Muon's Magnetic Mystery

Researchers from JSC computed an important contribution to the muon's magnetic moment, which has recently been published in *Nature* (DOI: 10.1038/s41586-021-03418-1). The muon is an elementary particle, a short-lived cousin of the electron. Since about 20 years the calculation of its magnetic moment disagrees with its measurement, indicating that a not-yet-known particle or force might be influencing the muon. An experiment at the Fermi National Accelerator Laboratory (FNAL) in the United States has blatantly confirmed this puzzling discrepancy with an announcement on 7 April 2021. The event has received significant media attention.

Nonetheless, thanks to the computing power of Jülich's JUQUEEN, JURECA, and JUWELS supercomputers, a new ab-initio calculation has challenged previous computations and brought the theoretical prediction closer to the experimental value. According to this result, no new forces or particles are necessary to explain the FNAL and previous measurements. The new calculation has a precision comparable to the experiment and previous theory computations.

As Kalman Szabo, co-author of the paper and leader of the Relativistic Quantum Field Theory research group, points out, "before claiming new physics, we have to understand the differences between our new result and previous theory computations, and new supercomputer calculations are essential for that." Thomas Lippert, another co-author, emphasizes that "this case shows again that Jülich's world-class HPC infrastructure is essential for doing world-class science in Europe." Beside Lippert and Szabo, JSC's Finn Stokes and Csaba Török belong to the research team, which also involves partners from Wuppertal, Marseille, and Budapest.

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Supercomputing against SARS-CoV-2

The first vaccines authorized for use are raising hopes for an end to the pandemic. What is still missing, however, is an effective cure. In the European project EXSCALATE4CORONAVIRUS (E4C), scientists are searching for molecules that block key proteins of the coronavirus. E4C is a public–private consortium backed by the European Commission's H2020 program that aims at fighting the coronavirus by combining the best supercomputing resources and artificial intelligence with state-of-the-art experimental facilities through to clinical validation.

In a recent publication, the Jülich E4C team headed by Prof. Giulia Rossetti from JSC and the Institute of Neuroscience and Medicine (INM-9) reports a new method to identify inhibitors of "Mpro", the main protease of SARS-CoV-2. The virus can no longer reproduce if Mpro is inhibited. When searching for drugs, researchers usually follow the lock-and-key principle: they take a library of known molecules, i.e. "keys", and run a computer test to see which molecule fits into the active-site of the enzyme, the "lock". The shape of SARS-CoV-2 Mpro, however, turns out to be extremely flexible, meaning that the lock is constantly changing. Therefore, the team reversed the search and started "from the lock side". Together with colleagues from E4C and the Human Brain Project, the Jülich team investigated more than 30,000 possible spatial arrangements of the active-site, which were used as a "blueprint" to search for the "keys": with the high-performance computing systems at JSC millions of molecules were screened. Two novel Mpro inhibitors were identified through computer simulations alone. Tests on cell cultures confirmed a moderate antiviral effect. The work appeared in *ACS Pharmacology and Translational Science* (DOI: 10.1021/acsptsci.0c00215) and reached the cover page.

This research demonstrates the value of interdisciplinary trans-European networks and infrastructures to pool expertise in developing new approaches.

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Lessons Learned from $DATA Incident in January 2021

On 26 January 2021, an improbable sequence of unrelated hardware failures in combination with a firmware bug happened, unfortunately leading to partial data loss on the $DATA file system at JSC.

After the system was brought into maintenance, a task force from JSC, together with the system vendor, software provider, and the disk and RAID manufacturers tried to restore and recover as much data as possible in a joint effort. A file system */p/largedata_restore/* was temporarily introduced, to provide access to data recovered from an unofficial backup that was created in January.

To avoid such a situation in the future, several new measures have been implemented. While $DATA was not backed up before – a full restore of this multi-PetaByte file system would take months to finish – $DATA will be split up into several smaller chunks, allowing for an implementation of a backup strategy. As an interim solution, JSC is performing a backup of the existing $DATA despite the well-known restore challenge.

Further information, together with a detailed timeline, can be found in the JUST system documentation on the $DATA incident.

JSC is very sorry for this unfortunate situation and apologizes for the inconvenience to those affected. The Data Services Support Team is happy to help if you have questions regarding the whereabouts of your data and will suggest potential additional steps as part of your recovery.

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New EuroHPC JU Project TIME-X Started

Recent successes have established the potential of parallel-in-time integration as a powerful algorithmic paradigm to unlock the performance of exascale systems. However, these successes have mainly been achieved in a rather academic setting, without an overarching understanding. TIME-X will take the next leap in the development and deployment of this promising new approach for massively parallel HPC simulation, enabling efficient parallel-in-time integration for real-life applications. Funded by the EuroHPC Joint Undertaking and national governments, the consortium of 10 institutions from Belgium, France, Germany, and Switzerland will develop software and novel algorithmic concepts for parallel-in-time integration on current and future HPC architectures. The partners will showcase the potential in three diverse and challenging application fields with high societal impact: weather and climate, medicine, and fusion. To achieve this, the inherently interdisciplinary TIME-X consortium unites all relevant actors at the European level from numerical analysis and applied mathematics, computer science, and the selected application domains in a joint strategic research effort.

This project is led by KU Leuven (Belgium). JSC will primarily work within the work packages “HPC & Implementation” (WP2) and “Impact Maximisation” (WP5). In WP2, JSC and the Hamburg University of Technology will start a joint PhD project on resilient, inexact parallel-in-time integrators, their efficient implementation, and their application. Leading WP5, JSC will furthermore manage training and tutorial activities. Other German partners include the Technical University of Darmstadt, the Technical University of Munich and the University of Wuppertal. The project started on 1 April and will run for three years.

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German and Russian Scientists Join Forces to Improve HPC Performance Tuning

High-performance computing is a key technology of the 21st century. However, exploiting the full power of HPC systems has always been hard and is becoming even harder as the complexity and size of systems and applications continue to grow. On the other hand, the savings potential in terms of energy and CPU hours that application optimization can achieve is enormous.

Key to understanding and ultimately improving the performance of HPC applications is performance measurement. Unfortunately, many HPC systems expose their jobs to substantial amounts of interference (aka noise), leading to significant run-to-run variation. This makes performance measurements generally irreproducible, heavily complicating performance analysis and modelling. On noisy systems, performance analysts usually have to repeat performance measurements several times and then apply statistical analysis to capture trends. Firstly, this is expensive and secondly, extracting trends from a limited series of experiments is far from trivial, as the noise can follow quite irregular patterns.

Prof. Felix Wolf of TU Darmstadt, Dr. Bernd Mohr of the Jülich Supercomputing Centre, and Drs. Dmitry Nikitenko and Konstantin Stefanov of Moscow State University are now addressing this problem in a joint project, named ExtraNoise. It is funded by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) and the Russian Foundation for Basic Research (RFBR). Moreover, Prof. Torsten Hoefler of ETH Zurich is contributing his expertise as an associated partner. In addition to making performance analysis more noise-resilient, the partners also aim to achieve a better understanding of how applications respond to noise in general and which design choices increase or lower their active and passive interference potential. The project, which will run for three years, is coordinated by TU Darmstadt.

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Events

Introduction to the usage and programming of supercomputer resources at Jülich (online event)
Instructors: Representatives of Atos, Intel and ParTec, JSC employees
Date: 17–20 May 2021, 13:00–17:00
https://fz-juelich.de/ias/jsc/2021/sc-1

For further events, talks, and training courses see, https://fz-juelich.de/ias/jsc/events