EXASCALE

Newsletter of Forschungszentrum Jülich on Supercomputing

JÜLICH
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Thanks to a certain combination of various polymers, water can also be used to lubricate joints and hinges. This was shown in simulations on Jülich's supercomputers. Water is much more fluid than oil and reduces wear and tear.

Dressing Extends Lifetime of Machines

Engineers are somewhat envious of nature: instead of applying viscous oil as a lubricant, it uses aqueous solutions, which are much more fluid. By means of simulations on supercomputers, scientists from Jülich and Twente (the Netherlands) have now discovered a way of mimicking nature. This could help to considerably reduce wear in machines.

Knee joints, pumps, ball bearings – there are places where moveable parts meet, both in nature and engineering. Lubricants prevent the parts from touching directly, which would cause wear and tear. For this purpose, nature uses an aqueous solution, while in engineering, oil is usually applied. Prof. Martin Müser, head of the NIC research unit Computational Materials Physics at the Jülich Supercomputing Centre (JSC), explains why nature performs better: "Oil produces greater friction than water. And friction usually leads to increased wear."

For a long time, researchers have been attempting to emulate nature. The problem is that fluids similar to water are displaced when the pressure increases. Oil, in contrast, becomes stiffer and stays where it is. Nature uses a trick here: on the cartilage of knee joints, so-called polymer brushes can be found. These chain-like molecules are charged in such a way that they attract water. Engineers could also use polymer brushes, but are experiencing difficulties in

doing so: the brushes become entangled, which causes damage. In the knee, the brushes regrow, but in machines, they don't.

Müser developed an idea that goes beyond the approach of nature. "Hydrophilic and hydrophobic polymer brushes are combined and a device is lubricated with a kind of salad dressing: a mixture of oil and water. This creates a layer which prevents the polymer brushes from becoming entangled," says the physicist. He and his former colleague Sissi de Beer, who currently works at the University of Twente, developed a model that simulates this process on a supercomputer on an area of 100 nanometres. Their approach reduced the abrasive wear caused by the lubricant by a factor of 100. This finding was also verified by de Beer in experiments. This may mean longer lifetimes for a variety of machines.
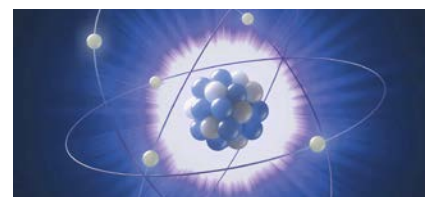
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Order Discovered in Chaos

Turbulence still puzzles physicists. Simulations on Jülich's supercomputer JUQUEEN have brought research one step further. An international team of scientists verified scaling laws that demonstrate the universality of small-scale turbulent fluid motion in three different generic fluid flows.

Turbulence is an everyday phenomenon: examples include gusts of wind, clouds, combustion in jet engines, and simply stirring milk into coffee. Turbulence is caused when gases or liquids flow rapidly. Large vortices are thus continuously generated, which then decay into smaller ones. This decay continues until molecular viscosity becomes dominant. The researchers headed by Jörg Schumacher, a professor for fluid mechanics at Technische Universität Ilmenau in Germany, however, were not concerned with this cascade of vortices. They were interested in the very fine shear layers between the various vortices. The scientists compared these shear layers in three very different turbulent flows and consistently found the same statistical laws for their statistical fluctuations.

The researchers' approach opens up a new method of verifying Kolmogorov's hypothesis on the universality of turbulence, which he postulated more than 70 years ago. According to this hypothesis, the random motion of the medium-sized and smaller vortices in a turbulent cascade always follows the same statistical laws. The simulation of such an extended vortex cascade still demands too much computing power for today's supercomputers. "However, this fundamental hypothesis on turbulence can be verified using the supercomputer technology available today if we
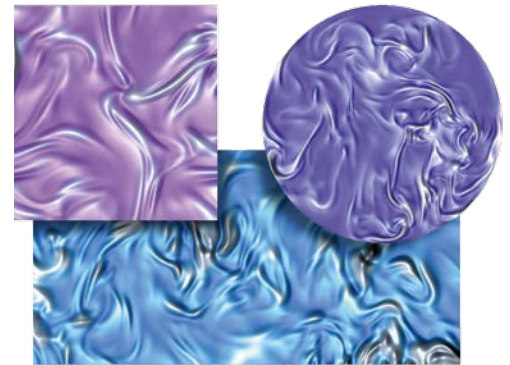
In the apparent chaos of vortices, rules reign – to be exact, in the shear layers, the transition zone between two parallel flows.

focus on the right physical quantities – namely, the shear layers instead of the flow vortices," says Jörg Schumacher.

PNAS, DOI:10.1073/pnas.1410791111

Staying One Step Ahead of Fire

Computer simulations are becoming more and more important in fire protection. Experts from Civil Security and Traffic at the Jülich Supercomputing Centre (JSC) are working together with colleagues from the University of Wuppertal to improve the modelling of fires. "We analyse the spread of fire and smoke, for example in simple buildings or complex underground stations. Then, we derive generally applicable statements, which are incorporated into the further development of computer models," says JSC scientist Dr. Lukas Arnold, who has headed the research team since 2012.

Fires are an extremely complex process in which numerous factors play a role: for example, the air flow and air temperature, the type of flammable materials, the combustion process itself, and what is known as radiative heat transfer. "In the case of a liquid fire, the electromagnetic radiation of the flames causes the liquid to evaporate releasing another flammable gas. If this type of heat transport is not taken into account, the fire in the simulation would stop burning," says the physicist.

In order to simulate the spread of fire and smoke, the scientists use computational fluid dynamics. Their simulations on Jülich's supercomputer JUROPA are much more detailed than applications used by engineers in industry today. Calculations can take up to several weeks on hundreds of processor cores. Only in this way can the researchers identify the important processes and discern the necessary numerical resolution. In the past, simulations split the volume of a room into equal subvolumes. The Jülich researchers are endeavouring to develop a model that will dynamically adapt the resolution of these volumes: very fine at the origin of the fire and coarser in areas farther away. This would considerably reduce the computation time without impeding the quality. The scientists are already thinking ahead. Their aim is to calculate fires in real time. "However, before we reach this stage, we have much research work to do," says Lukas Arnold.

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

Imminent danger: if an underground catches fire and the smoke cannot escape into the atmosphere, it fills the train station or tunnel within minutes. Jülich researchers simulate this process.

Insights into Exotic Nuclei

Extremely neutron-rich nuclei play a decisive role in the creation of elements in the universe. For example, gold or lead is created when stars explode as a supernova at the end of their lives. Prof. Achim Schwenk and his team at Technische Universität Darmstadt are using supercomputers to predict extremely neutron-rich matter in astrophysics and in exotic nuclei. His project entitled "The Strong Interaction at Neutron-Rich Extremes" was awarded the accolade of NIC Excellence Project 2014 by the John von Neumann Institute for Computing. This accolade grants the researchers in Darmstadt additional computation time on Jülich's supercomputer JUROPA.

The nuclear physicists will thus be able to advance novel many-body approaches. "The combination of JUROPA and state-of-the-art nuclear and many-body physics will facilitate new insights into the strong inter-action in exotic nuclei and in neutron stars," says Schwenk. Only half of the atomic nuclei held together by the strong interaction have been identified so far. Most of the unknown exotic nuclei are extremely neutron-rich isotopes that only exist for a very short time or under neutron-rich conditions. Isotopes are atomic nuclei that contain the same number of protons but different numbers of neutrons.

The Darmstadt researchers have already shown that three-body forces between neutrons and protons are essential for understanding neutron-rich isotope chains. The first calculations with two- and three-body forces impressively predicted the neutron-rich calcium isotope.

www.john-von-neumann-institut.de/nic/exzellenz-2014
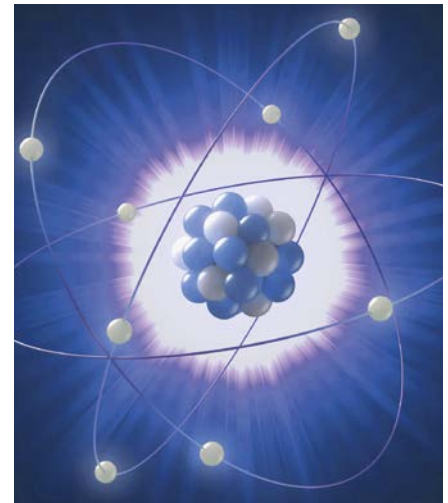
Exotic atomic nuclei are often short-lived, extremely neutron-rich isotopes. Researchers at Darmstadt have taken a closer look at calcium isotopes.

Outstanding Strategy for the Future

Prof. Wolfgang Marquardt took over as Chairman of the Board of Directors of Forschungszentrum Jülich in July 2014. The qualified process engineer is no stranger to supercomputing. From 2011 to 2014, he was Chairman of the German Council of Science and Humanities, which in the same period published one position paper each on supercomputing and simulation science.

Prof. Marquardt, what were the key messages of these papers?
The German Council of Science and Humanities has always emphasized that in order to be competitive in numerous scientific fields, Germany requires an appropriate infrastructure of supercomputers. A pyramid system with different levels of computing power and a small number of centres at the top has proven a successful solution. However, continual financial backing is required from the federal and state governments in order to cover the ever-growing demand. We also recommended closer coordination within Europe.

Now you are at the helm of such a centre. How well-equipped is Jülich?
Over the past few years, a splendid job has been done here. This was also confirmed by international experts who recently reviewed the research area of supercomputing on behalf of the Helmholtz Association. According to them, Jülich is one of the world's leading institutions. They specifically praised our outstanding strategy for the future.

What does this strategy involve?
We don't just operate supercomputers; we also provide expert advice and methodological support for our national and international users. Our experts develop solutions which are added to our range of applications, continuously expanding our portfolio. Two examples are simulations in brain research and materials science. In joint laboratories, we also work intensively with our industrial partners towards the major objective of realizing exascale. An important role is also played by collaborations within German and European networks such as GAUSS and PRACE.

Prof. Marquardt, thank you very much for this interview.

NEWS IN BRIEF

Tool Use in Industry

Siemens AG and Forschungszentrum Jülich are working together to improve the successful performance analysis tool Scalasca. The aim is to extend Scalasca in such a way that the performance of parallel programs used in industry can be measured and analysed more efficiently. The Jülich Supercomputing Centre (JSC) had initially developed the software for high-performance computing (HPC). However, programs in industry are usually based on programming models other than the Message Passing Interface (MPI) often used in HPC. The activities are part of Runtime Analysis of Parallel Applications for Industrial Software Development (RAPID), a joint project of the Corporate Technology Multicore Expert Center of Siemens AG and JSC.

www.fz-juelich.de/ias/jsc/EN/Research/ HPCTechnology/PerformanceAnalyse/ RAPID/rapid.html

Excellent Early-Career Scientist

Dr. Armel Ulrich Kemloh Wagoum from the Jülich Supercomputing Centre (JSC) received the 2014 Excellence Prize of Forschungszentrum Jülich. The prize endowed with € 5,000 is awarded by Forschungszentrum Jülich to honour early-career scientists who have achieved international success and whose ideas provide fresh impetus for research. The 31-year-old researcher works on pedestrian simulations, aiming to improve safety at large events. He received the award for his PhD project at the University of Wuppertal, which he carried out mainly at JSC. In his thesis, Kemloh investigates how the behaviour of large crowds can be simulated on a computer. He is continuing his research

at JSC's division Civil Security and Traffic. At the moment, he is working on a model for predicting pedestrian trajectories faster than real time.

www.fz-juelich.de/SharedDocs/ Pressemitteilungen/UK/DE/2014/ 14-06-14exzellenz-preis.html

Closer Coordination

Four large European supercomputing centres are combining their activities for the implementation of the European high-performance computing (HPC) strategy. This was agreed upon at a meeting that took place in Barcelona at the end of May between the Barcelona Supercomputing Center (BSC), the French Alternative Energies and Atomic Energy Commission (CEA), Consorzio Interuniversitario per il Calcolo Automatico (CINECA) in Italy, and the Jülich Supercomputing Centre (JSC). In their joint declaration, the four institutions agreed to coordinate their activities in research, development, and innovation more closely. Their aim is a European HPC Flagship industry covering all important areas of HPC.

www.hpc.cineca.it/news/signed-agree- ment-coordinate-development-hpc-technolo- gy-value-chain-europe

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UPCOMING EVENTS

Data Analysis and Data Mining with Python

17–19 November 2014
at the Jülich Supercomputing Centre

The programming language Python allows data to be analysed simply and efficiently. This course provides an overview of Python and an introduction to helpful analysis and evaluation programs for Python: matplotlib for visualization, pandas for time series analysis, and scikit-learn for data mining. The course will be taught in English.

Instructors: Dr. Jan Meinke,
Dr. Olav Zimmermann, JSC

www.fz-juelich.de/ias/jsc/events/ data-mining

Introduction to the Usage and Programming of Supercomputer Resources at Jülich

27–28 November 2014
at the Jülich Supercomputing Centre

In this course, users will be given an overview of the supercomputer resources at Forschungszentrum Jülich and their usage. The course will be taught in English. Course participants will also learn how to make optimal use of the resources allocated to them.

Instructors: JSC employees and representatives of IBM, Intel, and ParTec
www.fz-juelich.de/ias/jsc/events/sc-nov

Introduction to Parallel Programming with MPI and OpenMP

1–3 December 2014
at the Jülich Supercomputing Centre

This course provides an introduction to parallel processing in technical and scientific computing. The focus will be on the application of the Message Passing Interface (MPI), which is the most common programming model for systems with distributed storage. Another topic that will be covered is OpenMP, which is often used in systems with shared storage. State-of-the-art methods from MPI-3.0 will also be discussed, which were developed for the efficient use of today's computing architectures in supercomputers. The course will be taught in German.

Instructor: Dr. Rolf Rabenseifner,
HLRS Stuttgart

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

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