MISSION FOR CLIMATE RESEARCH
Across Europe with the Zeppelin

:: Faulty Folding – Catastrophic Consequences
:: Mathematical Prowess of a Quantum Computer
Part of a historical telegraph? By no means! Investigations are performed here for the telecommunications of tomorrow. The silver disc measures a mere ten millimetres. In a vacuum, researchers at Jülich produce thin layers of organic molecules on the disc by means of vapour deposition, and then study their potential for use in a new generation of semiconductor electronics, for example, in organic light-emitting diodes for smartphones (see “Strong Bonds”, p. 5). Here, the silver crystal is being heated to around 300 degrees Celsius. The white-hot filament can be clearly seen behind the crystal. The crystal is heated “from behind”.

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Diagnosing Schizophrenia Earlier

Scientists from Jülich, Düsseldorf and Detroit have found out that even in healthy offspring of patients with schizophrenia, communication between brain regions is disturbed. The researchers investigated the brain activity of test subjects and then used mathematical models to gain information on the interaction between different regions of the brain.

Using functional magnetic resonance imaging (fMRI), the researchers discovered that many interaction patterns in the brains of children whose parents suffer from schizophrenia are different from those of a control group with no family history of the disease, and similar to those found in individuals with schizophrenia. The mechanisms for processing emotions were weaker overall in the children whose parents had schizophrenia and their balance was different. The part of the brain where feelings of anxiety originate issues warning signals almost constantly without being calmed by other regions of the brain.

The scientists hope to use these findings to develop a test for early diagnosis. If schizophrenia is diagnosed and treated at an early stage, the chances of recovery are much better. Schizophrenia is a serious psychiatric disorder. It affects around one percent of the population, with relatives of those suffering from the disorder being at greater risk.

Fuel Cell Achieves 40,000-Hour Breakthrough

A planar solid oxide fuel cell from Jülich has clocked up more than 40,000 operating hours. This makes it the first in the world to achieve the equivalent of an operating time of five years, which is required for the cost-effective deployment of fuel cells in stationary applications. Due to good efficiency and high operating temperatures, development of this type of fuel cell is targeting stationary applications in particular, such as decentralized systems for private households.

The Jülich test stack is run on hydrogen, which is converted into electric current in the cell with an efficiency of 64 percent. Other fuels such as natural gas can also be converted, with higher efficiencies in some cases, as has been demonstrated in other tests. The test system is made of materials that could also be used to manufacture a commercial product. Before this stage, however, manufacturing costs must be reduced further and the system must prove itself under everyday conditions and not just in the test stand.
Flight into Icy Clouds

Mixed-phase clouds – made up of ice crystals and droplets of water – are important for climate models. Their properties are the focus of attention in the VerDI campaign ("Vertical Distribution of Ice in Arctic Clouds"). In April, the Polar 5 research aircraft set off for the Arctic from the Canadian town of Inuvik in a mission coordinated by the University of Leipzig. On board was the NIXE-CAPS spectrometer, which researchers from Forschungszentrum Jülich use to study cloud particles.

Clouds trap the thermal radiation of the earth in the atmosphere, while also reflecting the incident radiation of the sun, thus cooling the earth. The intensity of these effects in mixed-phase clouds depends above all on the fraction of ice particles they contain. And this is what NIXE-CAPS measures. Using a laser, it determines the size of each individual cloud particle, and it can also distinguish droplets of water from ice crystals. This allows conclusions to be drawn on how much ice is present in clouds.

Spin Spirals for Computers of the Future

How can computer data be reliably stored and read out in future when computers are getting smaller and smaller? Scientists from Jülich, Hamburg and Kiel propose to make use of magnetic moments in chains of iron atoms. This would allow information to be transported on the nanoscale in a fast and energy-efficient manner over a wide temperature range, while remaining largely unaffected by external magnetic fields.

Computers currently save data in magnetic domains on the hard drive referred to as bits. However, if the bits lie too close together, their magnetic fields overlap, making the writing and reading of data impossible. In order to make new functionalities possible, computer components will have to shrink even more.

“Spin spirals” could provide an alternative method of transporting data in the tiniest of dimensions and allow information to be compressed even further in the future. This is what the researchers call the spiral arrangement of the magnetic properties (spins) in chains of iron atoms. If one end of such a chain is connected to a magnetized object, then its magnetic orientation can be read out at the other end, a few atoms and up to three hundred thousandths of a millimetre (30 nanometres) further away. This type of information transmission can be compared to a screw: the iron atoms are the screw, the spin the thread. If you turn the screw head, the revolution proceeds right to the tip and the position of the screw head provides information about the position of the tip.
In May, the Zeppelin NT set off on a great adventure: it took off from Friedrichshafen and headed for the Dutch North Sea coast. Its mission: climate research. On board: high-precision measuring instruments, all of them specially developed for this commission.

To ensure that the data collected over a period of weeks are comparable, the instrument that measures the OH radicals must be regularly calibrated. This is done by a remote-controlled robot arm, which positions a calibration source above the measuring nozzle with millimetre precision.
On its travels for research lasting several months, the flying research platform sets course for the Netherlands, Italy and Finland. The Zeppelin NT flies through very different air masses: it cruises above heavily populated industrial areas and large cities, flies over the Adriatic, and floats above vast forests. However, it does so without the feeling of being on holiday. The many measuring instruments on board continuously analyse the chemical composition of the air during the long flying time and record the data for research purposes. Prof. Spyros Pandis, coordinator of the Pan-European Gas-Aerosol-Climate Interaction Study (PEGASOS) outlines the scientific context: “This mission is one of the most extensive campaigns measuring air quality in Europe, if not worldwide. Our aim is to create datasets that can then be used as a reference for international air-quality research.”

Within PEGASOS, the Zeppelin NT collects data for a total of 20 weeks coordinated by researchers from Jülich. Twenty-six partners from 14 European countries are working together with Israel in an effort to investigate the relationships between atmospheric chemistry and climate change. The findings will be used as a basis for climate protection measures throughout the EU.

In order to collect these data, the Zeppelin transports highly specialized measuring instruments with a combined weight of around 1,000 kilograms. Of this, 390 kilograms are installed on a platform on top of the Zeppelin. The reason is that the most important chemical processes in air are induced by light. Underneath the Zeppelin – in the shadow of the mighty airship – these photochemical reactions do not occur.

TRACKING THE INTANGIBLE

Understanding these photochemical reactions is one of the main priorities of the measurement campaign. At altitudes of 100 to 2,000 metres, scientists are investigating the self-cleaning ability of the atmosphere. The key molecule in this process is the hydroxyl radical (OH radical). It triggers the degradation of most pollutants and determines how long they survive in the atmosphere. The OH concentration is therefore a measure of the cleaning efficiency of the atmosphere. The hydroxyl radical is formed in the atmosphere from ozone and water molecules under UV radiation. In a natural cycle, it is initially consumed when pollutants are degraded, but in many cases it is then subsequently recycled (see “The Cycle of Radicals”, p. 11). However, in the last few years, Jülich researchers have come across discrepancies in the prevailing theory with respect to recycling. It is hoped that the Zeppelin flights will now clarify the matter.

Hydroxyl radicals are highly reactive – and they are elusive. The radicals only exist for a fraction of a second. In 10,000,000,000,000 (ten trillion) air particles, there is only ever a single particle of this atmospheric detergent. New measuring methods developed by Jülich scientists will now make it possible to reliably determine the concentration and lifetime of hydroxyl radicals in the atmosphere.

LIGHT, COMPACT, AND STABLE

Dr. Andreas Hofzumahaus from the Jülich Institute of Energy and Climate Research (IEK-8) says, “We have developed two main methods of measuring the OH radical. It triggers the degradation of most pollutants and determines how long they survive in the atmosphere. The OH concentration is therefore a measure of the cleaning efficiency of the atmosphere. The hydroxyl radical is formed in the atmosphere from ozone and water molecules under UV radiation. In a natural cycle, it is initially consumed when pollutants are degraded, but in many cases it is then subsequently recycled (see “The Cycle of Radicals”, p. 11). However, in the last few years, Jülich researchers have come across discrepancies in the prevailing theory with respect to recycling. It is hoped that the Zeppelin flights will now clarify the matter.

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"At the launch in early May, Federal Research Minister Prof. Annette Schavan familiarized herself with the scientists’ goals. Sitting opposite her is Robert-Jan Smits, Director-General for Research and Innovation of the European Commission."
radicals. The first is based on the fact that the intensity of laser light is reduced by the OH radicals, that means it is absorbed. The second method uses a laser to excite the OH radicals, causing them to fluoresce.

In an effort to ensure that enough of the rare hydroxyl radicals are recorded by the first method, the researchers reflect a laser beam back and forth more than a hundred times between mirrors placed around twenty metres away from each other. “Such a setup is used, for example, in our atmosphere simulation chamber SAPHIR – and in other locations where we have enough space,” explains Hofzumahaus. The second method is just as accurate but requires less space, making it an ideal candidate for the Zeppelin’s top platform, which is around five metres long. “Being able to use two different methods has the great advantage that we can verify the results obtained with the two measuring techniques against each other,” says Andreas Hofzumahaus. The second laser setup is not affected by changes in temperature or air pressure and functions perfectly at increasing altitudes on board the Zeppelin. The credit for this goes to engineers at Jülich’s Central Institute of Technology (ZAT). They first reduced the weight of the setup as a whole. “For aircraft transport, every gram counts – our aim was therefore to reduce the weight over and again,” says Knut Dahlhoff from ZAT. However, the equipment must remain robust. “The original ground instrument made a pretty reliable impression. But every time the ambient temperature dropped by only two degrees, it had to be readjusted,” Dahlhoff recalls. Together with colleagues from the Fraunhofer Institute for Laser Technology in Aachen, they developed a unique precision instrument that is light, compact and also robust enough for use on the long Zeppelin flights.

The team of scientists and engineers also scored a similar success with an instrument that determines how polluted
the air is. To do so, it measures the lifetime of OH radicals. This new device is known as AirTauOH. It sucks in an even flow of external air and illuminates it with a laser. This causes the immediate formation of OH radicals. The more reaction partners – or different types of molecules – can be found in the air, the shorter the lifetime of the OH radicals.

**FAST AND RELIABLE**

The decrease in concentration over time is registered exactly by another measuring cell. This allows conclusions to be drawn on how polluted the air is, but it does not help to determine whether the pollutants are natural or man-made. Other instruments on board record aerosols or molecules present in the air, such as formaldehyde. According to Hofzumahaus, “Space limitations mean that we can’t measure the entire range of all atmospheric molecules during the Zeppelin mission. But thanks to AirTauOH, we can determine how many reactive components are in the air at a particular point in time.”

A group of molecules has been identified as being particularly important for climate, namely volatile substances released by plants. After oxidation, these can form aerosols in the atmosphere, which later contribute to the formation of clouds. Clouds reflect solar radiation and can therefore be considered to counteract global warming. For this reason, another priority of the PEGASOS campaign is to verify and characterize the existence of aerosols above different regions.

Conifers, for example, predominantly release terpenes into the air which create the fragrant aroma in a forest. Deciduous trees, on the other hand, tend to emit a substance known as isoprene. The two substances react at different speeds with the OH radicals, which impacts on the formation of aerosols in the atmosphere, as Jülich researchers recently discovered. In their study, they demonstrated that aerosol formation is impaired when the isoprene concentration is high in relation to the terpene concentration, as is frequently the case in summer. Under these conditions, the isoprene molecules basically steal the terpenes’ reaction partners. This has considerable consequences. The volatile terpenes are no longer oxidized by the OH radicals and therefore no longer act as precursors for cloud nuclei. It is hoped that measurements above the extensive forest areas in Finland will provide data still lacking on the rivalry between the two plant substances.

“The Zeppelin follows flights routes set in advance to take into account existing ground measuring stations,” emphasizes Dr. Astrid Kiendler-Scharr. The researchers want to find out exactly what happens with the components of air on their way from the earth’s surface to an altitude of 2,000 metres.
Cycle of Radicals

Hydroxyl radicals (OH radicals) are formed in sunlight from ozone molecules. Other radicals known as HO₂ radicals are formed by the splitting of formaldehyde. These “detergents of the atmosphere” are short-lived and are present only in minute amounts in the atmosphere. Yet they are a decisive factor in determining the length of time that important trace gases (hydrocarbons, carbon monoxide, nitrogen oxides) remain in the lower atmospheric layers. The sooner trace gas molecules are degraded in reactions with radicals, the less they spread. However, the degradation of trace gases produces secondary pollutants such as ozone. On the other hand, measurements by Jülich scientists in China have revealed that there could be other degradation processes in which few ozone molecules are formed. The graphic shows the most important chemical processes involved in the degradation of trace gases by OH radicals and HO₂ radicals, which are converted into each other during the cycle in a matter of seconds. In each case, a carbon monoxide or a hydrocarbon molecule is oxidized. Depending on the level of nitrogen oxide pollution, an ozone molecule is either created or destroyed.

When this cycle has been repeated around ten times, the radicals then disappear forming nitric acid (HNO₃) and hydrogen peroxide (H₂O₂) and are no longer part of the “detergent cycle”.

OH radicals emit light when excited with a laser.
When neurons in the brain start firing synchronous electrical signals, this usually spells trouble: the consequences may be the typical tremor or rigidity of patients with Parkinson’s disease, or else pain or an unbearable ringing tone in the ear of people suffering from tinnitus. The Institute of Neuroscience and Medicine – Neuro-modulation (INM-7) is developing treatments for this abnormal synchronization promoting healthy chaos in the brain. They have now used computer models to demonstrate that even indirect stimulation counteracts this abnormal synchronization. This understanding could pave the way for new, non-invasive treatment options.

A probe implanted deep into the brain is often the last hope for patients with Parkinson’s or a tremor. This device, commonly referred to as a brain pacemaker, sends electrical “cross fire” into the affected regions of the brain. Some 75,000 patients have already undergone this neurosurgical procedure.

In order to avoid the risks involved in the operation and to be able to help a large number of patients, Prof. Peter A. Tass and his team are searching for alternatives involving neither a scalpel nor anaesthetics. The question is whether it is possible to treat diseases of the brain via indirect or even sensory stimuli so that, for example, the nerves in the auditory cortex of tinnitus patients can be taught to forget this synchronous mode by specific successions of tones.

Dr. Oleksandr Popovych (INM-7) specializes in calculating the communication in complex clusters of neurons. In computer models, he reconstructed the effects of direct and indirect stimulation. Direct stimulation means that an impulse is sent straight to those neurons firing synchronous signals. In the case of indirect stimulation, several neurons are used as relays, making the impulse’s path to its destination longer and more ramified. “The result is very encouraging,” says Popovych. “The computer simulations clearly show that indirect signals are also able to cancel out the abnormally synchronized neuronal signals. In our model calculations, we even found they had a more long-term effect.”

With his mathematical models, Popovych is also trying to find out how strong an impulse must be in order to have an effect. He has already found out that less is sometimes more. “Many important questions still remain to be answered. For example, we need to find out how to further optimize the parameter values for the treatment to be more effective. This requires advanced models and lots of computing time.”
“2,500 Patients Treated”

The Coordinated Reset® (CR®) method developed by Prof. Peter A. Tass is an approach that can help tinnitus patients as well as those affected by Parkinson’s or epilepsy. The positive effect of this method is even visible in the brain waves as reported by Tass and his team in recent scientific publications.

**Question:** Prof. Tass, what are the key results of the studies you have recently published?
**Tass:** The most important result of our controlled trial with 63 tinnitus patients is easy to summarize: 75 percent of patients clearly or very clearly benefited from the treatment. This means that the patients subjectively perceive their tinnitus to be much less noisy and also less annoying. Objectively, we demonstrated by means of EEG* measurements that the treatment has a positive effect on the patients’ brain waves and that the abnormally synchronized neuronal activity subsides. Even four weeks after treatment, the effect was still there – the tinnitus continued to be significantly better than before the treatment.

**Question:** Are the synchronously firing neurons blocked or their signals "camouflaged" by the frequencies used in your method?
**Tass:** No. This is what sets the CR® method apart from other approaches such as noise generators. We want to allow the synchronized neuron clusters to be active in their pathological frequency range – but they need to become desynchronized! The reason is that only active neurons are able to learn and unlearn anything. Suppression alone does not have any lasting effect.

**Question:** What further trials with patients are you planning?
**Tass:** In Germany, another application trial has just got under way. Doctors are treating 200 patients over a period of one year and will observe them subsequently for several months. In the UK, another trial with 100 patients is currently being prepared as well. We are also planning a series of tests at Jülich in order to objectively and individually personalize by means of EEG* the CR® treatment tones for the abnormal synchronization in each patient’s brain. To date, patients have been requested to identify the pitch of their tinnitus themselves, but even professional musicians are not always able to do this with the necessary accuracy. However, for our treatment to be successful, stimulation has to take place in the correct frequency range.

**Question:** Will the CR® method be part of the clinical routine anytime soon?
**Tass:** Yes, it will. In Europe, about 2,500 patients have already been treated successfully by our CR® method. The number of specialized CR® treatment centres is also increasing. In addition to existing centres in London and Budapest, we are establishing a large tinnitus centre together with the psychiatry section of University Hospital Salzburg in Austria.

Tinnitus patients with four points on the severity scale often suffer from depression as well. We would like to offer them CR® treatment in combination with psychiatric support.

**Question:** What other diseases could be treated using the CR® method?
**Tass:** Any disease that is characterized by abnormally synchronous neuronal activity in the brain, for example Parkinson’s or epilepsy, as well as dystonia, pain or ADHD**.

**Synchronous electrical signals cause tinnitus**

Ringing, swooshing, buzzing: three million Germans are affected by tinnitus. The causes can be found both in the ear and in the brain. Usually, the continuous tone is preceded by a hearing impairment. Loosely speaking, those neuron clusters responsible for the frequencies affected by a hearing loss are simply bored. They start firing synchronous electrical signals, which the patient perceives as a distressing noise. The Coordinated Reset® method developed at Jülich helps the neurons to unlearn their synchronous firing by means of carefully calculated impulses that are adjusted to each patient’s tinnitus to help their brain return to healthy chaos.

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**ADHD (attention deficit hyperactivity disorder): disorder characterized by massive attention and concentration problems combined with extreme hyperactivity in children and young people.*
Cyclotron for Medicine and Research

The large-scale device for medical research delivered to the Jülich campus in early May weighs in at 35 tonnes. A heavy-duty crane lifted the new compact cyclotron into its home, an underground concrete bunker. This is where, starting in summer 2013, it will produce radionuclides for the synthesis of radiopharmaceuticals that can be used to track down tumours, monitor metabolic processes and investigate the mechanisms of medical drugs.

The device developed in Belgium by IBA is the first of a new series capable of accelerating three different particles. Apart from protons* and deuterons* for the routine production of pharmaceuticals, it is also possible to generate alpha particles* with an energy of up to 30 mega-electron volts. "The new cyclotron, on the one hand, enables us to maintain a reliable supply of short-lived radiopharmaceuticals for patients and, on the other hand, to undertake ground-breaking research and teaching in nuclear chemistry here at Jülich," explains Prof. Heinz H. Coenen, director of the Institute of Neuroscience and Medicine – Nuclear Chemistry (INM-5).

And particularly the research promises to be exciting. If, for example, high-energy alpha particles hit chlorine atoms then potassium-38 is formed, which medical scientists use for detailed investigations of myocardial blood flow. Other radionuclides, such as samarium-153 for tracking down bone metastasis and astatine-211 for the irradiation of malignant tumours, can be very effectively produced with alpha radiation. Furthermore, research has recently started to focus on “partner isotopes”. These isotopes enable the production of bimodal tracers. Such tracers can be identified by both positron emission tomographs (PETs) and also magnetic resonance imaging (MRI) scanners. “We are thus able to make a decisive contribution to the further development of Jülich’s hybrid imaging, a combination of PET and MRI,” adds Coenen.

SIMPLER AND BETTER

And this is precisely the strength of Jülich researchers. Their expertise covers the entire range from understanding the individual nuclear reactions up to the production of radiopharmaceuticals for routine use. Coenen emphasizes: “One of our declared priorities is the investigation and development of new radionuclides. Such radionuclides are either more suitable for a specific purpose or they can be produced more easily by a new nuclear reaction – that is to say at less expense or with fewer side products.” As in the case of the extremely successful [18F] fluorodeoxyglucose, the tracer most frequently used for tumour diagnosis with PET, after successful introduction in clinical practice, researchers at Jülich leave the later mass production to industry.

Their efforts are better employed in developing new tracers. For example, selenium-73 as a new PET tracer. Its longer half-life of about seven hours means that slower metabolic processes can be investigated, for example the creation and degradation of proteins in the body. Or new radionuclides for appli-
Cyclotron applications even in plants. Carbon-11, which is often used in plant research, has a half-life of just 20 minutes. “We will now be able to make novel nuclides available for environmental research which cannot be produced with a conventional cyclotron,” explains Dr. Ingo Spahn, who specializes in the production of radionuclides at INM-5.

DAZZLING PROSPECTS

Installation of the new cyclotron also involves extensive building work. State-of-the-art laboratories are being constructed immediately adjacent to the cyclotron both for the routine production of radiopharmaceuticals and also for research. Above ground, the new Jülich translation centre is under construction. Its function is to ensure that medically relevant findings are incorporated in everyday clinical practice as soon as possible. Close by, the scientists of INM-5 plan to move into their new institute in 2014. This complex will have direct underground access to the cyclotron. “Here we are setting up two further target stations for the particle beam of the cyclotron,” says Spahn. “This will enable us to increase capacities for research and development in nuclear chemistry.”

This aspect is also of significance for neighbouring universities. “The two cyclotrons in Cologne and Hannover, which can also generate alpha particles, are due to be shut down for reasons of age,” says Coenen. “The new Jülich cyclotron will therefore be the only one in Germany with this equipment and capacity.” In the view of researchers at Jülich, this means that the traditionally close cooperation with universities in the region, especially with the University of Cologne in the field of nuclear chemistry, will be further intensified. The number of students enrolled in this subject has doubled in the past five years. “Graduates in this field are being urgently sought by medical facilities, energy utilities and also by regulatory authorities,” says Coenen. “Employment prospects are excellent, especially if they are trained in the state of the art,” he adds.

* Protons are stable positively charged building blocks of the atomic nucleus. Deuterium (D or $^2\text{H}$) is a hydrogen isotope that has one neutron and one proton in the nucleus. Alpha particles ($\alpha$-particles) are doubly positively charged helium ions ($\text{He}^++$). An alpha particle consists of two neutrons and two protons.
Mathematical Prowess of a Quantum Computer

Quantum computers were long a mere utopian vision in the minds of physicists. But now they really exist. Theoretical studies can be made of the problems which they may in future help to solve. In his studies, the physicist Privatdozent Dr. Thomas Neuhaus makes use of conventional but extremely powerful computers – the Jülich supercomputers.

The future has already started. At least that is what some people may think when they read that the Canadian company D-Wave has been marketing quantum computers since 2011. All conventional PCs, smartphones and supercomputers make use of bits as the smallest information units. These bits can only take on the values 0 and 1, but quantum computers operate with quantum bits, qubits for short, which consist of a large number of superimposed states. In contrast to conventional processors, quantum computers are basically able to perform multiple operations simultaneously in one switching process. This is why physicists have been hoping since the 1980s that quantum computers would be able to solve certain computational problems at an unimaginable speed.

NEW TWIST

To date, experts have largely pursued a concept in which the qubits are formed of particles – for example, atomic nuclei – whose quantum mechanical angular momentum, the spin, can be selectively influenced. “In such quantum computers, researchers try to transfer the logic that a normal computer uses for addition, multiplication and other arithmetic procedures, to the rotation of the individual spins,” explains Thomas Neuhaus from the Jülich research group “Quantum Information Processing”. The problem is that each individual spin must be very precisely adjusted, which is difficult enough for real systems of just four or eight qubits.

In contrast, Neuhaus is concerned with the theory of a new and even more astounding variant of the quantum computer. This variant, the adiabatic quan-
Tum computer, has been implemented in practice by D-Wave - with 128 qubits according to the company's information. “An adiabatic quantum computer does not need to make any calculations, that is to say it doesn’t need to solve equations or multiply anything in order to solve a difficult mathematical problem,” says Prof. Kristel Michielsen, head of the research group at the Jülich Institute for Advanced Simulation. She admits that the functioning of an adiabatic quantum computer (see “Travelling Salesman for Quantum Computers”) is rather mind-boggling.

**SOLUTION FOR THE UNMANAGEABLE**

Many experts hoped that quantum computers would outstrip conventional computers above all in solving those mathematical problems that are regarded as “unmanageable”. The classical example of this is the travelling salesman problem. The problem is to find the shortest route connecting finitely many points such that the traveller should visit each town just once and return to the starting point. This problem cannot be solved with mathematical precision. A solution can only be found that is as close as possible to the optimum. For such a problem, computing time on a conventional computer explodes with the number of towns to be included.

“We investigated a special unmanageable problem to discover how effectively it can be treated with an adiabatic quantum computer,” says Neuhaus. Since the Jülich theoreticians did not have a D-Wave quantum computer at their disposal they simulated the sequences on the Jülich supercomputers, which was extremely time-consuming. They achieved a spectacular if rather sobering result. The problem was just as unmanageable on a quantum computer as on any other computer. “Our research is also intended to continue to help assess the usefulness of quantum computers more realistically in the future,” says Neuhaus.

However, the Jülich physicist is still convinced that the adiabatic quantum computer does have a future. If D-Wave should succeed in increasing the number of qubits in their quantum computer to 512, then this could already exceed the performance of a present-day supercomputer. “And in doing so it would only consume about one thousandth of the energy required by a conventional supercomputer,” adds Neuhaus.

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**Travelling Salesman for Quantum Computers**

The user of an adiabatic quantum computer would first radically simplify the travelling salesman problem (see article) by, for example, arranging all the towns on a circle. This simplified problem would then be formulated mathematically with the aid of a Hamiltonian function, named after the Irish mathematician and physicist William Rowan Hamilton (1805–1865). This function describes the energy state of a quantum mechanical system. The familiar solution of the simplified travelling salesman problem corresponds to the energy minimum of such a quantum mechanical system, which is the central component of a quantum computer.

If the adiabatic quantum computer is to solve the travelling salesman problem for a real arrangement of towns then the original Hamiltonian function must be modified in controlled steps until it describes the problem. Due to a natural law, the quantum mechanical system is always in the lowest energy state at each step. If the system arrives at the Hamiltonian function that describes the real travelling salesman problem then the solution has been found, which is the energy minimum of the quantum mechanical state that has been reached.

Even the adiabatic quantum computer cannot solve problems without real effort. On the way to a real arrangement of towns, the computer comes across a quantum phase transition at which it has to perform a large number of small steps in order to remain in the minimum energy state.
Correct shapes matter if proteins are to fulfil their respective functions. If they are not properly folded, molecules may clump together and cause cells to die. This happens in a number of brain diseases, such as Alzheimer’s and Parkinson’s. An international team of researchers headed by Dr. Philipp Neudecker from Forschungszentrum Jülich and Heinrich Heine University Düsseldorf have now observed with unprecedented accuracy a decisive step at the beginning of this process. Their finding were reported in the renowned journal Science in April 2012.

When a new protein is formed, amino acids are initially threaded together like a string of pearls. However, this chain of protein building blocks immediately starts to fold up until it forms a three-dimensional structure. Within a few seconds, the amino acid string thus becomes either an enzyme, a muscle protein, an antibody, or one of a plethora of other proteins that fulfil a variety of tasks in our body.

When a molecule required for signal transmission in the cell folds up, it passes through short-lived intermediates, which can transform either into correctly shaped proteins, or sometimes a defective version with a tendency to join up
with others. As soon as this fatal procedure has started, more and more protein molecules attach themselves to the aggregate, which is at first tiny but then begins to form long threads – the dreaded amyloid fibrils. Unless they are broken down by the cell’s “clean-up squads”, they accumulate and ultimately destroy the cell. Its place in the brain is filled by the clumped fibrils, which are visible under the microscope as amyloid plaques in Alzheimer’s, Parkinson’s, and Creutzfeldt-Jakob disease.

Philipp Neudecker from the Institute of Complex Systems (ICS) analysed the intermediate stage of protein folding, which stands at the crossroads between the working protein and the dangerous fibrils. “This state is necessary for the protein to fold up properly within less than a second,” he explains. “However, this process is something of a balancing act, because it may also cause fibrils to be formed.” It only exists for an extremely short period of time, no more than a few thousandsths of a second. His team succeeded in observing these “borderline cases” closely during this fleeting moment and in analysing the process of folding in great detail using nuclear magnetic resonance spectroscopy. The method, NMR for short, shows the exact spatial structure of the short-lived unstable intermediate stage in atomic resolution.

ERRORS INCREASE WITH AGE

In his experiments carried out mostly at the University of Toronto, Neudecker found out that the arrangement of the last four amino acids in the molecule consisting of a total of 59 components plays a decisive role. This end of the chain normally forms a string that is aligned almost in parallel with the first building blocks of the molecule. This arrangement prevents further proteins from attaching themselves to the molecule. In the intermediate state, it is precisely this last protective section of the molecule that is not yet folded. The beginning of the protein is open to further protein molecules, enabling fibrils to form spontaneously.

It is not always clear why the balancing act ends in disaster in individual cases. “The formation of the initial aggregates – a process referred to as nucleation – is a relatively rare event,” reports Neudecker. “Of course, it only occurs when several such molecules meet, and is therefore extremely dependent on the concentration of the protein variant that tends to aggregate.” With increasing age, however, misfolded proteins are increasingly likely to accumulate. It is also assumed that the repair mechanisms able to either whip the protein molecules into shape or eliminate them become less effective with age. “Environmental impacts, such as natural or artificial chemicals, are also suspected of playing a role in the formation of amyloid fibrils, as are genetic defects,” explains Neudecker.

HOPE FOR TREATMENT

“Our research is of a very basic nature,” says the researcher, who came to Jülich from Toronto last spring. He nevertheless expects the results to provide great benefits, for example for the diagnosis and treatment of Alzheimer’s. “There is an almost alarming lack of knowledge on the fundamental mechanisms in the decisive initial stages of the disease – which constitutes a great barrier to the development of new drugs.” It was recently reported at a specialist conference in Paris that none of the 200 potential active ingredients for Alzheimer’s that have undergone clinical trials so far is actually used as a drug today. “By analysing the mechanisms that mark the beginning of such diseases, we can contribute to progress in this area,” says Neudecker.

Source

Materials with More Thermopower

In cars and numerous industrial production processes, a great deal of energy is lost in the form of heat. With thermoelectric materials, the waste heat could be utilized and therefore less energy squandered. Dr. Raphaël Hermann and his Helmholtz young investigators group conduct research on how these materials can be improved.

Raphaël Hermann, who hails from Belgium, says with satisfaction, “We have just undergone evaluation – with excellent results. This means that I can continue my work at Jülich.” By “we” Hermann means the Helmholtz young investigators group he established in 2008 and which he also heads. With its young investigators group programme, the Helmholtz Association (HGF) supports early-career scientists in conducting research independently and “offers them secure career prospects”, as HGF puts it. This means first and foremost a permanent contract – and nothing stands in the way of this for Hermann after the results of the latest evaluation.

Hermann’s objects of research include materials that can be used to build thermoelectric generators (TEGs). TEGs convert temperature differences into electrical energy. They could therefore help utilize the waste heat that is currently lost in cars with petrol or diesel engines. Car manufacturers believe that in this way fuel consumption can be reduced by at least five percent, which would curb carbon dioxide emissions as well. Excess heat is also released in many industrial processes and in combined heat and power plants. The reason why TEGs are not yet used, neither in these applications nor in cars, is that to date they only convert a small fraction of the excess heat into electrical power. Experts consider their efficiency to be too low: it is usually less than ten percent, even if the temperature difference between the hot and the cold side of the TEG is high.

THE GOAL: HIGHER EFFICIENCY

An increase in efficiency requires materials that conduct electric current effectively but have a low thermal conductivity. Unfortunately, high electrical conductivity usually goes hand in hand with a high thermal conductivity, be-
cause both properties are influenced by the mobility of electrons. “However, thermal conductivity is due not only to electrical charge carriers, but also to lattice vibrations. By reducing their share, it is possible to produce more efficient thermoelectric materials,” says Hermann, who lectures at the University of Liège in Belgium as a guest professor.

As the name of his young investigators group – “Lattice dynamics in emerging functional materials” – suggests, he specializes in experiments on lattice vibrations and mechanisms of heat transport. In fact, his group, which currently includes five PhD students and one postdoc, conduct research not only on thermoelectric materials, but also phase-change materials, for example, which are important for optical data storage.

In the labs of the Jülich Centre for Neutron Science (JCNS) on campus, the scientists measure elastic constants and other macroscopic properties of materials related to movements of the lattice. However, in order to take a look at lattice vibrations under the microscope, they require access to large-scale facilities at international research institutions. For example, they regularly use the measuring facilities of JCNS at the FRM-2 research reactor in Garching near Munich and at the Institute Laue-Langevin in Grenoble, France. Furthermore they study the materials at institutions such as the European Synchrotron Radiation Facility, which is also located in Grenoble, and at the photon source of the Argonne National Laboratory, USA.

ROLE OF LATTICE VIBRATIONS

Microscopic images of the lattice vibrations show that their energy is “quantized”, meaning that it can only take specific values. Quantized lattice vibrations are known as phonons – comparable to photons, which are energy quanta of light. There are three factors that determine heat transport by phonons: velocity, free path, and thermal capacity. “It can be compared to the transport of goods by road: the faster a truck goes, the less time it spends stuck in traffic jams and the larger its cargo space is, the more it can transport,” explains Hermann.

The researchers determined the key limiting factor for the thermal conductivity of phonons in thermoelectric materials described with chemical formulas such as $Y_{14}MnSb_{11}$, $FeSb_3$ and $Sr_{6}Ga_{13}Ge_{30}$. Hermann’s former PhD student Anne Möchel, now Anne Houben and working at the Max Planck Institute for Plasma Physics, received a young scientists award from the German Thermoelectric Society (DTG) for her PhD thesis in 2011. According to the DFG press release, her work represents an important step towards improving our understanding of thermal transport. Hermann is confident: “This understanding of heat transport is a key factor in the quest for thermoelectric materials with higher efficiency.” He adds that Jülich provides ideal conditions for him to continue to be successful with his research. He has obviously convinced the German Research Foundation (DFG) and the Federal Ministry of Education and Research (BMBF) as well. The funding they provide now considerably bolsters Hermann’s research budget from the Helmholtz programme.
Potatoes in the Scanner

Leeks, potatoes, onions – this sounds like the recipe for a tasty soup or a hearty stew. Jülich plant researchers at the Institute of Bio- and Geosciences, however, are not interested in peeling or chopping them. In fact, quite the opposite is true: they want to understand what exactly is going on inside these plants – while they are growing and without destroying them.

This is possible with methods that are normally employed in medical engineering: magnetic resonance imaging (MRI) and positron emission tomography (PET). MRI is used in medicine to visualize different types of tissue, but also lends itself to shedding light upon the inner structure of plants. It even allows insights into the growth of roots below the surface. PET provides information on the transport of photosynthesis products inside plants. Three years ago, Jülich researchers were the first to perform combined measurements with MRI and PET in plant research. Thanks to this technology, it is now possible to assign metabolic processes clearly to defined types of tissue in plants. For example, MRI-PET measurements show exactly where plants incorporate carbon and how this changes in different types of soil or under changing climatic conditions. One of the goals is to utilize plants more effectively as suppliers of useful substances. For this purpose, it is necessary to understand their properties in greater detail, for example in order to select plants that yield good crops even during dry periods or that get by with a smaller amount of nutrients (fertilizer).
Intricate structures
1 Roots of a maize plant
2 Potato
3 Barley roots
4 Roots of a sugar beet
5 Maize roots
6 Mandarin
7 Onion
8 Leek