projects are likely to be funded in future calls.”

DEISA has played a significant role in the Virtual Physiological Human projects.

”Without the computing resources provided by DEISA, many of the VPH Initiative projects would not have had access to sufficient computational resources to complete their research,” Zasada points out.

The community is managed by the VPH Network of Excellence. Initially the Network of Excellence surveyed the VPH-Initial projects to discover their computing requirements. Portions of the main Virtual Community allocation were then allocated to the VPH-I projects based on these requirements. ■

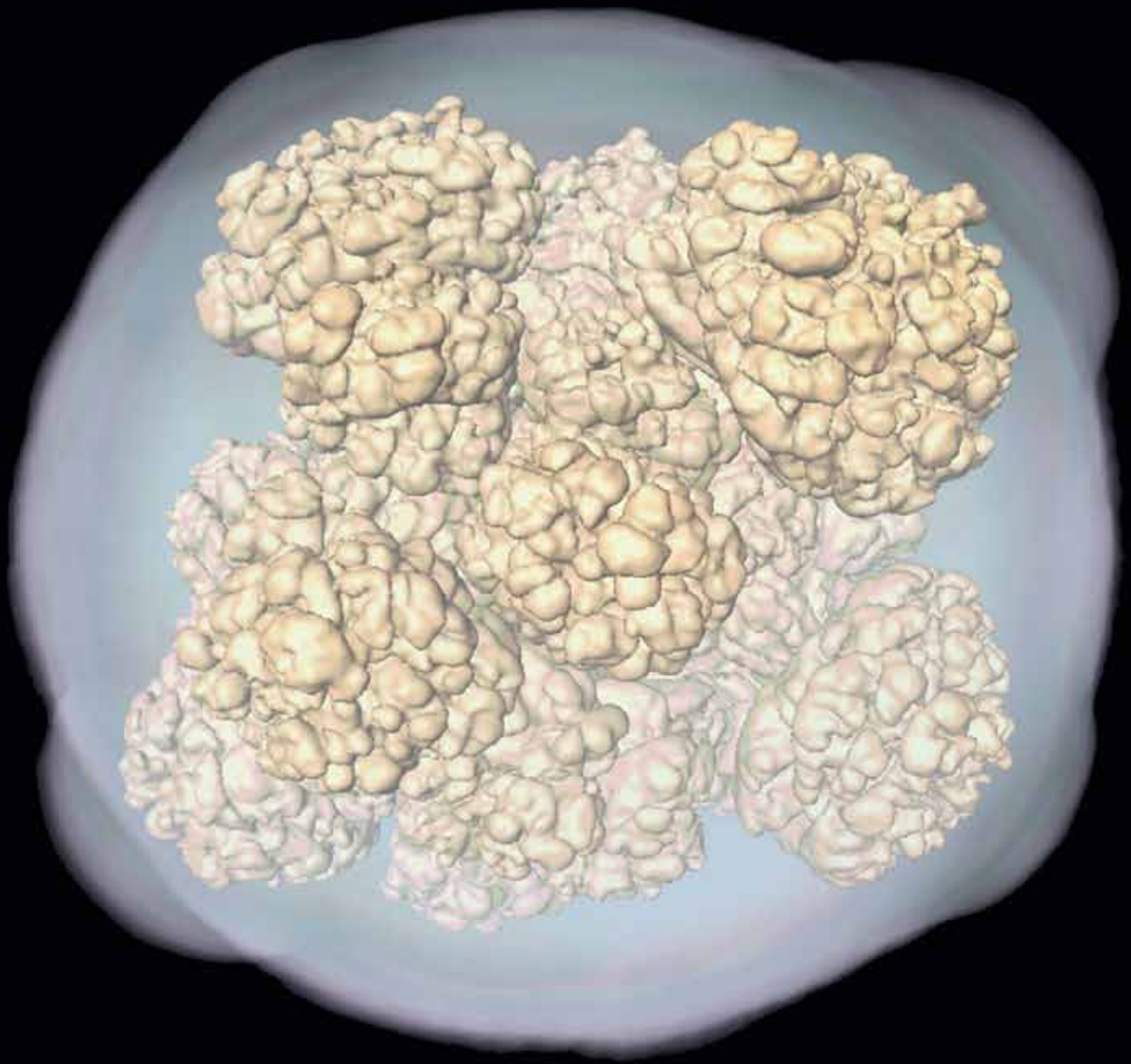
DEISA Resources:

Through the VPH Virtual Community, VPH researcher have used almost 4 million CPU hours on the DEISA infrastructure since 2008, with a further 1.6 million allocated for work in 2011. This work has been mainly carried out on the HECToR and SARA machines, but access has also been granted to RZG.

The VPH Virtual Community, consisting as it does of 15 VPH Initiative projects, uses a wide range of application codes, both home grown and established applications.

Simulating lighthouses of the Universe

Tiina Autio



Measuring distances in the Universe is a challenging task. By calibrating the brightnesses of Type Ia supernovae (SNe Ia), these cosmic explosions can be used as distance indicators to survey the geometry of the Universe. Friedrich Röpke's research group in the Max Planck Institute for Astrophysics, Garching, performed three-dimensional simulations of explosions of white dwarf stars that are able to reproduce global observed characteristics of SNe Ia. In the explosions, a thermonuclear flame incinerates the star and the flame propagation is modelled consistently with current knowledge.

"By calibrating their brightnesses, they can be used as distance indicators to measure the geometry of the Universe"

Type Ia supernovae (SNe Ia) are a sub-group of stellar explosions appearing in our galaxy once in roughly a hundred years, and fading away over a period of a few weeks. Professor **Friedrich Röpke** from the University of Würzburg says that they are among the brightest cosmic explosions we can observe today. "The amount of energy released by an SNe Ia is enormous. If it were to shine constantly at its present luminosity, the Sun would need about 10 billion years to radiate this energy. They produce the bulk of the iron in the Universe, drive shock waves into the interstellar medium and thus have significant impact on other astrophysical processes. By calibrating their brightnesses we can use them as distance indicators to measure the geometry of the Universe", he explains.

Röpke adds that when the first distance measurements with SNe Ia were carried out in the late 1990's, the expectation was to find an eternally expanding freely coasting universe or onein which the rate of expansion is slowing due to the gravity of the matter contained in it. "The most striking result was the discovery of an accelerating expansion of the Universe, which also gave rise to a revolution in the standard picture of cosmology. The reason for the acceleration is still unclear, but it has been confirmed by independent cosmological observation methods. Today, it is assumed that a "dark" energy form that dominates the Universe drives the accelerated expansion. This component makes up about 70% of the energy contained in the Universe. Its nature, however, is unknown", Röpke says. SNe Ia distance measurements can help to constrain its properties, but for this highly precise measurements are required. "This calls for an improved calibration of SNe Ia as distance indicators", Röpke says.

Progenitors of SNe Ia explosions

Type Ia Supernovae are believed to originate from thermonuclear explosions of white dwarf stars, which are the dense and compact end stages of the evolution of intermediate and low mass stars. "A leading scenario with an SN Ia is that the white dwarf explodes when it comes close to the limit of its stability. This is known as the Chandrasekhar mass, about 1.4 times the mass of the Sun. This limiting mass is reached by accretion of material from a binary companion star", Röpke says. After a complex ignition and combustion process the initial carbon-oxygen material of the star transforms to heavier elements such as nickel and silicon. "The energy release in the nuclear reactions causes the explosion of the white dwarf star. Radioactive nickel is produced in large amounts and its decay powers the bright optical display we observe from SNe Ia", Röpke notes.

"Our goal is to simulate these processes in detail and compare the results with astronomical observations of SNe Ia to assess the validity of this theoretical picture. We aimed at a specific mechanism of the explosion where the combustion wave ignites as a subsonic flame that later on undergoes a transition to a supersonic detonation. It has been shown that this "delayed detonation" mechanism is particularly promising for the explanation of a large part of the observed SNe Ia", Röpke says.

Sequence of cosmic explosion

The challenge of implementing such a scenario into numerical simulations lies in the vast range of relevant length scales. "While the radius of the exploding White Dwarf star amounts to about 2000 km, the width of a flame is typically less than a millimeter. In order

© Friedrich Röpke

Simulation of a Type Ia supernova explosion in the delayed detonation scenario. The exploding white dwarf star is indicated in blue. The snapshot is taken shortly after the subsonic deflagration flame (orange) made in some locations a transition to a supersonic detonation (shown in white).

explosion energy in the simulation are consistent with the observed brightness of normal SNe Ia", Röpke adds.

He notes that the propagation of a thermonuclear flame through a white dwarf star is a complex process. "Initially, when it is ignited, the "flame" is subsonic. Because of its slow propagation, it is subject to instabilities. Below the flame, hot burning products are found, and above it the fuel is dense and cold. This causes an inverse and unstable density stratification. At the interfaces, shear flows induce strong turbulence. This complicated flow pattern drags the flame around, corrugates it and increases its surface. As a consequence, the burning is strongly accelerated", Röpke explains.

"A subsonic flame, however, is not capable of producing the vigorous and bright explosions we observe as normal SNe Ia. Part of the reason for this inability is that the complicated unstable flow pattern on a large scale leads to downdrafts of fuel material into the center of the explosion where they are not reached by the flame and remain

© X-ray: NASA/CXC/SAO/J.Hughes et al, Optical: NASA/ESA/Hubble Heritage Team (STScI/AURA)

Picture shows soft green and blue hues of heated material from the X-ray data surrounded by the glowing pink optical shell which shows the ambient gas being shocked by the expanding blast wave from the 1A supernova.

unburned", Röpke says. For a complete burning, a second stage of combustion is necessary: a supersonic detonation. "Although the detailed mechanism of the transition is unknown and cannot be resolved in large-scale simulations that comprise the full exploding star, we can make physically motivated assumptions on when and where the transition happens. The supersonic detonation then propagates through the remaining fuel and burns it efficiently into nuclear ash. This was simulated in detail in our project", Röpke says.

Detailed three-dimensional simulations

According to the results, global characteristics of observed SNe Ia can be reproduced. The models of the flame propagation process are consistent with current knowledge and involve state-of-the-art techniques. "Whether or not the process we simulate reflects the nature of the real supernova event, however, has to be decided upon more detailed comparisons with astronomical observations. As we model the physical mechanism of SNe Ia, numerous new observations become available that constrain the models further. Ultimately, the goal is to converge to a consistent picture of the events. For now, establishing the feasibility of detailed three-dimensional simulations of the complicated model processes is quite an achievement", Röpke says. ■

DEISA Resources:

Computations of SN-DET-hires project were performed on the SGI Altix machine at the Leibniz computer center (LRZ) in Garching, Germany. In the research 512 CPU cores were used in parallel for one simulation. A total of approximately 500 000 CPU hours were invested in these simulations.

http://www.deisa.eu/science/deci/projects2009-2010/SN-DET-hires

More information on the simulations can be found in an article "Type Ia supernova diversity in three-dimensional delayed detonation models from variations in the central white dwarf density at ignition" at Monthly Notices of the Royal Astronomical Society (MNRAS).
A preprint is available on arXiv:
http://arxiv.org/abs/1012.4929

Drug design: medicine gets physical

Nina Morgan

Computational biophysics is opening up new pathways of understanding about the molecular basis of diseases and functions such as taste and smell. In the RNAHIV project, DEISA helped to make possible the computational biophysics that is paving the way for the development of a new class of drugs for anti-AIDS therapy.

Although most current drug treatments target proteins – not all infectious agents do. Retroviruses, such as HIV, target RNA. By developing a better understanding of the way drug molecules bind to RNA, researchers in the RNAHIV project are working to provide new insights into the development of drugs that target RNA.

"This is a very exciting project for several reasons," says **Paolo Carloni**, Professor of Computational Biophysics at the German Research School for Simulation Sciences, a joint graduate school of RWTH Aachen University and Forschungszentrum Jülich (FZJ), Germany.

"For a start, it really brings together physics and medicine to solve a very challenging problem."

"To tackle diseases such as HIV, you need to develop drugs that bind to the trans-activating response region (TAR) in viral RNA, rather than proteins. Because RNA is a more complicated molecule than proteins this is very difficult to do using normal drug design tools. Standard computational approaches are not very effective for designing RNA drugs because they are not able to accurately predict how drug molecules will attach to RNA. But by focusing on the physics that governs the interactions that occur when molecules bind to each other we are gaining good insights that might help in the development of RNA-based drugs."

Predicting predictions

In the RNAHIV project, which began in 2008 and was completed in 2010, Carloni and his colleagues from the University of Washington in the USA, ETH Zurich in Switzerland and SISSA/ISAS in Trieste Italy worked in collaboration with researchers from the University of Ho Chi Minh City in Vietnam to simulate the dynamics of the interaction between a drug molecule and RNA, and to study energetics associated with the binding.

Their work involved a three-step process. They began by drawing on their theoretical knowledge of biophysics to predict how the RNA and drug would interact, they used spectroscopy techniques in an experimental phase to test whether their predictions were correct. The spectroscopy data was then used in the simulations of the molecular dynamics.

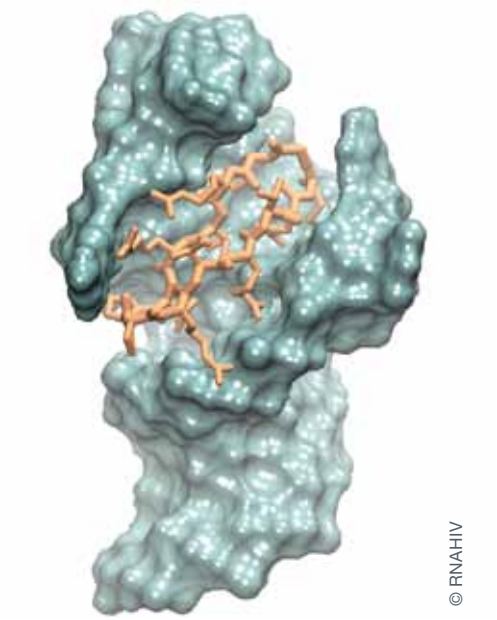
"We were dealing with several thousand atoms and to carry out simulations you have to know where each goes and be able to follow its motion," explains Carloni.

"This is something that requires a lot of computer power!"

Generating simulations in this way is a difficult process, but Carloni believes it offers a number of advantages.

"This method provides a much more rigorous description of the process by

"To tackle diseases such as HIV, you need to develop drugs that bind to the trans-activating response region in viral RNA, rather than proteins."



© RNAHIV

The same system as in TAR-complex (below) with surface representation for the RNA showing the deep binding pocket that the RNA forms around the peptide.

which the drug binds to the RNA," he notes.

"In conventional drug design, you end up only with a prediction of where the drug binds, but you don´t learn anything about the way that the drug molecule travels to the RNA and latches onto it. As well as suggesting a new way to design drugs, the methods we have developed can be applied to study any RNA – protein or DNA – protein interactions. That takes in an enormous number of processes in cells."

Promoting human health

The computing time provided by Deisa played an important role in the success of the RNAHIV project.

"But, Deisa has done more than just provide access to supercomputers. By supporting projects such as RNAHIV, Deisa also opened up the use of supercomputers for projects related to human health. And by making it possible for scientists from a developing country, like Vietnam, to participate, Deisa spread the benefits still further," says Carloni.

"Carrying out experimental research is difficult for our Vietnamese collaborators, but with computers they can work remotely. In our case, Deisa provided a wonderful opportunity for Vietnamese researchers to enter into the exciting field of RNA drug design, and to be able to bring the knowledge back home." ■

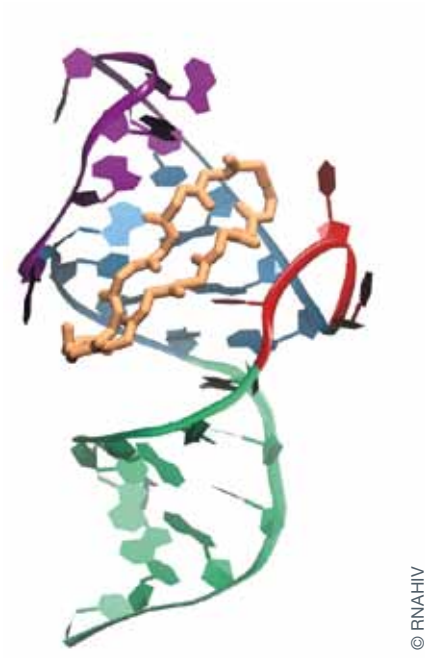
DEISA Resources:

Computations of the RNAHIV research project were performed on the Cray XT4/XT5 system at the CSC – IT Center for Science in Finland. There were 3 independent runs, which used up to 256 CPU cores each. About 250,000 CPU hours were invested on the core of the production simulations.

To construct the initial models, AMBER software package was used on local computers. An open-source software package GROMACS was used for classical molecular dynamics simulations (coded in C, parallelization via MPI). GROMACS were modified to allow the use of AMBER force fields to better describe RNA complexes. The plugin PLUMED was used in combination with GROMACS to perform metadynamics simulations.

Visualization and data analysis on local computers were done using GROMACS, VMD and APBS.

For more information: http://www.deisa.eu/science/deci/projects2008-2009/RNAHIV



© RNAHIV

NMR complex structure of the apical portion of HIV-1 TAR RNA (nucleotides G17–G45) and one of its potential cyclic peptide inhibitor designed by the project collaborators in the University of Washington, Seattle, USA. HIV-1 TAR RNA is a viral RNA that plays a crucial role in the HIV replication, and hence chosen as the drug target in our project. This NMR structure and its structural properties have been used for the first validation of our simulation protocols.

Damping down bad vibrations

Nina Morgan

Vortex induced vibration, caused by turbulent flow, can lead to fatigue and even failure in under the subsea pipelines and marine risers that link offshore oil production platforms and drilling rigs to the sea bed. Thanks to the supercomputing resources provided by Deisa, the results from the Cylinder project are smoothing the pathways to the study of turbulent flow, and aiding progress towards the development of simplified equations to aid the design of safer underwater structures.

When water flows around the surface of a cylinder, vortices – phenomena similar to the familiar spiral flow generated around the plughole when water is drained from a bath – are generated freely and form in the cylinder's wake. The forces created by the vortices on the cylinder can lead to vibration. The motion caused by this vortex induced vibration presents a problem in underwater pipeline and riser design.

The motion of fluids can be described by the Navier-Stokes equations. But although these equations have been around for 150 years, solving them accurately – even with the benefit of powerful computers – requires a lot of computing time. And once completed, the full solution to the calculations may not accurately simulate the conditions faced in real-life applications.

To gain a better understanding vortex induced vibration, the Cylinder project, which included scientists from the Universitat Politècnica de Catalunya, CTTC, in Spain; The Maritime Research Institute Netherlands (MARIN); and the Institute of Mathematics and Computing Science, University of Groningen in The Netherlands, worked to run a full simulation of turbulent flow and the resulting formation of vortices around a cylinder.

"Trying to understand these vortices represents a new approach in computational fluid dynamics," explains Dr. **Roel Verstappen** of the Institute of Mathematics and Computing Science at the University of Groningen.

"To do this we need to include information about the full flow field. This makes the calculations very, very expensive to run."

Following up

Currently designers tackle the problem of designing for vortex induced vibrations by carrying out experiments using physical models set up in tanks of water. After generating vibrations in the models they measure the effects and use these results to try to calculate the strength of materials needed for the

"The results of the Cylinder project are enabling us to develop simpler models that can be used in computations for engineering applications."

cylindrical structures such as risers and pipelines. Thanks to Cylinder, engineers may soon be able to turn to mathematical simulations to gather the data they need.

"The results of the Cylinder project," says Verstappen, "are enabling us to develop simpler models that can be used in computations for engineering applications."

Cylinder was carried out in 2009. As a follow-up and with support from the Dutch Maritime Innovation Platform (MIP) the group have gone on to devise a number of simplified models. These will then be tested to determine which is the most accurate.

"These simpler models will allow designers to use local parallel computing facilities to assist in their designs," explains Verstappen.

"Typically designers require many computer runs in the design phase. But, as a result of the Cylinder work and the follow up project, designers will not only require fewer runs. They will be able to carry them out using simpler computing facilities.

The same cannot be said for the Cylinder researchers themselves.

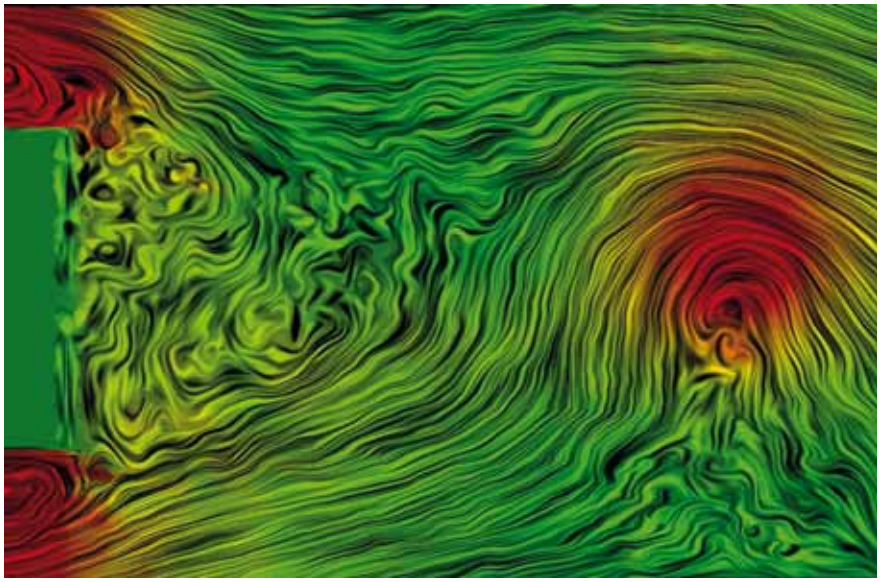
"Fluid flow is very complex," explains Verstappen.

"If you want get the full solution in turbulent flow you have to solve all physical scales in the flow. As well as solving the equations at the scale of the cylinder itself, you also have very small motions which are 1,000 – 10,000 times smaller than the diameter of the cylinder. Solving and evaluating at all these different scales is very costly in terms of computing time and can only be done using supercomputers."

Thanks to Deisa, Verstappen and his colleagues were able to carry out the full computation. Even though the group were careful to chose their parameters to take into account the amount of time on the supercomputer available to them, their calculations required around 650,000 hours of computing time.

"It sounds like a lot, but it isn't really," says Verstappen.

"If we had considered a more complex turbulent flow it could easily have required 10 or 20 or even a hundred million hours. If you want to carry out the kind of research we've been doing there is only one source of computing resources you can turn to – and that is Deisa. At the national level 1 million CPU hours is very difficult to obtain, especially not every year. Deisa has made the Cylinder project possible." ■



An instantaneous picture of vortical motion in the wake of a cylinder.

DEISA Resources:

Computations of the Cylinder research project were performed at Barcelona Supercomputer Center. There were a few try outs, which took about 50,000 CPU-hours. About 600,000 hours were invested on the main run. The code was developed at UPC - Barcelona TECH and University of Groningen. It was written in MPI-Fortran. Visualization and data analysis were done on local machines. A new visualization tool (developed in the Scientific Visualization and Computer Graphics Group at University of Groningen) was applied to track particle path lines.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/CYLINDER

Simulations to understand experiments in the

Wendelstein 7–X stellarator

Pirjo Rötkönen

The EUTERPE code has been extended for simulations to understand experiments in the world's largest fusion experiment of the stellarator type, Wendelstein 7–X, which will start operation in 2014.

EUTERPE is a global gyrokinetic code for three-dimensional geometry that simulates micro instabilities and related turbulence in stellarator geometry.

"We obtained the EUTERPE code from CRPP in Lausanne, Switzerland, where it was created. We have developed and extended it for many new applications. Originally, the code was electrostatic and linear. After development and optimization it is electromagnetic, non-linear and scales very well," explains Dr. **Ralf Kleiber** of the Max Planck Institute for Plasma Physics, Greifswald, Germany. Dr.Kleiber is responsible for developing the EUTERPE code and coordinating the EUTERPE project in the DEISA framework.

The Max Planck Institute for Plasma Physics has great interest in stellarator simulations because the large stellarator experimental facility, Wendelstein 7–X, is under construction in Greifswald. When it starts operation in 2014 it will be the world's largest fusion device based on an optimized stellarator. The purpose of Wendelstein 7–X is to evaluate the concept and technology for a future fusion reactor of the stellarator type.

"Our main goal is to carry out simulations for Wendelstein 7–X. It is very important that we understand the experimental results that will be obtained when the device is in operation," says Dr. Kleiber.

Two different concepts for fusion reactors

In Wendelstein 7-X the plasma will be confined for about half an hour by using superconducting coils. This experiment will be an important step towards a stellarator fusion reactor. The ITER device, which is being build at Cadarache in France, represents the other line of fusion devices, the tokamak concept.

"In the ITER reactor the temperature will be high enough to create fusion reactions, so it could actually yield more energy than is fed into the plasma by heating," Kleiber points out.

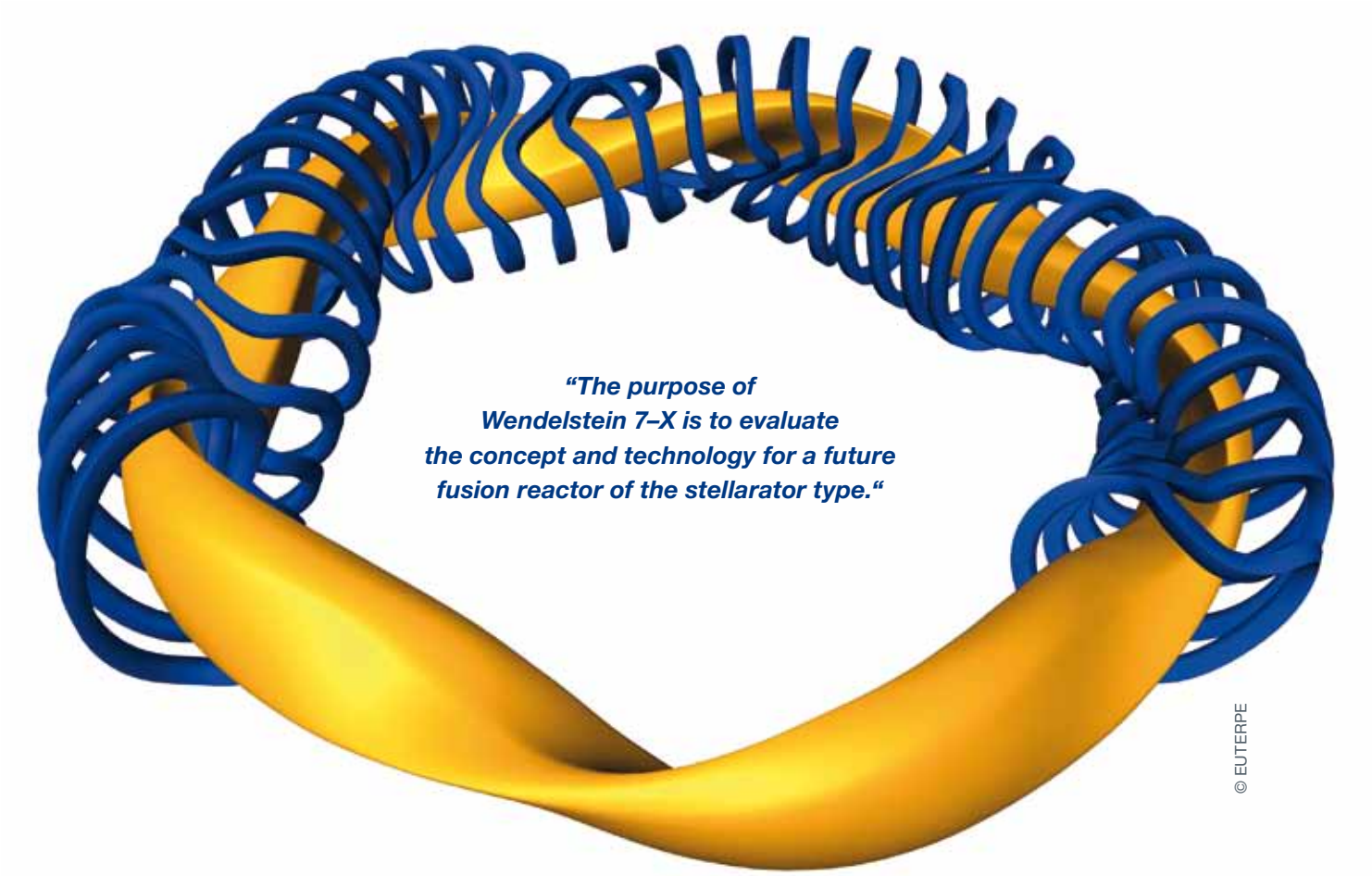
The stellarator has a three-dimensional geometry. It is mathematically more complex to describe, and harder to simulate and to construct, than a tokamak. However, a stellarator can operate in a steady-state and, unlike a tokamak, it has none of the variations of pulsed operations. These advantages have been sufficient to justify active development of this concept.

Comprehensive physical model

"The main part of our work has been the numerical development of the EUTERPE code. Physically it is a relatively complete model, including electro-magnetic effects, non-linear features and collisions," Ralf Kleiber explains.

"Using the code we study instabilities and turbulence caused by the ion-temperature gradient. We are focusing on effects produced by kinetic electrons and electromagnetic perturbations. All these studies are done in stellarator geometry. Also we want to use the code for neoclassical calculations."

The Max Planck Institute for Plasma



Graphics of coil system and plasma of the experimental fusion device Wendelstein 7-X, under construction in Greifswald, Germany. The power plant fusion research is concentrating on two different types of experiment, the tokamak and the stellarator. Both types feature ring-shaped magnetic fields. Tokamaks produce part of these fields by means of an electric current flowing in the plasma. Stellarators form the magnetic field cage solely by means of external coils. Stellarators are thus suitable for continuous operation, whereas tokamaks without auxiliary facilities can only work in pulsed mode.

Physics in Greifswald has three cooperation partners in the EUTERPE project – CIEMAT in Madrid, Spain; CRPP in Lausanne, Switzerland; and the Max Planck Institute for Plasma Physics in Garching, Germany.

Expertise and computing power from DEISA

"DEISA plays an essential role in the EUTERPE project. We get access to highly skilled people and computing time on powerful machines," Ralf Kleiber says.

"We identified the parts in the code that were not very well parallelized and DEISA provided us with experts who optimized the code for single processor and for parallel performance."

Stellarator simulations are complex. "They are very time-consuming and require a lot of computing power. They cannot be run on small clusters. That is why DEISA computing resources were extremely important for us." ■

Dr. Ralf Kleiber of the Max Planck Institute for Plasma Physics, Greifswald, is coordinating the EUTERPE project in the DEISA framework.

DEISA Resources:

The computations were performed at the Leibnitz-Rechenzentrum in Germany and CINECA in Italy.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/EUTERPE

Catalysing catalysis

Nina Morgan

Catalysts – substances that make chemical reactions go faster, without actually being consumed during the process – play an important role in many chemical processes. The supercomputing resources provided by DEISA helped the partners in the SIRE project to explore the mechanisms of chemical bonding and provide more clues about how catalysis works.

From cosmetics to clean energy, from petroleum refining to polymers, the chemical industry depends on the use of catalysts. Designing effective and efficient catalysts is a key to improving many chemical processes, making them more efficient and cleaner. But developing new catalysts still remains a bit of a 'black art' requiring lots of experimentation. Although it is often clear that a catalyst works – exactly how and why can remain a mystery. To really understand catalysis, it is necessary to gain a better understanding of chemical bonding.

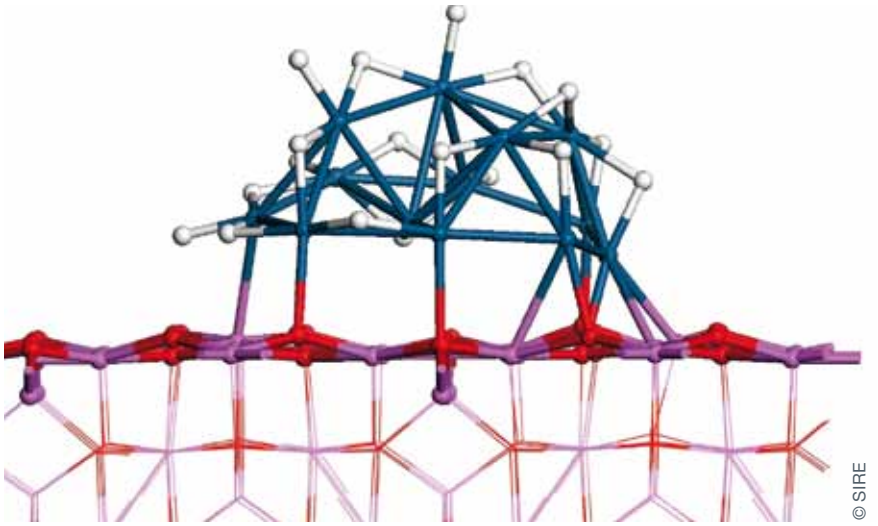
"Chemical bonding lies at the crossroad of a large number of natural or industrial processes, not only in chemistry but also in life, materials, earth and environmental sciences," explains Dr **Philippe Sautet**, of the Laboratory of Chemistry at Ecole Normale Supérieure de Lyon, France, the principle investigator in the project.

"Catalysts play an important role in the breaking and formation of chemical bonds. The ultimate goal in the Simulation of Reactivity at Interfaces (SIRE) project, which began in 2009 and was completed in 2010, was to gain a better understanding of how catalysts operate at an atomic scale. This knowledge could lead to improved designs for catalysts."

Back to basics

Electrons play a key role in chemical bonding. To achieve greater insight into chemical bonding, the group, which

"Designing effective and efficient catalysts is a key to improving many chemical processes, making them more efficient and cleaner."



Simulation of nanometre sized platinum particles (shown as blue balls) on an alumina support, submitted to a pressure of hydrogen. The simulation shows, for the first time, that a nanometre sized particle can accomodate a very large number of hydrogen atoms. This has important implications in catalysis.

included colleagues at the Institute Français du Pétrole (IFP) Energies Nouvelles, the University of Montpellier II and the Ecole Nationale des Ponts et Chaussées in France, went back to the basics of theoretical chemistry, by applying the laws of physics that govern the behaviour of electrons. Their first step was to develop a computer code to solve the basic Schrödinger equation – an equation used in quantum physics and made famous by the thought experiment involving Schrödinger's cat – which governs the stability and structure of molecules.

"The equation itself is simple," explains Sautet. "But it is not possible to solve it analytically using equations on a blackboard. To get a good approximation of the results numerically we needed to carry out the calculations on a supercomputer."

As part of the project the group also developed some new methods to explore reaction pathways and gain a better understanding of how bonds are formed and broken at the surface of molecules. This, in turn, allowed them to carry out simulations and to explore various aspects of catalyst systems – such the reactivity of metallic nanoparticles deposited on an oxide support.

"A supercomputer was essential for this too," notes Sautet. "It was the access to CPU hours that Deisa provided that enabled us to do the real science in SIRE. The access to the CINECA machine that Deisa provided enabled us to look at systems that were significantly more complex than we could have studied using our own local computing facilities."

Appliance of the science

"By trying to get as close as possible to a realistic description of the catalytic system we were aiming to develop a model for catalysis that is not too far from reality," he continues.

"The ultimate goal is to make it possible to develop catalysts and make chemical reactions work more efficiently."

The group chose to focus on metallic catalysts, which have applications in fine chemistry, and in the refining of hydrocarbons and petroleum-based fuels, and to explore the structure and reactivity of small platinum clusters stabilised on an alumina support. This work, which will help catalyst designers to find ways reduce the amounts of expensive platinum used in catalysts, is due to be published in ChemCatChem, a top ranking academic journal for the catalysis community.

But, as Sautet is quick to point out, the results from the SIRE project will lead to a better understanding of all types of catalysts – not just metallic catalysts.

"The insights gained in the SIRE project will be very beneficial both in terms of catalyst development and for increasing the understanding of how catalysts work," he points out.

And along the way, it has also provided important new insights into the very basis of chemical bonding. ■

Philippe Sautet is the principal investigator in the SIRE project.

DEISA Resources:

All calculations have been performed with the periodic density functional theory code VASP (G. Kresse, J. Hafner, University of Vienna) at the CINECA in Italy on the BCX and SP6 machines. The DECI funding permitted to perform parallel calculations, up to 128 nodes, and to run long molecular dynamics which are needed for such systems.

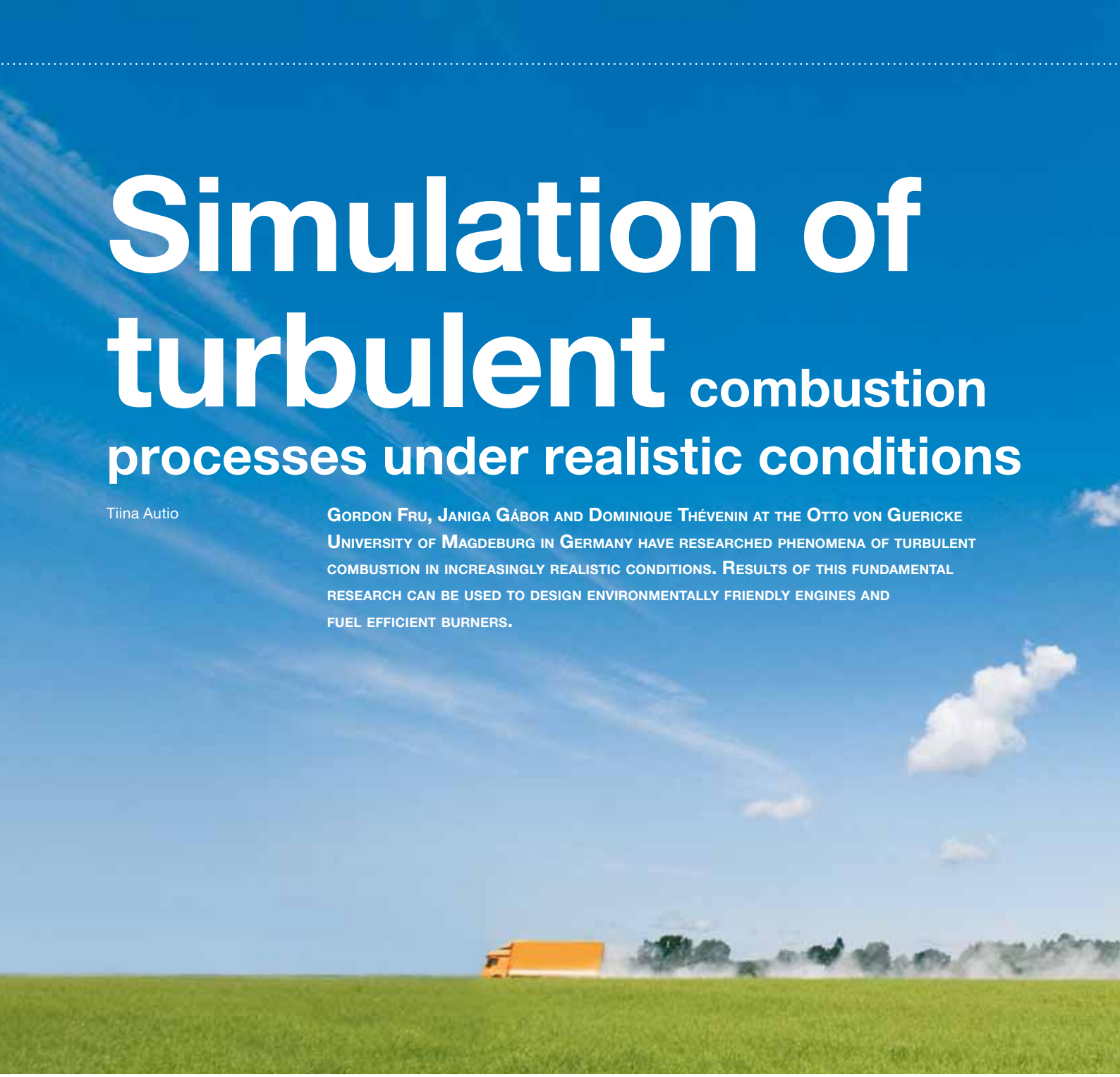
Initial models were constructed on local computer using Materials Studio software. Reaction pathways searches were performed with the local code CARTE.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/SIRE

Simulation of turbulent combustion processes under realistic conditions

Tiina Autio

Gordon Fru, Janiga Gábor and Dominique Thévenin at the Otto von Guericke University of Magdeburg in Germany have researched phenomena of turbulent combustion in increasingly realistic conditions. Results of this fundamental research can be used to design environmentally friendly engines and fuel efficient burners.



Combustion under turbulent conditions is widely used for industrial applications because turbulence accelerates mixing processes between fuel and oxidizer. For many decades a major part of energy needed in power plants and transportation will still be covered by combustion of fossil fuels. It is therefore essential to understand and improve combustion processes to reduce fuel consumption and pollutant emissions.

Researchers **Gordon Fru** and **Gábor Janiga** have examined phenomena of turbulent combustion in the research group of Professor **Dominique Thévenin** at the Otto von Guericke University of Magdeburg, Germany. As a method, they have used Direct Numerical Simulation (DNS) coupled with detailed physicochemical models. DNS is an essential tool for the investigation of turbulent combustion because it does not rely on any model for turbulence.

"The research focused on quantitative investigations of turbulent reacting flows for turbulent Reynolds numbers up to 7 300", Gordon Fru says. Turbulent flow occurring at such high Reynolds numbers, which is a measure of the ratio of inertial forces, reflects increasingly realistic turbulent conditions.

"The research also concentrated on the impact of the traditionally neglected volume viscosity on turbulent flame structures for highly turbulent premixed hydrogen-air, syngas-air and methane-air flames", Fru adds. In terms of fluid properties, viscosity plays a major role for combustion applications due to the fact that it directly controls dissipation processes, and because temperature and composition variations lead to large spatial and temporal changes in viscosity. As a consequence, viscosity is one of the most important terms coupling turbulence and combustion.

Essence of high Reynolds number combustion DNS

"Research verified that analysing direct numerical simulation results at high

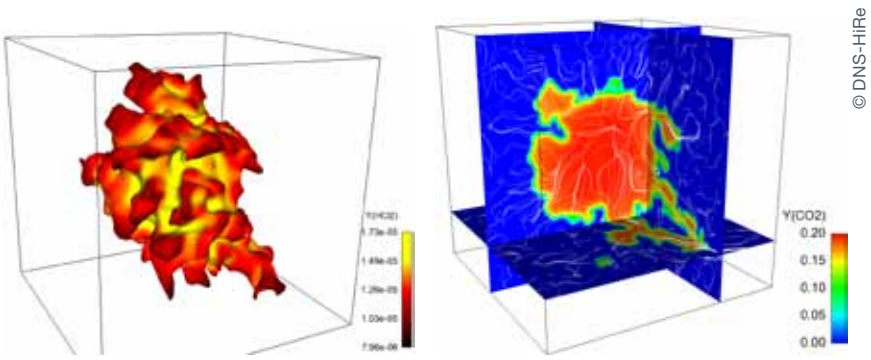
"These findings are crucial and can be used to design more fuel efficient and low emission engines and burners for instance by allowing more compact combustion chambers with reduced losses."

Reynolds numbers is essential to obtain realistic information for modeling purposes", Fru summarises. As Reynolds number exceeds considerably 1000, the turbulent flame structure is reformed with numerous perforations and considerable structural modifications as a result of sustained flame-flame interactions and local re-ignition fronts. "Flame thickening predominates for turbulent flames. However, saturation is observed at higher Reynolds numbers", Fru says. He adds that flame speed rapidly increases when turbulence stirring is increased: both local and global gas phase quenching is observed, leaner mixtures shows stronger quenching effects and turbulence alone cannot increase the speed of flames incessantly, in accordance with experimental results.

According to the results, Probability Density Function (PDF) of flame curvature and strain rates becomes broader and flatter with increasing turbulence intensity. Also, peak conditional profiles of heat release and major and minor species mass fractions are lowered with increasing turbulence intensity.

For computations where volume viscosity effects are included, it is shown that viscosity leads to noticeable instantaneous differences in turbulent flows. "The results show that for methane, >

Researcher Gordon Fru's responsibilities in the research project included code development and optimization, preparation and execution of all simulations and post processing and analysis of resulting simulation data.



(a) (b)

DNS of turbulent premixed methane–air flames with detailed physicochemical models, showing (a) the mass fraction of CO^2 colored by the HO^2 and (b) the mass fraction of CO^2 slices with stream lines (thin white lines), revealing the heavily wrinkled flame front after interacting with the three-dimensional time-decaying homogeneous isotropic synthetic turbulent velocity field for 0:8 ms [1].

volume viscosity has a minor impact in all considered cases on global flame properties. For turbulent flames burning hydrogen and syngas fuels, the inclusion of viscosity leads to noticeable differences for the local and global flame structure", Fru says.

The chaotic nature of turbulence amplifies small instantaneous differences with time, eventually leading to completely different evolutions for the turbulent flames burning hydrogen-containing fuels. As a consequence, taking into account volume viscosity leads to noticeable differences even before reaching the characteristic turbulent time.

"This effect is clearly visible locally, changing for instance the local flame structure. But it is also observed with a considerable magnitude on all global flame properties and it increases with time", Fru says. He adds that these observations are more intense for the pure hydrogen flames compared to when using syngas as a fuel. For these hydrogen-containing fuels, the influence of volume viscosity appears to be independent of the turbulent Reynolds number even though the peak value of volume to shear viscosity ratio increases timidly. Methane flames on the other hand show no convincing modifications in the presence of volume viscosity, even for ensemble averaged quantities. "The inclusion of volume viscosity effects in multi-component multi-dimensional turbulent premixed flame computations is therefore recommended for all hydrogen-containing fuels", Fru notes.

Preliminary tools for more efficient combustion processes

The results of the research can be used to support the development and optimisation of simplified models for engineering level computations using for instance computational fluid dynamics techniques such as the Reynolds Averaged Navier-Stokes and the Large Eddy Simulation. These tools are capable of tackling practical large scale industrial configuration like fuel and air injection into normal car engines.

"Our research using Direct Numerical Simulations has confirmed the strong dependency of fuel consumption rate to turbulence intensity. We also found that turbulence cannot increase the burning rates incessantly. There is a saturation point beyond, which further increases in turbulence intensity results in both local and global gas phase quenching, depending on the mixture ratio and burner configuration. These findings are crucial and can be used to design more fuel efficient and low emission engines and burners for instance by allowing more compact combustion chambers with reduced losses. However, direct numerical simulations studies are fundamental in nature and do not help directly engineering applications yet", Fru says. ■

DEISA Resources:

The High Performance Computer (HPC) systems and data storage facilities in three DEISA centers across Europe were used: the IBM BlueGene/P (BABEL) at IDRIS in France, the CRAY Vector (HECToR X2) and the IBM Power5 Cluster (HPCx) both at EPCC in Scotland.

Eight full-scale three-dimensional direct numerical simulations were realized involving two different fuels. A typical simulation involving volume viscosity took approximately 10 days when employing at least 512 processing cores.

Both BlueGene/P and Cray X2 vector machines used the same code. Parcomb3D has been developed over 20 years and contains now more than 30 000 lines of code. It is coded in Fortran95 and parallelized with MPI.

Parcomb3D has been successfully developed with a view toward efficient parallelization using up to several thousand processors. However, the advantages of vector processors are still taken into account for the low-level loops, leading to an acceptable efficiency on vector supercomputers as well. Various architectures are automatically detected and loops are vectorised accordingly. Nevertheless, the code is clearly more at ease with "classical" parallel supercomputers, delivering its full potential for such architectures.

More information

http://www.deisa.eu/science/deci/projects2008-2009/DNS-HiRe

Fru, G.; Janiga, G.; Thévenin, D. Direct Numerical Simulation of the impact of high turbulence intensities and volume viscosity on premixed methane flames. J. Combustion 2011, submitted.

Fru, G.; Janiga, G.; Thévenin, D., Direct Numerical Simulation of turbulent methane flames with and without volume viscosity. In 8th Euromech Fluid Mechanics Conference (EFMC-8); Bad Reichenhal, Germany; 2010; pp. MS2–9.

On the paths towards improved climate models

Tiina Autio

Clouds above Florida. In a warming world in the current century, high clouds move upwards and cloudiness at mid-latitudes is reduced. If the low-level cloud cover is reduced in the tropical region, global warming will escalate.

One of the general aims of climate modeling research is to improve the accuracy and reliability of climate models. Research Professor Heikki Järvinen and senior research scientist Petri Räisänen from the Finnish Meteorological Institute have studied how the climate simulated by the ECHAM5 model depends on the parameterization of cloudiness and atmospheric radiative transfer.

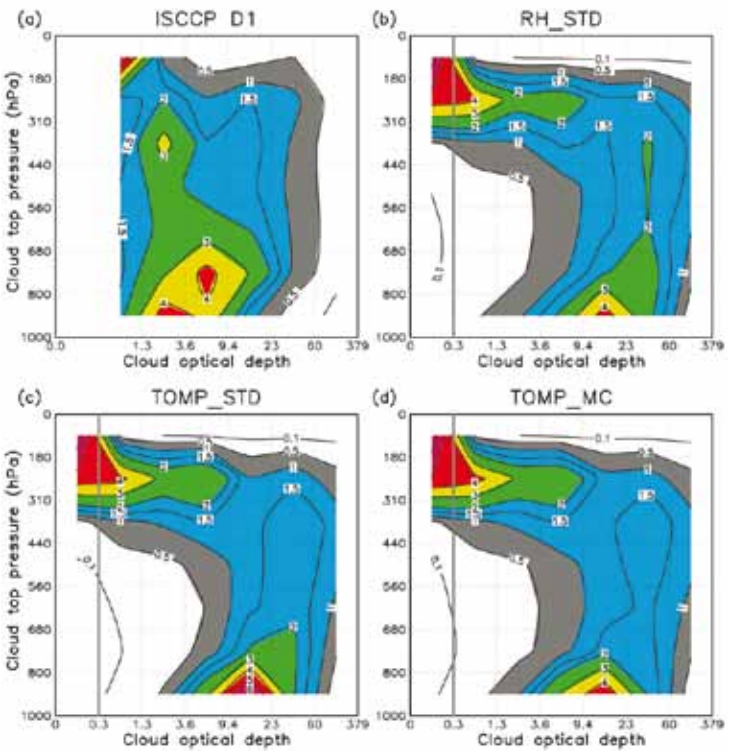
They used three different model versions and found that changing these parameterizations had relatively little effect on simulations of the present climate in, for example, regional distributions of temperature and precipitation. In spite of this, the different model versions showed clear differences in the simulation of climate change: in the most sensitive model version an increase in atmospheric carbon dioxide (CO_2) caused almost 50% more warming compared with the least sensitive one.

Climate models are used, for example, in long-term predictions of climate change. These predictions involve significant uncertainty. For example, in the most recent report of the Intergovernmental Panel on Climate Change (IPCC) the global temperature is expected to rise by 1.1 to 6.4 °C during the 21st century. There is a wide range of uncertainty relating partly to the future development of greenhouse gas concentrations and partly to the climate models themselves. “The most important individual uncertainty factor in climate modeling is changing cloudiness,” says **Petri Räisänen** from the Finnish Meteorology Institute.

Climate models are generally in agreement about high-level clouds moving upwards and mid-latitude cloudiness decreasing in conjunction with climate warming during the current century. At northern latitudes, for example in Finland, cloudiness is likely to increase during winters, and hence winters will gradually become darker than they are now. The greatest uncertainty concerns changes in low-level clouds in tropical and subtropical regions. “Should low-level clouds increase in the future, more solar radiation will be reflected into space, which would then work against global warming. Then again, should low-level clouds recede, global warming will escalate,” says Räisänen.

The long-term research goal is to improve the accuracy and reliability of climate models. The accuracy of climate models in simulating current climate has continuously improved. The models contain prediction equations for various parameters, such as temperature, wind >

"The experiments performed in this work represent the most extensive climate modeling study ever conducted in Finland."



Comparison of the joint frequency distribution of cloud optical depth and cloud top pressure in (a) ISCCP D1 satellite observations and (b)-(d) for the three versions of ECHAM5: RH_STD, TOMP_STD and TOMP_MC. The values are shown as percentages of all cases, for daytime data between latitudes of 60 S and 60 N. The gray vertical line at optical depth of 0.3 in (b)-(d) shows the approximate lower limit of cloud detection in ISCCP data.

speed, and air humidity content, and they are integrated forward over time. Prognostic descriptions of clouds are used to predict changes occurring in the amounts of cloud liquid water and ice during each model time step. "The most important problem here is insufficient resolution. The model atmosphere consists of grid cells with a typical area of 200x200 km and a height of 0.5–1 km. Many processes affecting the generation and properties of cloud formation occur on a much smaller scale. In climate models the effect of these processes must be parameterized, i.e. they must be presented based on the information that is available based on the model-specific resolution," says Räisänen.

Comparing physical parameterisations

Heikki Järvinen and Petri Räisänen have studied the effects of parameterisations related to cloudiness and radiation on climate simulated with the ECHAM5 atmospheric general circulation model. The testing was performed using three different model versions. The first version (RH_STD) involved a simple parameterisation of cloudiness, in which cloud fraction is calculated based on relative humidity. The second model version (TOMP_STD) involved the Tompkins cloud scheme that predicts subgrid-scale variations (i.e. variations at a scale smaller than the grid resolution). In the third version (TOMP_MC) the Tompkins cloud scheme was combined with a new stochastic method for radiation calculations, known as the Monte Carlo Independent Column Approximation; (McICA). This method accounts for variations smaller than grid resolution by dividing the cloud field into sub-columns, which are generated by using random numbers in addition to variables predicted by the model.

"The validity of the versions was studied using different model configurations. One test run employed only the atmospheric model with fixed sea surface temperatures specified from observations. The runs performed with this configuration covered a 29-year time span. The aim was to investigate how the changes in the model affect the cloud field and the radiative fluxes simulated by the model. The purpose of this experiment was to understand how the parameterization changes impact the system behavior in a fairly simple model setting."

"We also used a fully coupled model that contains an atmospheric and an oceanic general circulation model. The configuration was used to run 240-year simulations. The third experiment was a hybrid of these two: an atmospheric model coupled with a simple description for oceans, called the mixed-layer ocean model. The purpose of this experiment was to investigate the response of the model versions to increased CO_2," says Räisänen.

In the experiments that used the mixed-layer ocean model, two 100-year long runs were conducted with each model version: one at the pre-industrial CO_2 concentration of 286 ppm, and another at a higher-than-present concentration of 450 ppm. The differences between these runs were used to evaluate the strength of climate change predicted by each model version, and to determine the reasons behind the differences between the three versions.

Surprising results

"From the point of view of simulating the current climate, the differences between the three model versions were relatively small. When the structures of the simulated cloud fields were compared with observational data derived from satellite imaging, similar systematic errors were found in the different model versions," says Räisänen.

Surprisingly, in spite of similar performance for the present climate

simulation, the different model versions showed clear differences in climate change simulations. “The first version, used as the starting point, indicated climate warming to be less than that produced by the two other versions. The third version showed the highest response to increased CO_2 and a warming almost 50 percent stronger than that in the first version.”

“The result is explained by the fact that in the two versions based on the Tompkins cloud scheme, global warming reduces low-level cloudiness. This means that solar radiation reflected back to space is reduced, but the amount of thermal radiation escaping from Earth into space is not much changed. Hence, this generates a positive feedback phenomenon that strengthens global warming. But it is currently unknown what is ultimately causing the reduction in low-level cloudiness,” says Räisänen.

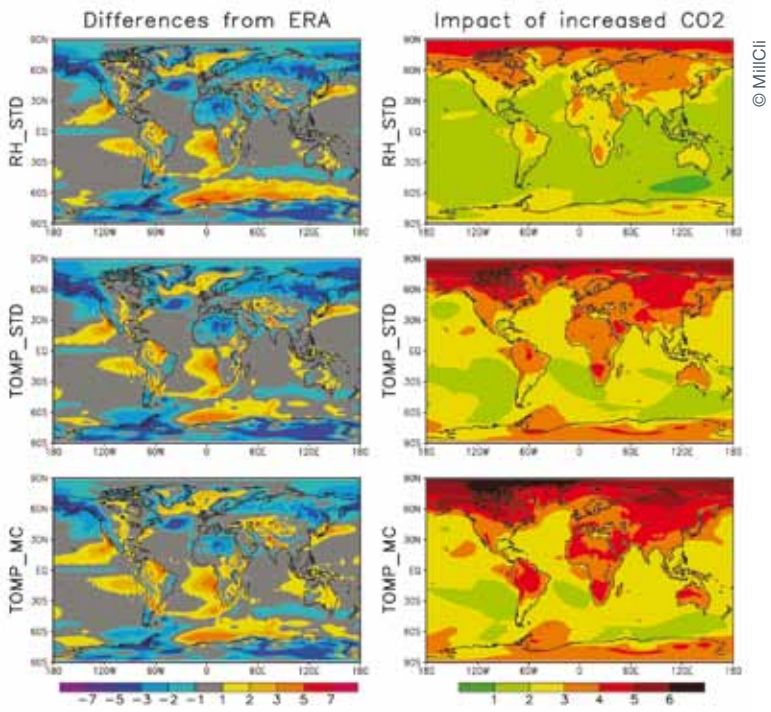
According to Räisänen, the results support the conclusion that although the models seem to produce quite similar simulations of present climate, they can still produce notable differences in the strength of climate change. Therefore, it is difficult to assess the reliability of climate change predictions based on merely how well the model performs in simulating the present climate – at least it is advisable to investigate more than just simple time averages. “A general question that still lacks good answers is which features in simulating current climate are critical for simulating climate change,” says Räisänen.

The experiments performed in this work represent the most extensive climate modeling study ever conducted in Finland. They are also of international significance, since even globally, this is so far the most in-depth study of the impact of subgrid-scale cloud features on climate simulation. ■

© MillCli

The problem: Climate models work by dividing the atmosphere into a grid with resolution of 100-300 km in the horizontal directions and at least several hundred meters vertically, but clouds feature a lot of smaller-scale structures. (Modified from an original figure by Adrian Tompkins, European Centre for Medium-Range Weather Forecasts).

“The accuracy of climate models in simulating current climate has continuously improved.”



© MillCli

Left column: Mean errors in simulated near-surface air temperature for the three model versions, as compared with ERA-Interim reanalysis data, in experiments with the fully coupled ECHAM5-MPIOM atmosphere-ocean climate model. Right column: temperature change due to increasing atmospheric CO_2 concentration from 286 to 450 parts per million, in experiments with ECHAM5 and the mixed-layer ocean model. Note that in spite of similar temperature errors for the present climate, the three model versions show substantial differences in their response to increased CO_2, with global-mean warming of 2.0 K for RH_STD, 2.7 K for TOMP_STD and 3.0 K for TOMP_MC.

DEISA Resources:

To carry out this research, Heikki Järvinen and Petri Räisänen used about 400,000 CPU hours of DEISA resources on the Nec SX8 at the HLRS computing center in Stuttgart and the SGI Altix supercomputer in Leibniz. While each single run used a relatively small number of processors (8 processors on NEC SX8 and 20–30 on SGI Altix), several models runs were conducted in parallel.

Additional information:
http://www.deisa.eu/science/deci/projects2008-2009/MillCli

Räisänen, P. and Järvinen, H. (2010), Impact of cloud and radiation scheme modifications on climate simulated by the ECHAM5 atmospheric GCM. Quarterly Journal of the Royal Meteorological Society, 136: 1733–1752. doi: 10.1002/qj.674
http://onlinelibrary.wiley.com/doi/10.1002/qj.674/abstract

Enhancing efficiency of aircraft wings

Nina Morgan

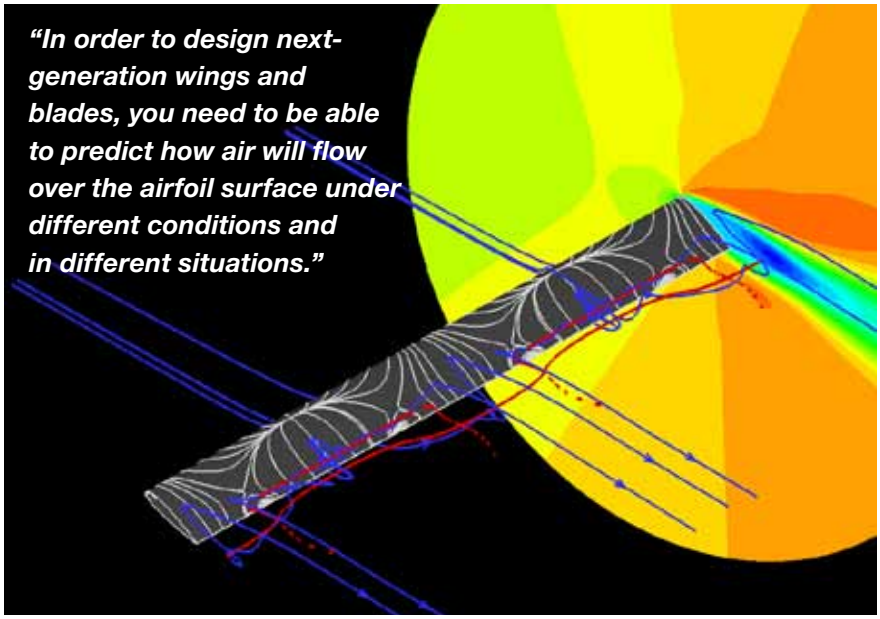
Better design of the lifting surfaces of wings and blades can enhance the efficiency of aircraft wings, wind turbine blades, aircraft engines and the wide range of other applications whose performance relies on air flowing over rotating blades. New methods of calculating the Navier-Stokes equations in three dimensions developed during the GATUS project with help from DEISA can reveal a more accurate picture of airflow – and help wing and blade design take off.

Why do commsercial planes take off and land only between a certain range of angles, rather than taking off nose steep up or landing nose steep down? The answer lies in the way that air flows over airplane wings. If a plane takes off too steeply, the airflow around the wing of the plane no longer flows smoothly around the contour of the airfoil, or wing surface. As a result stall cells form on the wing surface, leading to loss of lifting capacity.

Although the effects of stall cells have been well known for decades, their origin has never been unravelled.

"One reason is because of the way that the Navier-Stokes equations, which describe fluid motion, are generally solved," says Professor **Vassilis Theofilis**, of the School of Aeronautics at Universidad Politécnica de Madrid (UPM), Spain.

In the GATUS project Theofilis and Dr **Daniel Rodríguez**, worked during 2009 to develop a more efficient and effective way to analyse the three-dimensional stability of flow around a two-dimensional airfoil or blade.



© GATUS

Stall cell structures on a wing surface, as calculated by the GATUS project.

Predictive power

"Although industry also carries out three dimensional simulations using the Navier-Stokes equations, these draw on existing models of turbulence. They also adjust constants of the model in order to predict their application. As a result, the solutions they come up with are appropriate for one set of parameters only. In contrast, the alternative three-dimensional calculations we've developed do not rely on assumptions from the existing models of turbulence. As a result our calculations make it possible to more accurately predict the way air will flow over airfoil under different conditions," says Theofilis.

These more accurate predictions of airflow behaviour are an important key when it comes to improving efficiency in wings and blades.

"In order to design next-generation wings and blades, you need to be able to predict how air will flow over the airfoil surface under different conditions and in different situations," explains Theofilis.

"We still fly on technology developed by the Germans during World War II. And we still see planes are shaped like cigars with wings! One reason that the basic aircraft designs haven't changed very much is because the aircraft industry has become very good at optimising something whose behaviour it thoroughly understands. Up to now there hasn't been a good way of modelling airflow in three dimensions. But by making it possible to get closer to being able to solve turbulence equations for real world situations, the methodology we have developed during the GATUS project will help and encourage industry to work to design better aircraft wings and blades. Reducing the noise emitted from wind-turbine blades is another problem that our methodology will help to solve."

Computing provides power

Although the new method of calculating the Navier-Stokes equations in three dimensions developed by the GATUS project is more efficient, it still involves solving coupled linear systems composed of around a million equations.

"This is where access to super-computers is essential," Theofilis says.

"The calculations carried out in GATUS require large amounts of computing time. This is something his other research contracts did not provide. Without Deisa we wouldn't have been able to do carry out this work. But thanks to the Deisa award we've been able to produce results that have led to the publication of five papers in high impact journals over the past two and a half years, along with 10 or so conference papers. The computing time we received from Deisa, made all the difference!" ■

DEISA Resources:

Computations of the GATUS research project were performed at JUGENE in Juelich. Over 200 runs were performed, the most demanding of which used 4096 CPU cores and 24 hours each. A total of 8 million CPU hours (2.5 million CPU hours were granted initially) were invested on the computations.

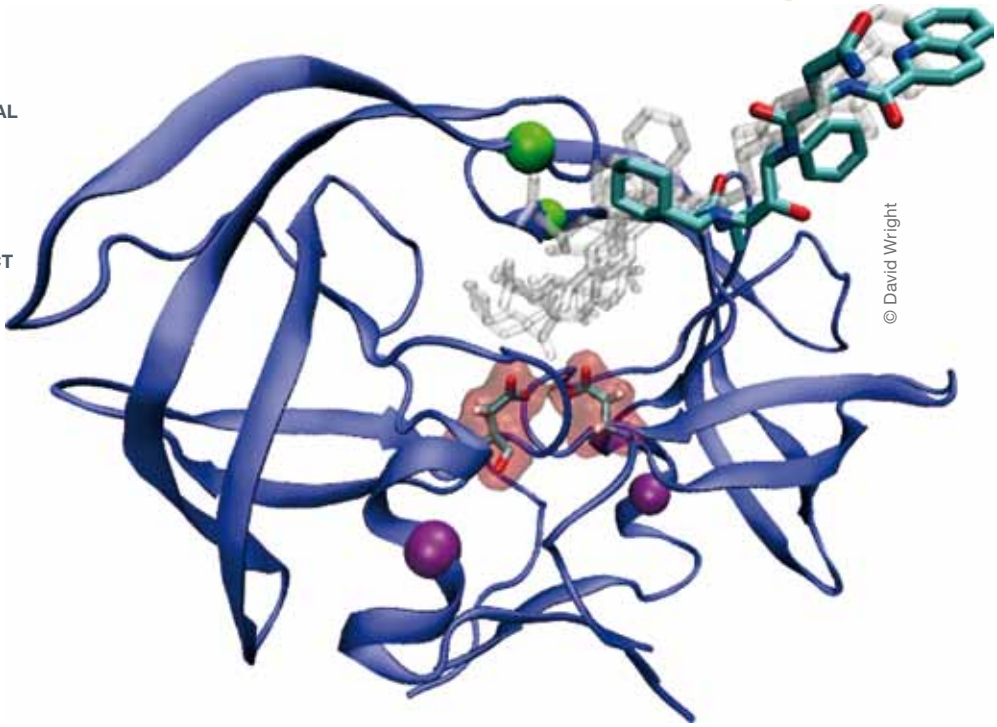
An own-developed code was used for the computations. This code, written in FORTRAN, makes use of the open-source libraries ScaLAPACK and BLACS for linear algebra operations, and MPI communications.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/GATUS

ViroLab enhances selection of HIV drugs

Tiina Autio

AIDS continues to be a major global health priority. University College London (UCL) is participating in a project to enhance existing HIV clinical software tools. The project has developed a virtual laboratory called ViroLab. This software supports doctors in their decision-making: they simply provide the viral sequence of the strain of HIV infecting their patient and receive the selection of drugs available to them. ViroLab has been trialled in six hospitals across Europe.



The inhibitor drug, saquinavir exiting the HIV-1 protease. In the crystal structure the drug is bound to the protease via the catalytic dyad (shown in red). Using steered molecular dynamics we are able to investigate the lateral exit pathway used by the drug. Mutations at position 48 and 90 (shown as green and purple spheres respectively) were seen to alter the ease with which the drug can use this exit pathway. The HIV-1 protease is the folded form in blue colour. The drug is marked with multi-colours in the top right. The trajectory followed by the drug is shown by the grey outlines.

In 2009 about 33.3 million people worldwide were living with HIV. The World Health Organization reported that 1.8 million people died due to AIDS in the same year. HIV undergoes mutations at a very rapid rate, which complicates the development of an effective vaccine.

The aim of the ViroLab project, which was started in 2006, is to enhance existing HIV clinical software tools. Tools available range from models of therapeutic drugs at the molecular level to models of the populations in which the disease spreads. The purpose of the project is to connect these models in the belief that the understanding gained will help to inform future clinical practice.

Effective software environment

”The major achievement of the project has been the virtual laboratory. ViroLab is the integrated software environment, which provides a unified interface to a wide range of different tools centred around the comparative drug ranking system including literature mining, an anonymised patient database and tools to run molecular dynamics simulations”, says researcher **David Wright** from University College London (UCL).

ViroLab automatically retrieves data from a variety of sources. The resistance interpretation rule sets are provided by the frequently used HIV drug resistance interpretation systems within the comparative drug ranking system: Rega, HIVdb and ANRS. Anonymised patient data is drawn from databases held at the participating hospitals. The literature is extracted from the US National Library of Medicine, Pubmed’s database of abstracts.

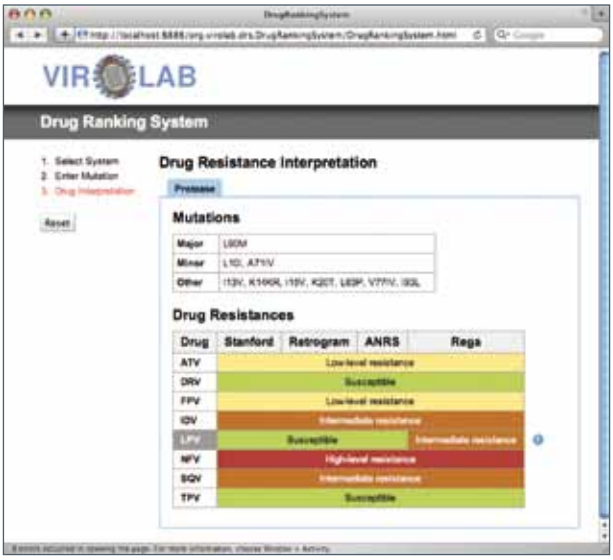
Recommendation of drugs

Researcher David Wright says that ViroLab is a useful tool for doctors whether a patient has just been diagnosed with HIV or has been infected for a long period of time.

”Doctors already routinely send samples of the virus infecting patients to be genotyped. The sequence that is returned to them is entered into clinical decision support systems, which produce recommendations on which drugs are likely to be effective against that particular strain”, Wright explains.

”The software provided by ViroLab enhances this existing system by incorporating multiple different assessment systems and showing the doctor the basis upon which each reaches their decision. It also provides integrated access to data from other individual patients with similar

The comparative drug ranking screen from the virtual laboratory software. ViroLab is an integrated software environment, which provides a unified interface to a wide range of different tools centred around the comparative drug ranking system. The software also allows the running of simulations based on the patient data.



"ViroLab is a useful tool for doctors whether a patient has just been diagnosed with HIV or has been infected for a long period of time."

sequences and their response to treatment", Wright adds.

In a rule based system a patient sequence is compared to a set of rules and the sequence flagged if certain mutations or groups of mutations are present. Depending on which rule causes the flagging, the sequence is assigned to one of three categories: susceptible, intermediately resistant or fully resistant.

"A simplified example rule might be that for the drug lopinavir, if the sequence contains alanine at position 82 and valine at position 84 then the sequence is deemed resistant. The real rules encode information based on the treatment outcomes of thousands of patients", Wright explains.

Modelling drug binding affinity

The UCL research group has recently published a study validating the Binding Affinity Calculator (BAC) tool for the case of lopinavir binding to a series of HIV protease mutants of increasing resistance. Following on from this they are now using BAC to investigate the sequence of a particular patient for whom the three different algorithms used in the comparative drug ranking system provided differing results.

"We found that the mutations considered by the decision support software do not induce any change in the strength of binding but that there was evidence that the full patient sequence exhibited intermediate levels of resistance", Wright says.

Researcher David Wright from UCL conducted molecular dynamics simulations as part of the virtual patient experiment. He is working to extend the protocol used to new targets such as the HIV reverse transcriptase.

"These results are meaningful as they suggest that molecular modelling can allow us to obtain quantitative assessment of the impact of HIV mutations on drug binding. By using simulations that provide atomic level insight into the system we can probe how resistance associated mutations interact with one another and cause changes in drug binding. This could then be used to assess the existing rules used to select drugs but also to inform future drug design", Wright adds. The BAC tool automates the full workflow of setting up patient specific models of the HIV protease, running molecular dynamics simulations and analysing the results.

ViroLab collaboration involves universities and hospitals throughout Europe as well as the Polish company, GridwiseTech. The prototype of ViroLab is available at *https://portal.virolab.org*

DEISA Resources:

Molecular dynamics simulations are generally computationally expensive and in order to gain the level of sampling needed to get reproducible results the research group required around 80,000 CPU hours for each sequence simulated. Researchers wish to be able to show that such simulations can be turned around on a timescale relevant to clinical applications. In order to obtain sufficient sampling from the molecular dynamics simulations the research group used the computing resources through DEISA at EPCC, in the United Kingdom, RZG and LRZ computing centres in Germany and Huygens supercomputer in the Netherlands. For each protease sequence that the research group studied they ran 50 independent simulations differing only in the initial conditions. Each run contained 6ns of simulation, with each nanosecond taking 4 hours to simulate on 64 cores. The submission of jobs to computers on the DEISA grid and data transfer between sites is orchestrated by a tool developed in the research group and called the Application Hosting Environment (AHE).

More information:
http://www.deisa.eu/science/deci/projects2008-2009/ALBECCIS

A prototype of ViroLab:
https://portal.virolab.org

S. K. Sadiq, D. W. Wright, O. A. Kenway, P. V. Coveney, "Accurate Ensemble Molecular Dynamics Binding Free Energy Ranking of Multidrug-Resistant HIV-1 Proteases", Journal of Chemical Information and Modeling, 50, 890-905, (2010), DOI: 10.1021/ci100007w.

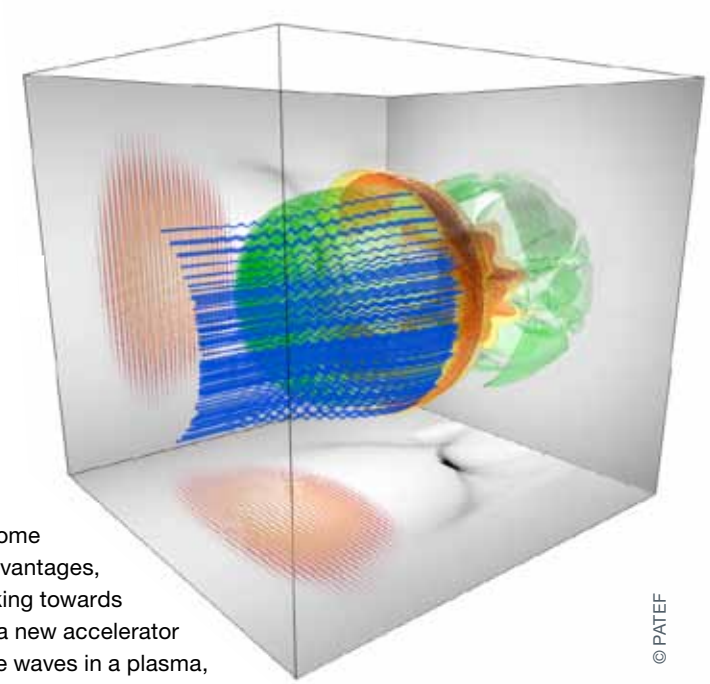
Laser plasma accelerators:

Powerful and compact

Nina Morgan

Nina Morgan

In hospitals and research labs, accelerators have a multitude of uses, but current accelerators are expensive. When researchers in the PATEF project were looking for extra computation resources to allow them to run simulations to help in the development of cheaper and more compact high energy plasma laser accelerators, they turned to DEISA.



© PATEF

The inhibitor drug, saquinavir exiting the HIV-1 protease. In the crystal structure the drug is bound to the protease via the catalytic dyad (shown in red). Using steered molecular dynamics we are able to investigate the lateral exit pathway used by the drug. Mutations at position 48 and 90 (shown as green and purple spheres respectively) were seen to alter the ease with which the drug can use this exit pathway. The HIV-1 protease is the folded form in blue colour. The drug is marked with multi-colours in the top right. The trajectory followed by the drug is shown by the grey outlines.

In applications ranging from fundamental physics to chemistry, biology, and materials science, high energy particle accelerators are an important tool in many different fields of science and technology. They have many medical applications too. In hospitals accelerators are also used to generate radiation, including x-rays and gamma rays to probe materials and tissues. They also play an important role in many cancer therapies where they generate the energetic particles used to kill cancer cells.

In particle accelerators very large electric fields are used to accelerate atomic particles to very high energies. When beams of accelerated particles collide, sub atomic particles are produced. In conventional accelerators microwaves propagating inside accelerator tubes are used to accelerate particles, but this approach has its drawbacks. For example, the size of the electric field is limited because of the properties of the metals the walls of conventional accelerators are made of. In addition, the accelerators themselves are large and very expensive. To overcome some of these disadvantages, researchers are looking towards the development of a new accelerator concept – one where waves in a plasma, or ionised gas, are used as an accelerating structure for electrons.

A new approach

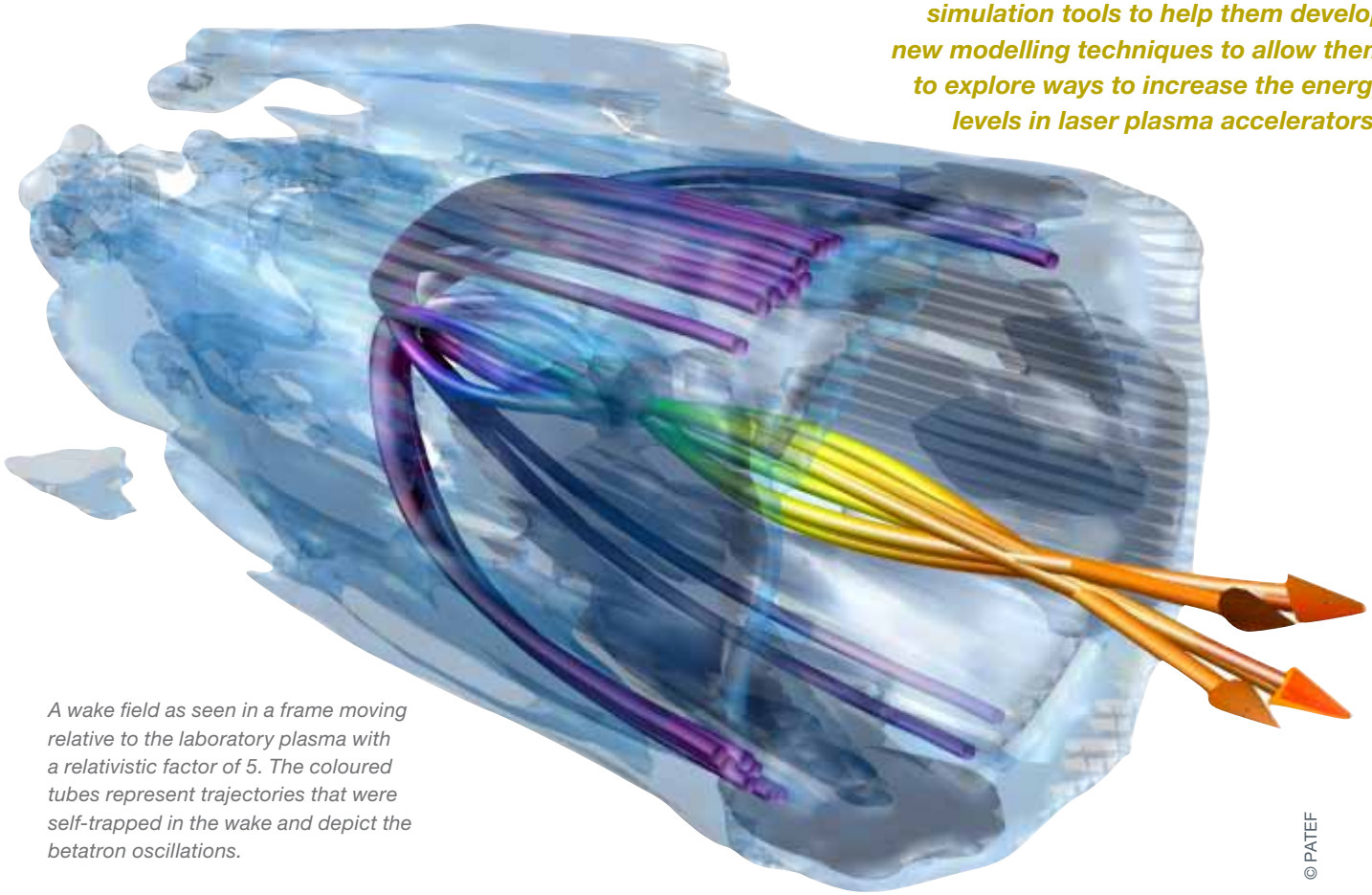
In laser plasma accelerators, also referred to as laser wakefield accelerators, an intense, short laser pulse is sent through a plasma to generate a wave wake.

"Particles 'surf' on this wake to reach very high energies," says Professor **Luis Silva** of Instituto Superior Técnico, Portugal, who worked on the PATEF project with colleagues from the University of California, in Los Angeles, US and STFC/Rutherford Appleton Laboratory in the UK.

"Because the electric field is determined by the density of the plasma, we can actually sustain as big an electric field as we want."

Laser plasma accelerators also have many convenient features, and as well as being more powerful than conventional accelerators, they are also cheaper and more compact. As a result, they could potentially be used for a

"Silva and his colleagues used a set of simulation tools to help them develop new modelling techniques to allow them to explore ways to increase the energy levels in laser plasma accelerators"



A wake field as seen in a frame moving relative to the laboratory plasma with a relativistic factor of 5. The coloured tubes represent trajectories that were self-trapped in the wake and depict the betatron oscillations.

much wider range of applications in, for example, hospitals. And because they are potentially so powerful they could also open up new avenues for fundamental scientific research, and might potentially contribute to the development of a future particle collider at very high energies or to a new light source.

Crucial contribution

Numerical simulations play a critical role in determining the optimal laser and plasma parameters. They also serve as an essential tool to explore new concepts and configurations. In the PATEF project, which began in 2009 and was completed in 2010, Silva and his colleagues used a set of simulation tools to help them develop new modelling techniques to allow them to explore ways to increase the energy levels in laser plasma accelerators.

"The new modelling techniques were essential," says Silva.

"It is very difficult to model the plasma accelerator system using standard techniques. Throughout our research this posed significant computational challenges. Carrying out a project like this requires a lot of computing time."

The 2 million CPU hours of computing time provided to PATEF by DEISA represents just the starting point and a fraction of the CPU hours the group used for the project.

"The DEISA contribution was crucial." The group have been awarded a further grant from the Partnership for Advanced Computing in Europe (PRACE) which will buy then a further 31 million hours of CPU time. The PATEF work has also generated proposals for two further projects that focus on different aspects of the original PATEF research.

"None of this would have been possible without the support we received from DEISA," says Silva.

"DEISA has helped to make it possible for us to become involved in more and more challenging projects." ■

DEISA Resources:

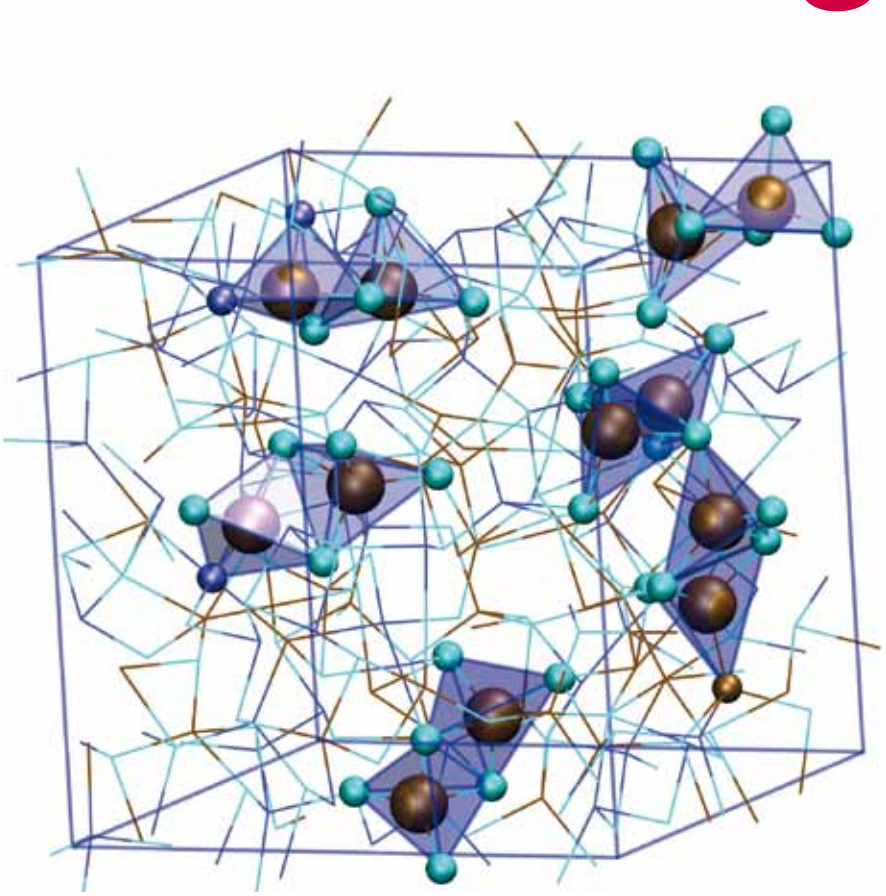
Computations on the PATEF project were performed on Jugene, at FZJ in Germany, with 10 production runs, running on approx. 10,000 CPU cores each, for a total of more than 1 million CPU hours. The simulations were performed with OSIRIS, a massivelly parallel particle-in-cell code, generating up to 100 GB of particle data and 1 TB of diagnostic files. The simulation data was analyzed with visXD, a home-grown visualization infrastructure for particle-in-cell simulations, on local dedicated visualization machines/small visualization clusters.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/PATEF

Nature Physics:
http://www.nature.com/nphys/journal/v6/n4/abs/nphys1538.html

Phase change memories enable better data storage

Tiina Autio



Marco Bernasconi from the University of Milano-Bicocca and Sebastiano Caravati, a member of Michele Parrinello's group at the Swiss Federal Institute of Technology Zurich (ETH) have studied the phase change memory properties of amorphous materials. Their simulations have provided a reliable microscopic description of the amorphous phase, which is the starting point for an atomistic description of all the functional properties of phase change materials. Phase change memory has a huge potential to change the architecture of non-volatile memories widespread in electronic devices and automotive systems.

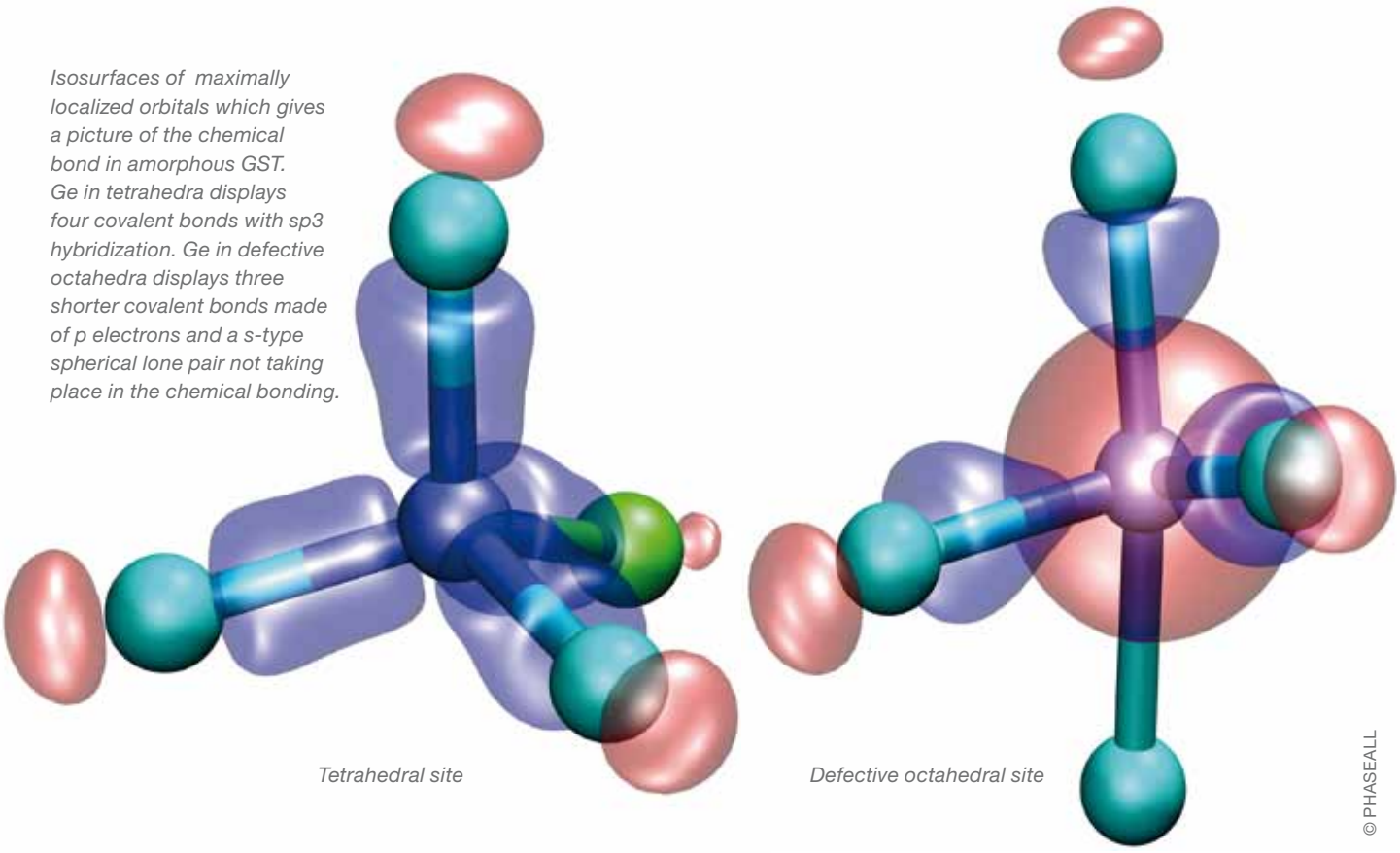
Professor **Marco Bernasconi** from the University of Milano-Biocca says that relentless advances in information technology rely largely on the availability of high-speed and large capacity memories. "In this segment, mainstream Flash technology based on silicon has demonstrated an unexpected longevity, driving for twenty years the non-volatile market and applications. Nowadays, however, it is clear that these devices are facing physical limits and compromises must be made on performance and reliability. In this scenario, alternative memory concepts are being widely studied and phase change memories (PCMs) are gaining wide acceptance as a leading, emerging non-volatile technology."

New memory architectures of the future

A phase change memory is essentially a resistor of a thin film of a tellurium (Te)-based alloy, which can easily change its phase from amorphous to crystalline and vice versa, when subjected to proper temperature variations. A similar principle can be found in optical storage media, such as rewritable CDs and DVDs, where two different phases are discriminated on the basis of their different optical reflectivity. "In phase change memories, instead, the two logical states, which correspond to crystalline and amorphous phase, are discriminated by their different electrical resistance, which changes by up to three order of magnitude across the phase change", Bernasconi explains. He adds that reading of phase change memory corresponds to a measure of resistance. "Programming the memory consists of heating up the chalcogenide alloy and inducing the phase change, either the melting of the crystal and subsequent amorphization or the recrystallization of the amorphous. Due to the high program speed (few tens of nanosecond), the superior cycling endurance and the low integration costs, phase change memory is regarded not only as competitor and

capacities

Isosurfaces of maximally localized orbitals which gives a picture of the chemical bond in amorphous GST. Ge in tetrahedra displays four covalent bonds with sp3 hybridization. Ge in defective octahedra displays three shorter covalent bonds made of p electrons and a s-type spherical lone pair not taking place in the chemical bonding.



Tetrahedral site

Defective octahedral site

potential replacement for Flash components, but also as an enabler of new memory architectures", Bernasconi notes.

"From the materials side, most of the industrial development has been made using the compound, Ge2Sb2Te5 (GST, including germanium, antimony and tellurium), which guarantees a 10-year data retention up to 85–105°C. Although the first commercial products based on this compound are expected within the next years, some consumer products and all automotive systems would require operating temperatures up to 125°C, beyond the reach of GST", Bernasconi explains. Specific examples of the application of non-volatile memories in automotive technology are engine control units and transmission control units. "Change in the composition of the alloy or doping of GST for instance with nitrogen are under scrutiny in most of the leading semiconductor companies", Bernasconi adds.

Microscopic description of the structure of the amorphous phase

Marco Bernasconi, **Sebastiano Caravati** and **Michele Parrinello** studied the structure of the amorphous phase of Ge2Sb2Te5 and related materials by means of ab-initio atomistic simulations. Models of the amorphous phase were generated by quenching from the liquid phase by means of ab-initio molecular dynamics. Large simulations cells (200–500 atoms) and long simulation time (100 ps) to cool the system slowly from the melt were needed to provide reliable models of the amorphous phase.

"The simulations have provided a microscopic description of the structure of the amorphous phase and of relations between the structure and the composition of the alloy. These results have made it possible to rationalise the experimental trends on the dependence of the crystallisation temperature, a crucial parameter for phase change memory operation, on alloy composition. We have also shed light on the microscopic origin of the changes in >

"The simulations have provided a reliable microscopic description of the amorphous phase which is the starting point for an atomistic description of all the functional properties of phase change materials."

reflectivity and conductivity across the phase change exploited, respectively, in DVDs and phase change memory", Bernasconi says.

Small defects in composition improve feasibility

"In the crystalline phases, atoms are in an octahedral environment bound to six neighboring atoms. The simulation revealed instead that the amorphous phase of phase change materials displays a coexistence of octahedral-like and tetrahedral-like environments", Bernasconi says.

He notes that also the octahedral-like environment differs from the crystalline one since atoms are under-coordinated with respect to the crystal; in the amorphous phase tellurium is bonded to three atoms, while antimony and germanium are bonded to four atoms. "We called these bonding geometries defective-octahedra (octahedral with neighboring vacancy sites). Most of the atoms are in defective octahedra, but a fraction of germanium (between twenty and thirty per cent) and most of indium (sixty per cent) are in the tetrahedral-like bonding geometry. For germanium, the tetrahedra are promoted by the presence of germanium-germanium and germanium-antimony bonds, which are not present in the crystal", Bernasconi explains.

"We also considered a small change in composition with respect to $Ge_2Sb_2Te_5$, i.e. deficiency or excess of germanium or antimony by at most ten per cent as in the $Ge_2Sb_{1.8}Te_5$ alloy. Small defects in stoichiometry are always present in these materials grown by deposition by different means. It turned out that while these defects in composition have dramatic effects on the electronic properties of the crystalline phase, they do not change the electronic properties of the amorphous. The crystal and the amorphous phases at perfect stoichiometry ($Ge_2Sb_2Te_5$) are actually semiconductors with a very similar band gap and low conductivity", Bernasconi says. However, a small deficiency in antimony or germanium turns the crystal into a degenerate p-type semiconductor with a very high conductivity while the amorphous is flexible enough to accommodate the defects in stoichiometry without changing its electronic properties. "We believe that this is one of the key features responsible for the large change in conductivity across the phase change exploited in a phase change memory device", Bernasconi says.

Tailoring the composition of the alloys

The simulations have provided a reliable microscopic description of the amorphous phase which is the starting point for an atomistic description of all the functional properties of phase change materials. "The availability of a model of the amorphous phase already allowed us to confirm the idea put forward very recently to explain the large change in optical reflectivity between the amorphous and crystalline phases which is a rather peculiar feature of materials in this class exploited in DVDs. Moreover, the outcome of the simulations suggests a possible strategy to tailor the composition of the alloys in order to increase the crystallization temperature, namely to introduce species suitable to display a tetrahedral environment (germanium or indium) and to increase the concentration of wrong bonds (germanium-germanium or germanium-antimony), for instance by moving off the pseudobinary line", Bernasconi notes. ■

DEISA Resources:

The Phaseall project was run on the Cray XT4 and Cray XT5 at CSC- IT Centre for Science in Finland. Sixty-four cores were used mostly with a maxium memory of 1.5 Gbyte per core. A typical single run took 500 core-hours. Two million core-hours were used in total.

"We used ab-initio molecular dynamics simulations in which one generates the trajectory of the ions by solving numerically the Newton equation of motion. The forces acting on the ions are obtained in turn by solving the quantum-mechanical problem for the electrons (the Schroedinger equation) at each configuration of the ions within the so called Born-Oppenheimer approximation which assumes that the electrons are at the ground state for each ionic configuration", Bernasconi explains. This is achieved within a well established framework for electronic structure calculations, the Density Functional Theory. "The method is ab-initio since it is based on the solution of the basic equation of physics without making use of any experimental information but for the chemical composition of the system we are interested in. We used the code QUICKSTEP, part of the open source project CP2K (*http://cp2k.berlios.de*)", Bernasconi says.

"In particular, we also made use of a new scheme for ab-initio molecular dynamics (T. Kühne et al., Phys. Rev. Lett. 98, 066401 (2007)) which is based on a predictor-corrector extrapolation of the electronic wavefunctions which allowed reducing the computational cost of the simulation of 200/300-atoms supercells by a factor of thirty with respect to traditional methods", Bernasconi says.

More information

http://www.deisa.eu/science/deci/projects2008-2009/PHASEALL

R. Mazzarello, S. Caravati, S. Angioletti-Uberti, M. Bernasconi, and M. Parrinello, Signature of tetrahedral Ge in the Raman spectrum of phase change materials, Phys. Rev. Lett. 104, 085503 (2010); DOI: 10.1103/PhysRevLett.104.085503.

New possibilities for exploring the history of the universe

Dark matter simulations predict missing galaxies

Pirjo Rötkönen

Simulations of the universe produce a lot of substructures in large galaxy clusters but observations do not find as many. This problem can now be investigated after the simulations.

Galaxies accumulate from small clumps of dark matter which grow by subsequent mergers to large galaxies. Each large galaxy is then accompanied by a number of smaller unmerged dark matter clumps in its halo. These small clumps are generally associated with the dwarf galaxies observed in the halos of all major galaxies. Cosmological simulations of dark-matter halos predict about a thousand dwarf galaxies, but the Milky-way galaxy has only 24 dwarf galaxies. This discrepancy is the missing dwarf galaxy problem. By means of simulations a better understanding of the evolution and distribution of dark matter and dark energy can be obtained. The computer simulation performed in the Gravitational Billion Body Project (GBBB) was the highest-resolution dark-matter simulation ever conducted.

According to Professor **Simon Portegies** Zwart of the University of Leiden, the resolution of the simulation is so high that it opens up new possibilities for exploring the history of the universe and the origins of merging histories of galaxies.

"With these simulations we expect to obtain a better understanding of the evolution and distribution of dark matter and dark energy. Together they comprise more than 98 percent of the universe whereas the stuff we are made of is only about 2 percent. All we know at the moment is that dark matter is gravitationally attractive, like black holes, and that it does not interact with visible matter via light or other electromagnetic radiation. This is why it is called dark matter."

"We still have at least two years to go with analyzing the data and improving our understanding of dark matter of the universe. In the meantime we will apply for new computer time to follow-up and to pinpoint studies of particularly interesting areas of the calculation."

Four computers instead of two

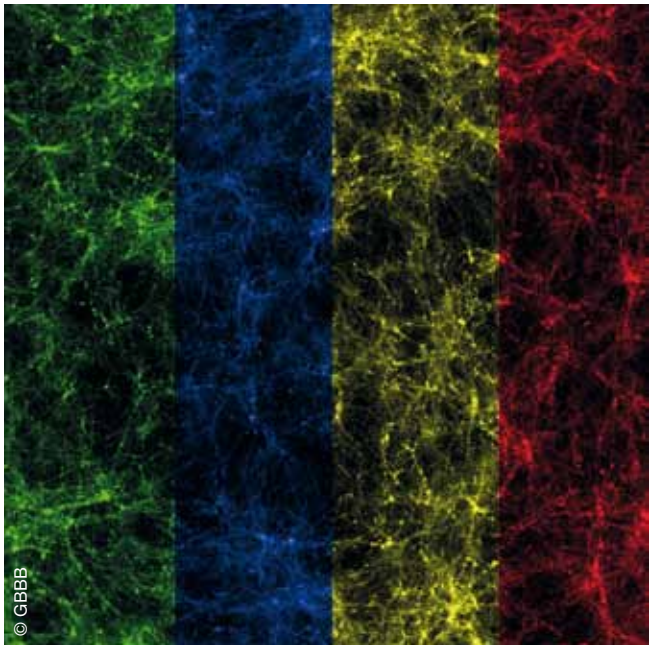
Three years ago four researchers – **Steve McMillan**, **Halden Cohn**, **Jun Makino** and Simon Portegies Zwart – met at Princeton IAS. Professor Simon Portegies Zwart of the University of Leiden explains: "We had access to two brand new supercomputers – one in the Netherlands and the other in Japan. We wanted to find out how to perform one calculation on two computers concurrently, and how to store the data on the other side of the globe. Our storage facility was in Bloomington, Indiana, USA."

"We came up with the idea of running a large-scale cosmological simulation to solve a cosmologic problem called the missing dwarf galaxy," Professor Portegies Zwart continues.

"We believed that large-scale simulations would enable us to find the solution if we did not concentrate on promising structures, but instead simulated a large cosmological volume in one go."

This is where DEISA came in.

"We got the resources to run this simulation on four supercomputers concurrently. It was our Gravitational Billion Body Project or GBBP. Many people thought I was crazy."



The various colored slabs give the parts of space that was computed on the different computers.

"The resolution of the simulation in GBBP-project is so high that it opens up new possibilities for exploring the history of the universe and the origins of merging histories of galaxies," says Professor Simon Portegies Zwart. Cold Dark Matter simulations are widely used to test cosmological predictions, because the Cosmological Dark Matter model has proven to be more successful than any other cosmological model. According to this model, halos (in which galaxies form) originate by accumulating small clumps of dark matter. Subsequent mergers between such clumps in turn form large halos. Clumps do not necessarily merge, however. Many small conglomerates survive the aggrandizing conditions inside a galaxy halo. The surviving clumps are often associated with the dwarf galaxies observed in the halos of major galaxies.

The four supercomputers were spread across two continents, three in Europe and one in Japan.

"It turned out to be a lot of fun to run the simulations concurrently and we demonstrated that it is feasible and even quite efficient," says Portegies Zwart.

100 terabytes of simulation data

The project produced more than 100 terabytes of simulation data, which are now being analyzed.

"Before you start to analyze all the data, you have to perform statistical and consistency studies to establish whether the results are consistent, and to find how much they deviate from earlier published results. We have to be sure

that we have not made mistakes. These tests have now been completed and we have reached the level of really recovering new science from the data."

"DEISA allowed us to run four supercomputers concurrently, a challenging enough task. Without the resources of DEISA this kind of simulation would not have been possible. The total amount of supercomputing power was equivalent to running four computers continuously for four months."

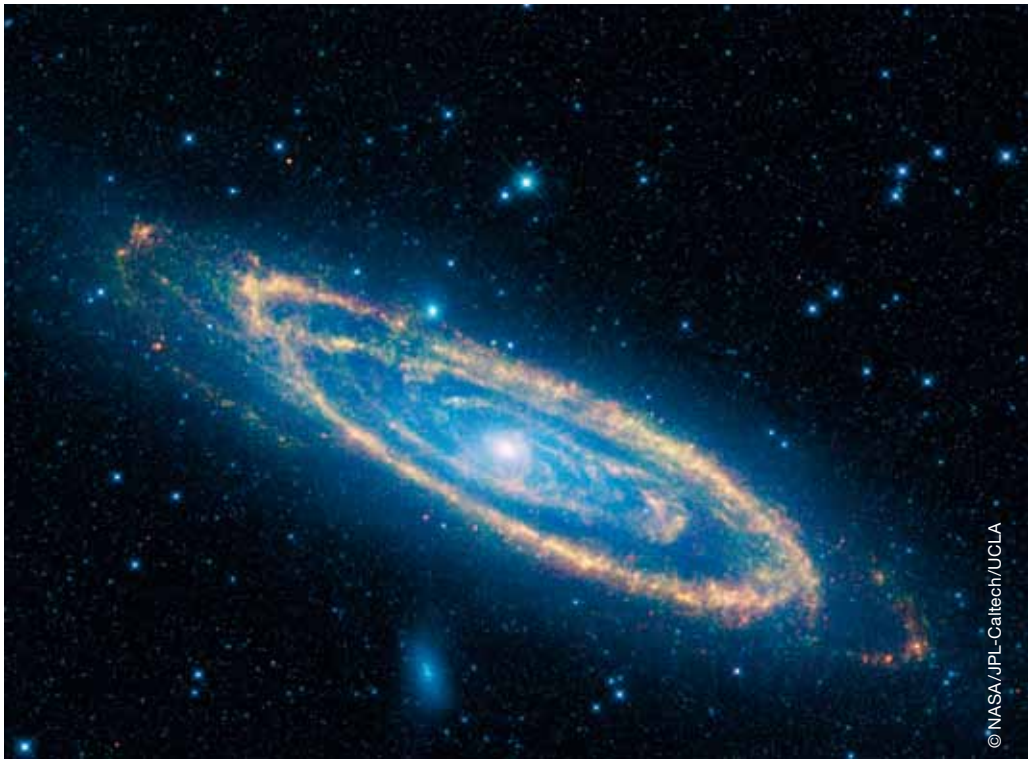
The research group studied in particular the final snapshot of their cosmological simulation. Nevertheless the unprecedented time resolution allows them to also study the formation and history of individual dwarf galaxies.

"In previous large scale simulations to study the missing dwarf-problem, there were usually two steps. The first step consisted of a large simulated volume with a relatively low mass-resolution. A specific part of the first simulation was then hand-selected for a rerun at higher resolution."

In the GBBB project simulations were sufficiently large, in volume, and sufficiently detailed, in terms of mass-resolution. Thus the research group does not have to hand-pick any structures but can perform an unbiased statistical study of the mass distribution of the dwarf galaxies.

"It turns out that the spread of the mass distributions varies over more than an order of magnitude from galaxy to galaxy. The selection of one particular galaxy cluster to study its substructure in more detail is therefore affected by the way in which the galaxy cluster was selected. Due to the large volume and high resolution of our simulation it is not necessary to make such a selection. It turned out that the amount of substructure in the massive galaxy halos depends on the environment of the halo, and therewith provides an elegant solution to the missing dwarf galaxy problem."

"At the moment we are further analyzing the data that was produced in the simulation. In the coming years we expect to study various aspects of merging halo morphologies and the history of the growth of void galaxies." ■



*Andromeda galaxy. The **dwarf galaxy problem** is one that arises from numerical cosmological simulations that predict the evolution of the distribution of matter in the universe. Dark matter seems to cluster hierarchically and in ever increasing number counts for smaller and smaller sized halos. However, while there seems to be enough observed normal-sized galaxies to account for this distribution, the number of dwarf galaxies is orders of magnitude lower than expected from simulation.*
The local group of galaxies, of which the Milky Way and Andromeda are the two largest galaxies, exhibits some 30 smaller satellite galaxies. According to Simon Portegies Zwart the conglomerates that mimic the local group in cosmological dark matter simulations generally exhibit many hundreds of smaller structures; a discrepancy with the observations of more than a factor 100.

Professor Simon Portegies Zwart at the University of Leiden is the Principal Investigator of the GBBP project.

DEISA Resources:

The calculations were performed on the supercomputers at Cray XT4 at the Center for Computational Astrophysics of National Astronomical Observatory of Japan and the national academic supercomputer centre SARA in Amsterdam, the Netherlands, Cray XT4 at CSC – IT Center for Science in Espoo, Finland and HECToR at EPCC in Edinburgh, Scotland.

For more information:
http://www.deisa.eu/science/deci/projects2008-2009/GBBP

Adsorption energy of water on carbon surfaces

Tiina Autio

The chemical interaction of water with carbon is an essential topic for science and technology. Professors Dario Alfè and Angelos Michaelides from University College London have researched the bond between water and carbon by simulating water on graphene using the quantum Monte Carlo method. The research showed that water binds weakly to graphene and isolated water undergoes ultrafast diffusion on the graphene surface.

Water covers the majority of Earth`s surface and is present in liquid, solid and gaseous forms. On the other hand, carbon is one of the most widely used elements in many fields of industry and research. Wherever carbon is used outdoors or in biological media, it interacts with water. In this context it is obvious that the water-carbon interaction and its strength are studied more precisely.

Research interests of Professor Dario Alfè at University College London are the Earth's core, surface catalysis and Quantum Monte Carlo method.

Professor **Dario Alfè** from the University College London says that the interaction of water with graphite, for example, is of relevance on earth to lubrication phenomena and emerging nanotechnologies, and in outer space to reactions in the interstellar medium. "It is important to understand the properties and function of carbon nanotubes in biological media. In particular, it is not established if these tubes fill with water or not, which would give them very different properties when immersed in water and when in contact with

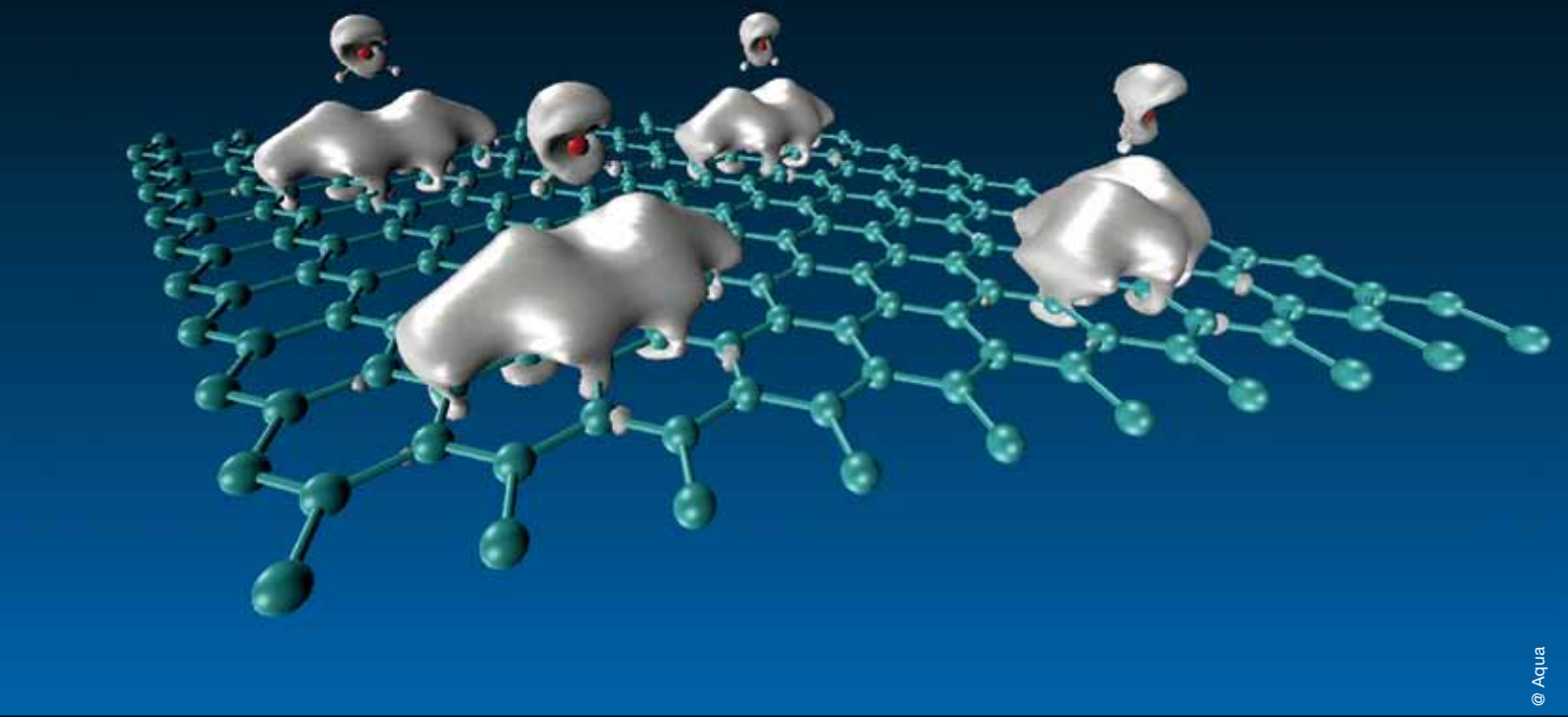
biological tissue. It all depends on the strength of the interaction between water and the graphitic surface."

He adds that establishing reliable adsorption energies for water monomers with carbon surfaces, and solid surfaces in general, is a major challenge for both experiment and theory. "Experiment is stymied because water forms clusters. Theory finds it difficult because water interacts with materials via dispersion (van der Waals, vdW) and hydrogen bonding. These are interactions which density functional theory (DFT), the most widely used electronic structure theory, does not normally describe with high enough precision", Alfè notes. He says that in previous studies about the subject water on graphite or graphene has been used as a model system with which to benchmark the water-carbon bond strength. "Generally, fused benzene rings (a finite cluster model) have been adopted, enabling the application of explicitly correlated quantum chemistry approaches. Adsorption energies from these approaches range from 100 meV to more than 200 meV, with the most recent values being about 130 to 140 meV. However, none of these calculations apply to truly extended models for graphene and hence a priori neglect correlation contributions from the bands close to the Dirac point", Alfè says.

Weak binding energies

Professors Dario Alfè and A**ngelos Michaelides** researched the bond between water and carbon with a parameter free quantum Monte Carlo simulations for water on graphene. The simulations were carried out with the parallel code CASINO leading to the first reliable theoretical estimates of the strength of the bond between water and two forms of carbon.

"We found that water binds to



The image shows how electrons rearrange when four water molecules bind with a sheet of graphene

© Aqua

graphene rather weakly, with a binding energy between 70 and 95 meV. The research also showed that on graphene an isolated water molecule undergoes ultrafast diffusion, one order of magnitude faster than the typical diffusion in bulk water. This explains why it is so difficult to perform experiments on this system: the ultrafast diffusion means that water molecules travel quickly on the surface and when they meet they stick together. Therefore experiments will always deal with water clusters rather then isolated water molecules", Alfè says.

Quantum Monte Carlo as a method

Researchers used the quantum Monte Carlo method (QMC), which can be seen as a stochastic method to solve the Schroedinger equation of the system, and in principle it is able to provide the exact ground state. "Although exact in principle, this method is not exact in practice as it requires two main approximations to be run. These approximations are known as the fixed nodes and the pseudopotential approximation. However, it has been demonstrated that the quantum Monte Carlo method can deliver results of very high accuracy, much more accurate than any density functional theory available", Alfè says.

Professor Angelos Michaelides' research interests involve water, surface chemistry and catalysis.

"In particular, we showed that for a similar system, namely water adsorbed on benzene, the quantum Monte Carlo method could deliver binding energies accurate to within only ~ 3 meV, which is ten times better than so called "chemical accuracy", the precision needed to make useful predictions for systems at ambient conditions. High accuracy comes with a cost though, which is about four orders of magnitudes more expensive than the density functional theory. This is the reason resources like those provided by DEISA are needed", Alfè explains. ■

DEISA Resources:

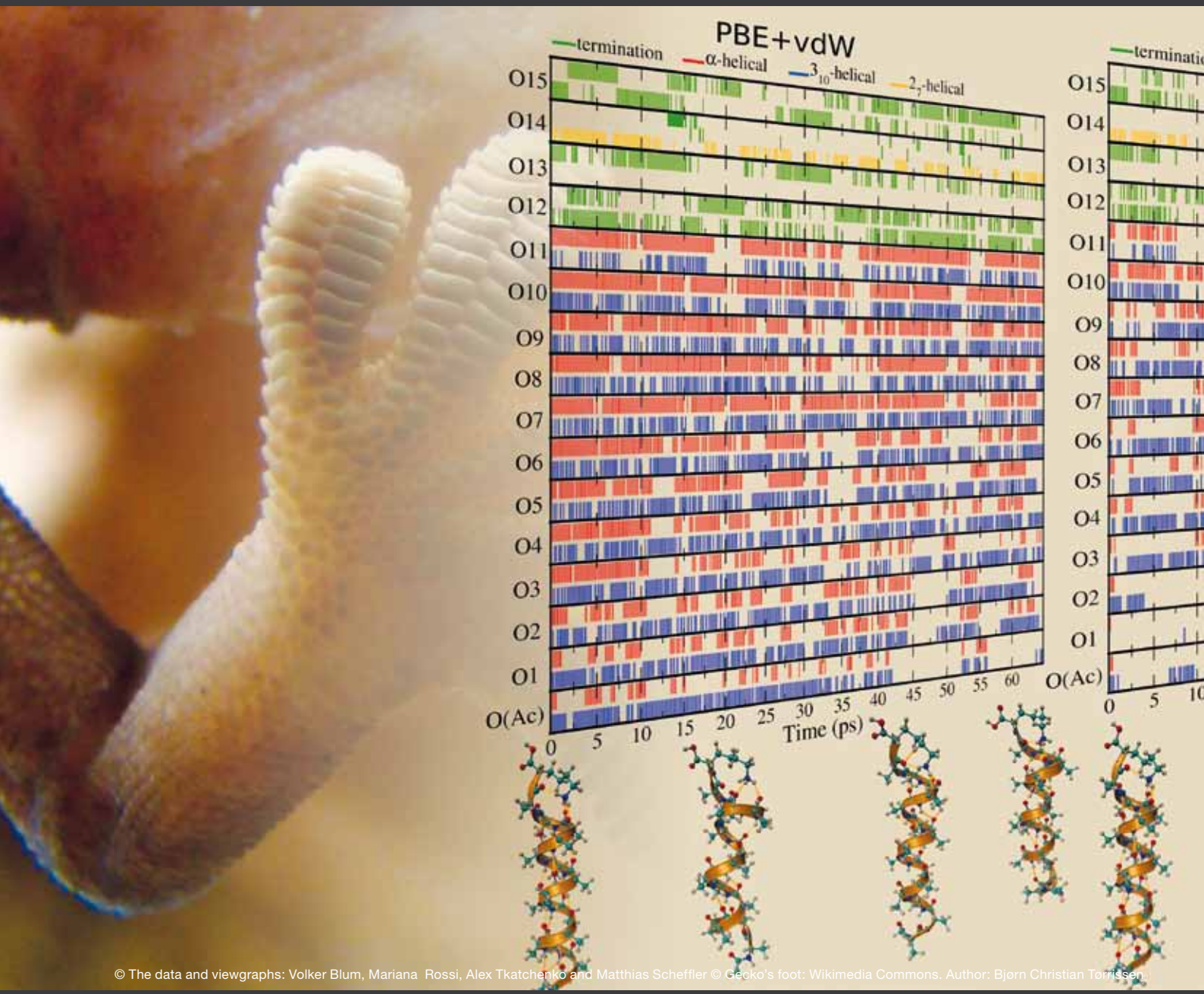
The researchers used 1.7 million CPU hours for their Aqua project. The research was run on the Cray XT4/XT5 supercomputer at the CSC – IT centre for Science in Finland.

For more information:
J. Ma, A. Michaelides, D. Alfè, L. Schimka, G. Kresse, E. Wang, Towards a reliable first principles description of water on graphene: Adsorption and diffusion, submitted

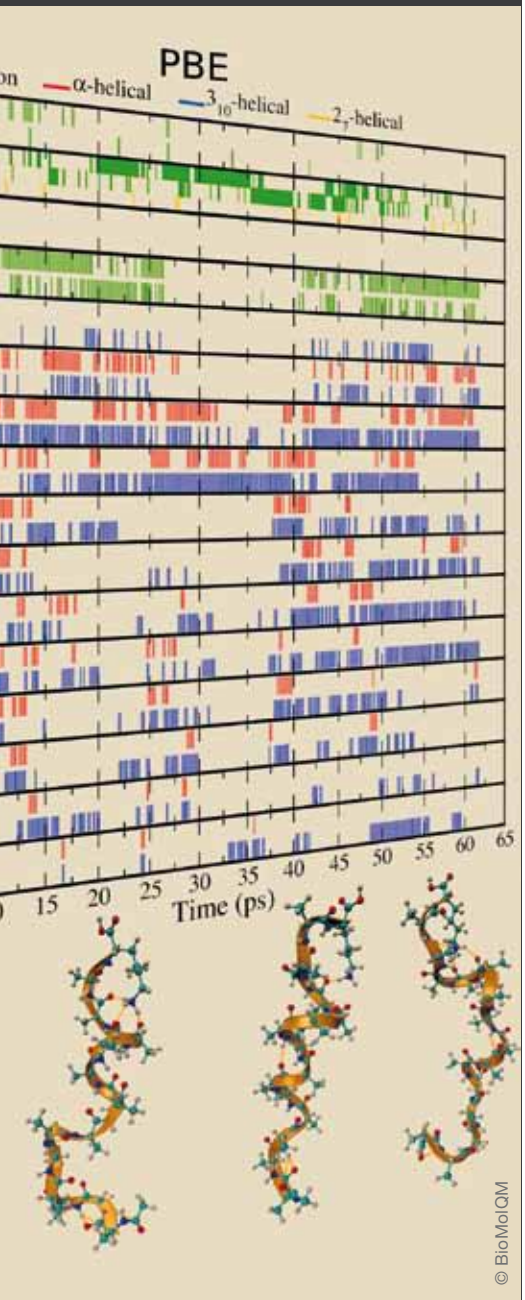
http://www.deisa.eu/science/deci/projects2008-2009/AQUA/

How a “weak” interaction shapes the structure of peptides

Tiina Autio



Mariana Rossi, Alex Tkatchenko, Volker Blum and Matthias Scheffler from the Fritz Haber Institute (FHI) of the Max Planck Society have investigated the structure and unfolding dynamics of polypeptides by direct quantum mechanical simulations. Their research shows how strongly the proper inclusion of so-called "weak" van der Waals (vdW) type intramolecular interactions changes the conformational landscape of polypeptides.



Folding and unfolding processes play an important role in the function of proteins, which consist of amino acid chains of various lengths. Short amino acid sequences (some tens) are called (poly)peptides. Citing an often used example, the FHI research group notes that if a protein folds into a non-native conformation and this misfolded form is replicated over and over again, diseases such as mad cow disease and some forms of diabetes can result – and that understanding the structure and dynamics of proteins could lead to a better understanding of these diseases.

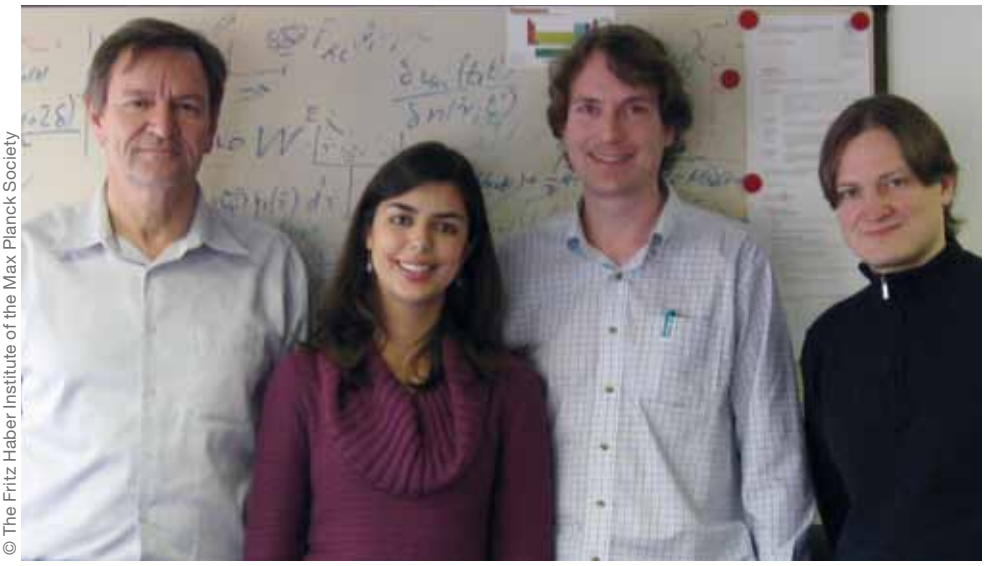
The amino acid sequence formally defines a given protein, but the actual three-dimensional structure and function of a protein is the result of a complicated interplay of many variables – including both environment variables and those intrinsic to the molecule itself. According to the research group, in principle, the underlying mathematical theory determining any chemical system, including the structure of proteins, is well known: quantum mechanics as embodied in the Schrödinger equation is often referred to as the scientific "first principles" on which our understanding of the chemical bond is founded. The research group attempted to extend the reach of this 'first-principles' accuracy to a peptide of a meaningful size (16 amino acids) with present methods.

In any practical treatment of Schrödinger's equation for real molecules, approximations must be made. The particular method used by the group to reach the necessary system sizes and times for molecular dynamics is known as density functional theory. The crux is that density functional theory as it is normally employed provides very good accuracy for bonded structures, but fails altogether to capture a weak, distant (non-local) class of interactions within molecules. These intramolecular forces are known as van der Waals (vdW) dispersion forces.

To achieve the necessary accuracy, the group included a carefully benchmarked correction for vdW interactions into its first-principles molecular dynamics simulations. "Inclusion of van der Waals interactions is essential – if there were no van der Waals interactions in the world, the structure formed by any peptide or protein could be completely different from what it is in reality. This would in turn change the function of the peptide or protein fundamentally", the group says. A direct comparison to gas-phase experiments by other groups confirms the need for this correction.

"We picked a series of peptide molecules for which a very good model for the structure exists. Gas phase experiments are the basis for this model, i.e., the molecule is essentially completely isolated. These experiments provide an ideal reference to which theory can connect", the group says. "Our attempt was to probe the structure and stability of the helical secondary structure in peptides, specifically a polyalanine peptide called Ac-Ala_{15}-$LysH^+$, by direct simulations with the full accuracy of a first principles calculation. A particular goal was to examine the various interaction contributions such as the Hydrogen bond strength with peptide length, the role of the termination and van der Waals interactions. This helix is known to be stable in a vacuum up to temperatures of ~700 K, far above the normal, biological stability range. Verifying this remarkable stability was one of our primary questions". >

A gecko hanging on to a pane of glass with the detailed "hydrogen bond patterns" that emerge from some of our simulations, with and without van der Waals. Van der Waals forces are ubiquitous in nature. Although often called "weak" in a chemical sense (covalent or ionic bonds are individually much stronger, for example), the combined effect of van der Waals interactions in biology can be significant. One of the most striking examples in popular science is the ability of a Gecko's foot to attach to a pane of glass. At the molecular scale, the group has demonstrated that a proper account of van der Waals interactions is essential for the formation of so-called "secondary structure" in peptide and protein molecules. Here, also, other interactions (hydrogen bonds or electrostatics) are often thought to constitute the main forces that stabilize the structure. However, the helical structure known from experiment for the molecule shown (Ac-Ala_{15}-$LysH^+$) is stable in theory over a few tens of picoseconds only if vdW interactions are properly accounted for, but not otherwise. The plots visualize the type of hydrogen bond formed during our simulations, separate for each C-O group in the peptide residue [O(Ac)-O(15)].



Matthias Scheffler (left) works as a director and Volker Blum as a group leader at the Fritz Haber Institute of the Max Planck Society. Mariana Rossi did the simulations as a part of her PhD thesis. Alex Tkatchenko (right) is a postdoc and expert on the van der Waals methodology used by the research group.

“Van der Waals interactions are crucial for the weak interlayer binding in graphite, and they can be influential in protein–protein and drug–protein binding inside our bodies. However, their role in protein secondary structure has not been fully established. Our work clearly demonstrates that “weak” interactions are even more ubiquitous than is generally appreciated.”

Weak interactions stabilize the structure of peptides

The study of the research group revealed the remarkably influential role that van der Waals interactions play as intramolecular forces stabilizing the structure of the investigated peptide up to the extreme temperatures observed in experiments.

“By using state-of-the-art electronic structure calculations on cutting edge supercomputers, we show that the extreme thermal stability of gas-phase peptides stems from the so-called “weak” van der Waals (vdW) interactions.

Van der Waals interactions are crucial for the weak interlayer binding in graphite, and they can be influential in protein–protein and drug–protein binding inside our bodies”, the group explains. However, their role in protein secondary structure has not been fully established. “Our work clearly demonstrates that “weak” vdW interactions are even more ubiquitous than is generally appreciated”, the group says.

“What is remarkable is that we could not only verify and quantify the impact of intramolecular van der Waals interactions for protein structure stability indirectly, by static benchmark calculations. We were also able to verify and visualize the impact of van der Waals interactions directly in first-principles molecular dynamics. On a time scale of ~50 ps in multiple, temperature dependent molecular dynamics simulations across several temperatures, we could show directly how the secondary structure is stable up to ~700 K when vdW interactions are appropriately included. In contrast, the same secondary structure clearly falls apart on the same short time scale when the standard theory neglecting van der Waals was applied”, the group explains.

The group’s present calculations show that it is possible to realize the potential of treating such molecules with the accuracy of quantum-mechanical “first principles” if all the relevant interactions are included. By considering van der Waals forces in the density-functional theory they were able to perform direct first-principles simulations of the structure and dynamics of peptides with several hundred atoms with an essentially converged energy landscape.

”The theory used by us is a parameter free way to describe the structure and structure changes of any molecule. If the environment is treated correctly and with sufficient computer power, this can lead to a reliable “screening” of molecules for many purposes, including medication. The same exact theory covers almost all materials and molecules known to us with great accuracy, and allows materials predictions as well as understanding”, the group notes. ■

DEISA Resources:

The researchers used altogether 3 000 000 computational hours on their Deisa project named BioMolQM. The simulations were run with the following supercomputers: Huygens at SARA in the Netherlands, Vip at the Rechenzentrum Garching (RZG) of the Max Planck Society and the IPP in Germany, HECToR at EPCC in the United Kingdom, Louhi at CSC – the IT Center for Science in Finland and HLRB at the LRZ computer centre in Germany. Approximately 500 individual runs were made.

http://www.deisa.eu/science/deci/projects2008-2009/BioMolQM

DEISA services and DECI to be continued in PRACE

- **PRACE, the Partnership for Advanced Computing in Europe, is a unique persistent pan-European Research Infrastructure (RI) for High Performance Computing (HPC).**
- **The PRACE RI is governed by an international non-profit association with its seat in Brussels. Twenty countries are presently members of the association 'Partnership for Advanced Computing in Europe AISBL'.**
- **Find more information about how to apply for resources at: www.prace-ri.eu/hpc-access.**
- **Access to the RI is open to researchers from recognized European academic institutions and industry for projects of merit based on peer-review governed by a PRACE Scientific Council.**

www.prace-ri.eu

The preparation and implementation of the PRACE RI receive EC funding under grants RI-211528 and FP7-261557.

Distributed European Infrastructure for Supercomputing Applications

DEISA

DEI SA IS A CONSORTIUM OF LEADING NATIONAL SUPERCOMPUTING CENTRES THAT OPERATES A PRODUCTION QUALITY, DISTRIBUTED SUPERCOMPUTING 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.

WWW.DEISA.EU

e-infrastructure

The DEISA Consortium receives funding from the European Community's Seventh Framework Programme (FP7) under the grant agreement n° RI-222919.