Mass spectrometry uses molecules in the gas phase to analyse, for example, the structure and composition of substances. In this process, oligonucleotides, the building blocks of DNA, change their structure as shown by simulations on the JUQUEEN supercomputer.

**Surprising Discovery:**

**Transposition in Building Blocks of DNA**

Belgian and Spanish researchers came up with very intriguing results. They had been using mass spectrometry and classical computer simulations to investigate the building blocks of DNA, so-called oligonucleotides. Surprisingly, the results were not in agreement. The puzzle could only be solved by ab initio molecular dynamics simulations performed on the JUQUEEN supercomputer by a team from their partners at Jülich headed by Prof. Paolo Carloni from Computational Biomedicine. Such simulations have the advantage that they do not just investigate the structure and dynamics of a system but also chemical processes on the atomic level. It turned out that in the gas phase hydrogen atoms swap places within a fraction of a second.

This discovery was a great surprise. In mass spectrometry, molecules are transferred from an aqueous solution to the gas phase. Previous studies had always shown that the results from the gas phase can be readily applied to aqueous conditions – that is to say to the conditions found in real living systems. “The results of such investigations will be examined more critically in future and changes such as those taking place with oligonucleotides will no longer be ruled out categorically,” says Jülich scientist Dr. Jens Dreyer.

The work performed by Carloni’s group shows that supercomputers such as JUQUEEN are also starting to play a major role in molecular biology. “Molecular dynamics is a good example. The continuously increasing performance of supercomputers opens up improved opportunities for us to use this method to face the grand challenges in biomedicine,” explains Paolo Carloni. Ab initio molecular dynamics uses quantum mechanical calculations making it possible to simulate the complex interaction of atoms and molecules even more precisely. In this way, researchers can derive even better structural information and physical parameters from the simulations, as in the case of the oligonucleotides. However, to describe these complex phenomena, these simulations require a tremendous amount of computing capacity. In total, the project required 11 million processor hours.

Angewandte Chemie, http://dx.doi.org/10.1002/anie.201406910
Expertise Combined in New Centre

IBM, NVIDIA, and Forschungszentrum Jülich have set up a new competency centre: the POWER Acceleration and Design Center. It offers scientists and engineers support in performing simulation calculations on OpenPOWER-compatible systems with GPU accelerators. “The POWER Acceleration and Design Center will help scientists and engineers to address the grand challenges facing society in the fields of energy and environment, information, and health using the most advanced HPC architectures and technologies,” explains Prof. Thomas Lippert, director of the Jülich Supercomputing Centre.

The three partners want to improve the programming, porting, and optimization of scientific codes, to develop new software solutions, and promote the configuration of a new supercomputer architecture. This work is part of the collaboration fostered by the OpenPOWER Foundation set up in 2013, which involves more than 70 companies and research establishments. The Foundation champions the use of open technologies for the POWER architecture developed by the IT corporation IBM to enable innovative hardware and software solutions for computer centres. Chip manufacturer NVIDIA contributes its GPUs to this endeavour.

The Jülich Supercomputing Centre already cooperates with both partners on different levels – for example, with IBM in the Exascale Innovation Center, which is developing new solutions for the future exascale class, and with NVIDIA in the NVIDIA Application Lab.

First Non-American to Chair SC

In 2017, the most important conference for high-performance computing (HPC), networking, storage, and analysis – the Supercomputing Conference (SC) in the USA – will be chaired by a non-American for the first time ever. The SC Steering Committee elected Jülich scientist Dr. Bernd Mohr as General Chair of the SC17 in Denver. Not long after the announcement, the portal HPCwire listed Mohr as one of the people to watch in 2015.

Established in 1988, the annual SC conference attracts scientists and users from all over the world who come together to discuss current developments. More than 10,000 people now participate in SC each year. The conference is sponsored by the Association for Computing Machinery (ACM) and the Institute of Electrical and Electronics Engineers (IEEE). In order to be elected General Chair, candidates go through a multistage application procedure. Colleagues persuaded Bernd Mohr to throw his hat into the ring. “I didn’t really think I’d have a chance. In the end, when the mail came announcing the decision, all I thought was: unbelievable!” says the researcher from the Application Support division of the Jülich Supercomputing Centre.

Why does he want to take on such a mammoth task? “I like organizing things,” he says quite simply. He has previous experience in helping to organize SC, most recently serving as a member of the SC Steering Committee. The fact that the open and communicative researcher doesn’t mind speaking in front of thousands of people is immediately obvious. He is also known for his ability to make good contacts. He has particularly close connections in the USA dating back to his research stay of several years in the mid-1990s. “I got to know many people back then who have gone on to make a significant impact on our field,” he says.

Now, it’s time to build on these personal networks. After all, work for SC17 is already well under way. One of the most important tasks is putting together his core team, around which some 500 volunteers will gather in the coming months. He’s also started to think about fine-tuning the topics for 2017: “An even stronger international focus and linking HPC more closely to topics such as big data analytics and visualization are two potential directions.”

The most important conference for high-performance computing, networks, storage, and analysis will be chaired by JSC expert Bernd Mohr in 2017.

www.hpcwire.com/people-watch-2015/
How Small Dust Clumps Turn into Planets

A star is rarely alone. In the vicinity of a star, debris left over from its birth leads to the formation of planets, so to speak. Science has not yet been able to completely solve the puzzle of how this actually happens. Researchers from the Max Planck Institute for Astronomy intend to use simulations on the Jülich supercomputer JUQUEEN to find out more about these planetesimals - the precursors and building blocks of planets.

When a star like our Sun is born, a disc of gas and dust is always also formed around it. In the course of millions of years, matter collides and sticks together in this disc leading first to clumps a few centimetres in size and later to bodies measuring several kilometres. There is, however, one problem. Scientists call it the metre barrier. Experiments have shown that the clumps should not be able to grow any larger than a tennis ball. The Max Planck researchers seem to have found an answer explaining how these enormous blocks originate. “Our computer simulations show that there are turbulences in the disc, where small clumps rapidly agglomerate into planetesimals several kilometres in size,” says Dr. Hubert Klahr, head of the project Gravoturbulent Planetesimal Formation: A Key to Understand Planet Formation.

He and his colleagues are using their computer model to discover what a realistic mass distribution of planetesimals should look like, taking into account important factors such as gravity, magnetic fields, and turbulences. JUQUEEN is needed to calculate about 64 million particles; 60 million computing hours have been made available for this purpose. However, since the processes only develop very slowly and a high resolution is required, this time will soon be used up.

“If our simulations are as successful as we hope, we will be able to predict when, where, and in what dimensions planetesimals originate in the discs. This would be an important step towards understanding the genesis of our solar system,” says Klahr.

The Enigma of Continental Drift

Our continents move around. Better said, it’s the continental and oceanic plates that shift over millions of years. This continental drift causes land masses to separate from each other or mountains to form. The physical processes behind it are still an enigma for research. Geoscientist Prof. Boris Kaus and his team from Johannes Gutenberg University Mainz are using simulations on the Jülich supercomputer JUQUEEN to learn more about these processes. The John von Neumann Institute for Computing (NIC), which allocates computation time on the supercomputer, named this project on the numerical modelling of lithospheric and crustal-scale deformation on geological timescales the NIC Excellence Project 2014.

“We can determine the current positions of the plates at any time using geological data and geophysical measuring techniques. Based on this, we can estimate how fast and where the plates are moving,” says Boris Kaus. The plates are about 100 to 200 kilometres thick and they lie on top of rock strata. To fully understand the processes responsible for the displacements, the team from Mainz couple the geological information with numerical 3D deformation models. They have developed a special software package for this. “The Lithosphere and Mantle Evolution Model (LaMEM) allows us to additionally incorporate the complex material behaviour of rocks,” says the geoscientist.

The 15.4 million hours of computation time on JUQUEEN makes it possible for the researchers to calculate models with dimensions of 2000 x 2000 x 700 kilometres – with a resolution of 2.5 kilometres in each direction. With a standard PC, only 20 kilometres are possible. The researchers are investigating events such as the collision of India and Asia, which led to the formation of the Himalayas and the Tibetan Plateau. They are also simulating how the plates under the Alps move and they are looking at how salt domes are formed.

Interactive Supercomputers

Work developing the central element of the Human Brain Project has begun. At the Jülich Supercomputing Centre, three consortia are each installing one pilot system for an interactive supercomputer. The system that is ultimately selected will be used by the EU-funded project to simulate the human brain in its entirety right down to single neurons. The three consortia are Dell/ParTec/Extoll, IBM/NVIDIA, and three subsidiaries of Cray from Germany, the UK, and Switzerland. They came out on top in a pre-commercial procurement (PCP) process.

Now available for smartphones and tablets!

Exascale Newsletter
www.exascale-news.de

effzett (magazine app)
www.fz-juelich.de/app

International Research Laboratory

The Jülich Supercomputing Centre recently became a member of the Joint Laboratory for Extreme Scale Computing (JLESC). In the international partnership, supercomputer centres from the USA, France, Spain, and Germany work together on software solutions for complex high-performance computers. JLESC grew out of the Joint Laboratory for Petascale Computing, founded by the US University of Illinois and the French national computer science institute, Inria, in 2009. http://publish.illinois.edu/jointlab-esc/

OPTIMIZATION REWARDED

A team from Jülich came second in the international CASP competition for computational biology. Junior professor Gunnar Schröder, head of the young investigators group at Jülich for computational structural biology, and his team member Dennis Della Corte were up against some 50 other teams in the category for structure optimization. Their task was to use their own computer models to correct defective, three-dimensional structural models of protein molecules. The necessary computation time was provided by the Jülich Supercomputing Centre. On the JUROPA supercomputer, Schröder and Della Corte simulated the folding of amino acid sequences – the building blocks of proteins. Such computational techniques are becoming increasingly important. The structural analysis of many proteins is either impossible using experimental methods or involves huge effort. Schröder and his group have developed several methods to optimize protein models which have already been successfully applied in various studies. www.predictioncenter.org/casp11

EXASCALE NEWSLETTER of Forschungszentrum Jülich
Published by: Forschungszentrum Jülich GmbH | 52425 Jülich
Conception and editorial work:
Dr. Anne Rother (responsible according to German press law), Tobias Schöller, Christian Hohlfeld
Graphics and layout: Graphical Media, Forschungszentrum Jülich
Translation: Language Services, Forschungszentrum Jülich
Images: p. 1 top: © DigitalGenetics/fotolia.com; p. 1 centre: Walter Nadler/JSC; p. 1 bottom: Andreas Schreiber/Max-Planck-Institut für Astronomie; p. 2 top: NVIDIA; p. 2 bottom: Forschungszentrum Jülich; p. 3 top: Hubert Klahr/Max-Planck-Institut für Astronomie; p. 3 bottom: Johannes-Gutenberg-Universität Mainz; p. 4 © Sagittaria/fotolia.com
Contact: Corporate Communications | Tel: +49 2461 61-4661 | Fax: +49 2461 61-4666
Email: info@fz-juelich.de
Printed by: Schloemer & Partner GmbH
Print run: 200

SCIENTIFIC WORKFLOWS AND DATA MANAGEMENT with UNICORE
16 June 2015
at the Jülich Supercomputing Centre
www.fz-juelich.de/ias/jsc/events/unicore

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