DATA IN NEW DIMENSIONS



KEY TOPIC: DATA IN NEW DIMENSIONS



BACKGROUND

Faster and smarter

When large research facilities such as the X-ray free-electron laser SwissFEL and the Swiss Light Source SLS are operating at full speed, they produce huge amounts of data. Capturing, processing, and analysing it is an enormous task.

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BACKGROUND Solving the unsolvable

PSI and ETH Zurich have founded the Quantum Computing Hub, where top researchers work together on concepts for quantum computers. One day these machines should comfortably outperform conventional computers in certain computing tasks.

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Step by step – or all at once

The quantum computer is revolutionising computer technology. Because its qubits are interconnected and simultaneously assume many different states, it can perform computational tasks that classical computers can never solve.

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of a financial institution's test centre.

What are you up to, Mr Rüegg?

The war in Ukraine is putting many people in extreme hardship, and it challenges us to reflect on our fundamental values. Director Christian Rüegg explains what measures PSI is taking to extend a helping hand to those affected and discusses how science is being challenged right now. Mr Rüegg, the war in Ukraine is causing great suffering for many people. How can PSI, as a research institute, provide support here?

For one thing, we are supporting Ukrainian researchers affected by the war. PSI is a member of the international network Scholars at Risk, and we participate in the Swiss National Science Foundation's offers of assistance. In addition, we have decided to extend expiring work contracts for Ukrainian staff members until at least the end of the year. Direct, personal exchange on the individual level is also important to us. We are talking with our Ukrainian colleagues and trying to find individual solutions to address their concerns and needs.

In what way does a situation like this challenge the self-image of the scientific community?

We must communicate our values more strongly to the outside world. Science thrives on open and international exchange. There's no room for national, ideological and political boundaries in our self-image. Colleagues from more than 60 nations – including Ukraine and Russia – work at the Paul Scherrer Institute, peacefully pursuing the common goal of advancing science and research for the benefit of all people. Science builds bridges. It doesn't tear them down. This is a precious good that we must protect.

What developments do you expect for the future? We have to fear that this war is leading to a new reality in which political systems are irreconcilably opposed to each other and the fronts between different world views become increasingly hardened. We must learn to deal with this tension. It is especially important in this difficult time to treat each other with respect, to seek dialogue, and not to exclude anyone. This also includes being mutually supportive and not blaming anyone for a situation they did not cause.

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Lock and key

Humans not only like to have all sorts of things at their disposal - they also want to control access to them. So roughly 3,500 years ago, ingenious minds invented a mechanism that helps accomplish this: locks and the corresponding keys. The first exemplars of this mechanical control device were little more than hooks that could be slipped through a small opening in a door. This kind of key was precisely constructed to enable one to reach a bolt and then push it back. Over time and through the work of many more inventors, this system became increasingly refined to keep others right where you want them: outside and locked out, or inside and locked in. In the process, human ingenuity has concentrated mainly on constructing ever more sophisticated locks, fit by keys that were ever more complex and difficult to reverse engineer. The principle that a key with its particular shape must be compatible with a very specific lock extends from mechanics into today's digital world, where people similarly work with keys - though not to guard troves of gold and jewels, but rather to protect valuable information.

& **RESEARCH**

Tracking and docking

It's nearly 130 years since the publication of an article in 1894 in which the chemist - and later Nobel Prize winner - Emil Fischer drew an analogy between the lock and key and the way biological molecules function. In doing so he relied on studies of enzymes, those building blocks of the human body that mediate or accelerate reactions, for example in digestion, or make them possible in the first place. He wrote: "To use an image, I want to say that enzyme and glucoside are like lock and key and must fit together to be able to exert a chemical effect on each other." To date, researchers have found numerous biological systems for which this lock-and-key principle plays a crucial role, for example in our immune system. Within this defence system, so-called antibodies are important. They specifically recognise certain structures on the surface of undesirable intruders or abnormal endogenous cells. They then dock on these structures. PSI researchers exploit this, for example, for radiopharmaceutical diagnosis and therapy, using special antibodies to bring radioisotopes to tumour cells in a targeted way, to detect or eliminate them.



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Data in new dimensions

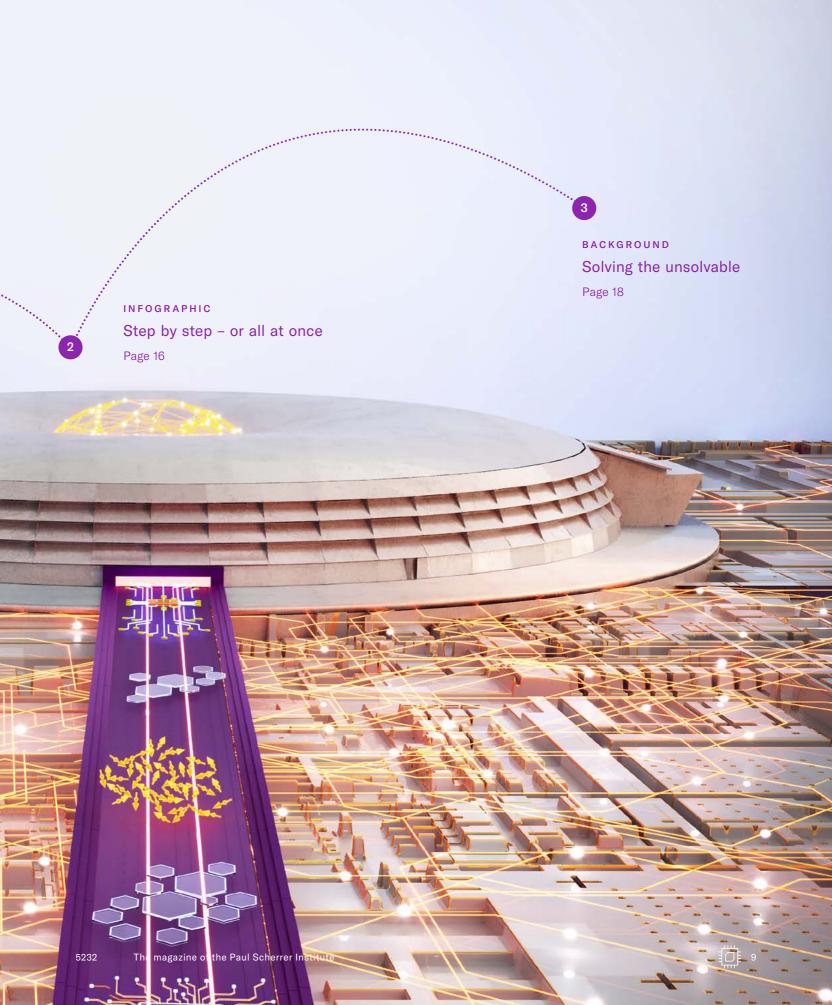
KEY TOPIC

mit

Researchers working at PSI are optimally networked – among themselves as well as with other institutions in Switzerland and worldwide. Among other measures to ensure it stays that way in the future or runs even better, a new research division for Scientific Computing, Theory, and Data has been established at PSI, as well as a Quantum Computing Hub jointly founded with ETH Zurich. This opens up new perspectives for working with data.

Text: Bernd Müller

BACKGROUND Faster and smarter Page 10



Faster and smarter

When large research facilities such as the X-ray free-electron laser SwissFEL and the Swiss Light Source SLS are operating at full speed, they produce enormous amounts of data. To interpret the data and use it, for example, to develop new drugs or materials, PSI is now concentrating its expertise in a new research division: Scientific Computing, Theory, and Data.

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Text: Bernd Müller

Alun Ashton ensures that researchers at PSI can make use of an excellent IT infrastructure. Alun Ashton's research career began in the 1990s, virtually in the Stone Age with regard to the use of computers. "As a student, I saved the data from my measurements on floppy disks," the biochemist and computer scientist recalls. For anyone who doesn't know what he's referring to: floppy disks were interchangeable magnetic storage media that could hold, in their most modern version, a then-phenomenal 1.4 megabytes. "If I had to store the data that is generated today in just one experiment at the Swiss Light Source SLS on such floppies, I'd need millions of them – and several lifetimes to change the floppy disks."

Luckily, information technology has advanced so rapidly that Ashton is able to use his time for more meaningful things. Even large amounts of data from the experiments at PSI are processed and stored quickly enough. So far, at least. By 2025 at the latest, when SLS 2.0 starts operating after an SLS upgrade, the researchers at PSI will face a major problem. After the upgrade to SLS 2.0, experiments can have up to a thousand times higher performance than with today's SLS and other configurations, and can therefore produce much more data than before. In addition, better and faster detectors with higher resolution are coming. Where today's SLS beamline generates one data set per minute, with SLS 2.0 it will generate such amounts of data in less than a second. And that is by no means the end of this rapid development. At SwissFEL, the brand new Jungfrau detector at its full speed could actually generate 50 gigabytes per second; a conventional PC hard drive would be full to the brim after just a few seconds. Overall, the experiments at PSI are currently yielding 3.6 petabytes per year. When SLS 2.0 is fully operational, the experiments there alone could generate up to 30 petabytes per year, which would require around 50,000 PC hard drives. If, for some reason, you want to convert this to floppy disks, add six more zeros.

Wanted: fresh ideas

It has been clear for years: the new challenges at PSI cannot be mastered with old concepts. Fresh ideas are needed on how to master the huge amounts of data in order to answer the increasingly demanding and numerous research questions. And this calls for a new dedicated research focus, with a corresponding organisational structure. The result is the new Scientific Computing, Theory, and Data Division, or SCD for short, which was established in July 2021. The SCD links existing units such as the Laboratory for Simulation and Modelling, whose interim manager is Andreas Adelmann, and new units such as the third site of the Swiss Data Science Centre at PSI, which complements the two locations at EPFL and ETHZ. Around seventy people in four departments are already conducting research and development and providing support; soon there will be a hundred. While the three laboratory heads Andreas Adelmann, Andreas Läuchli and Nicola Marzari are primarily concerned with scientific methods in their respective disciplines, Alun Ashton, with the Scientific IT Infrastructure and Services Department, leads a service unit that provides professional support to scientists at the research division Photon Science, SCD and throughout PSI.

"The research departments should conduct research and should not maintain their own IT departments," Ashton says. That is why centralisation in the SCD is the right step. "We're not reinventing the wheel, but nevertheless with the SCD we have a unique selling point," agrees Andreas Adelmann. The new research division should be better able to take advantage of synergies, distinguish itself in the international scientific community, and attract good people. Adelmann: "The SCD is more than the sum of its parts."

One of his most interesting "customers" is Marco Stampanoni, says Alun Ashton with a wink. The ETH Zurich professor's team has dedicated itself to tomographic X-ray microscopy, which places extremely high demands on computing power and storage. For example, to investigate how a warm gas penetrates a metallic liquid foam during the synthesis of a new alloy, the software has to calculate a three-dimensional snapshot from the data every millisecond. These are huge amounts of data that must be generated and processed. Other colleagues in the same lab are working on computational microscopy and, in particular, ptychography. This enhances conventional X-ray microscopy, which works with lenses but does not reach the fine resolution that would actually be possible with X-rays. In ptychography, an iterative algorithm reconstructs the X-ray image from the raw data of the detector, which is placed far away from the sample, without a lens in-between, and fully leverages on the coherent properties of a synchrotron source. The underlying mathematical operation is computationally very demanding and must be performed thousands of times. With SLS 2.0, the demands on such computing power will increase significantly, and this will make the use of the supercomputer at the Swiss National Supercomputing Centre in Lugano indispensable.

Xavier Deupi studies biomolecules such as light sensors at PSI. To understand exactly how they function, you have to know their structure. In the process of exploring them, immense quantities of data accumulate.

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You can't rely on Moore's law

And the performance gap is likely to widen further, because the researchers at PSI and in many other scientific disciplines can no longer rely on Moore's law. Intel co-founder Gordon Moore predicted in 1965 that the number of transistors, which roughly corresponds to computing power, would double every 18 months – some sources quote a figure of 12 or 24 months. Moore's Law still applies today and will probably continue to do so during this decade. Unfortunately that's not enough. "The brilliance of sources such as SwissFEL or SLS 2.0 is increasing at a faster pace than Moore's law," warns Marco Stampanoni. "This requires smarter solutions rather than just more and more computing power."

One might be machine learning "It's a truism: there's much more in our data than we have been able to utilise up to now," says Andreas Adelmann. Machine learning might find this hidden knowledge amid the huge mountains of data. And it can help save expensive beamtime at SLS and SwissFEL. In the past, the scientists took the data home after completing their measurements to analyse at their leisure. But experiments can also go wrong, and this is often not noticed until months later. Fast models based on machine learning can provide an indication of whether or not the measured values are plausible while an experiment is still running. If not, the experimenters have time to adjust their measuring equipment. Adelmann: "The data collection in experiments and the data analysis are moving closer together."

Here Marco Stampanoni sees the SCD as an important partner. Several users and researchers working at PSI have nothing to do with IT and can be overwhelmed by it. "Physicians do not need to know how a synchrotron works or how and where exactly the data is stored." If they are interested in the effect of a drug on the stability of bones, they do not want to have to work through the ten terabytes of data that a tomographic experiment at the synchrotron has delivered. All they need is a simple graphic from which they can read off the most important results. "In the future," Stampanoni hopes, "the SCD will make a contribution here so that users can interrogate their data questions and generate scientific impact in a reasonable amount of time."

Taking advantage of synergies

Xavier Deupi has no doubt that this will succeed. For the scientist in the Condensed Matter Theory research group, setting up the SCD was inevitable. "PSI needed to consolidate scientific computing in one organisational unit in order to be able to take advantage of synergies." Now that the data scientists are in the same department, they can answer questions from Deupi's team more quickly and start joint projects. "From their IT know-how and our knowledge of biology, new tools for research on proteins are being created."

Deupi describes himself as a "heavy user" of the high-performance Merlin computer at PSI and the supercomputer in Lugano. For one experiment, he uses hundreds of processors that run for hundreds of hours, sometimes even several months. But that's still not enough. Despite the long computing time, Deupi can only simulate changes in proteins that last a few microseconds. But when a molecule binds to a protein - for example adrenaline to receptors in heart cells - it takes at least milliseconds. Around one-third of all drugs bind to the proteins that Deupi studies. If it were possible to watch the entire process as if in a three-dimensional video, that would be a breakthrough for the development of such drugs. But even the most powerful computers are not yet able to do this.

So why make it so complicated when it can also be done simply? Many have been asking this question since Google introduced AlphaFold, a software that uses artificial intelligence to build models of such proteins much more rapidly and accurately. You just enter the sequence and AlphaFold spits out the structure. "AlphaFold is extremely good," praises Deupi. Yet the end of structural biology that some are already prophesying is not in sight. And he's not worried about his job either. Because, firstly, the Google algorithm does not predict the entire structure of a protein and, secondly, you cannot simply infer the function of the protein from the structure. "AlphaFold makes no statements about how such proteins move." This is precisely why large research facilities such as SLS and SwissFEL are still needed. "AlphaFold doesn't replace these machines. Rather, they complement each other."

Seeing the transformation through

The SCD is exactly the right place to test such new tools. To do this, experimenters, theoreticians, computer experts, engineers, and many more have to talk to each other. This is necessary so that computer scientists can find the right solutions for them, according to Marie Yao. She was hired at the SCD specifically to overcome the Babylonian confusion of languages and see the transformation through to ensure the best possible scientific results. If she worked in a company, she would call herself a manager for strategic alliances. "Change isn't always easy," says Yao, who worked for several years in a similar position at Oak Ridge National Laboratory in the USA. Some employees might cling to old processes out of fear that they will lose their value. She sees her role as promoting teamwork and creating an environment in which everyone feels secure and appreciated to contribute to better technical solutions.

Within Alun Ashton's team at the interface between the SCD and other PSI divisions, Yao is coordinating development for the start of SLS 2.0 in 2025 and is also contributing to the development of technical solutions. By then, hardware, software, and networks must be ready and able to cope with the enormous amounts of data. A holistic approach is important, according to Yao: "The whole data pipeline is only as strong as its weakest link."

An increasingly weak link in science, as in other areas of the economy, is the shortage of skilled workers. If there are no suitable experts, they have to be trained, often in interdisciplinary areas, says Yao. "Society gives us well-trained professionals, so we should give something back to society – one of the ways is by getting engaging with the education of the next generation."

Tomorrow's researchers have a lot of work ahead of them. Software for solving scientific problems is often 20 years old and in some cases is not efficient enough. Overcoming the deficits with even more computing power no longer works today. Scientific software must be made fit for the rapidly growing amounts of data and for trends in high-performance computing, such as the use of graphics processing units instead of conventional central processing units. "The SCD can help to attract people who can do just that," Marie Yao believes.

Machine and modelling

That has already succeeded in the case of Andreas Läuchli. He, along with Andreas Adelmann and Nicola Marzari, is head of the third scientific laboratory at the SCD, which deals with theoretical and computational physics. A year ago he came from Innsbruck to PSI and EPF Lausanne, where he also holds an academic chair. Läuchli is expected to strengthen the theory but also work hand in hand with the experimental physicists and give them ideas for new experiments, especially at SwissFEL and at SLS 2.0. Läuchli considers establishing the SCD a good decision. "Experiments and theory are becoming more and more complex. So whoever wants

"Whoever wants to do research and publish successfully needs a good machine and good modelling."

Andreas Läuchli, head of the Laboratory for Theoretical and Computational Physics

to do research and publish successfully needs a good machine and good modelling." He views the SCD as an important component of this synthesis.

Läuchli's hobbyhorse is many-particle systems, which in physics includes everything that is more than a single hydrogen atom – in other words, almost all matter. All paths towards determining energy levels in these systems pass through the Schrödinger equation. It provides exact results for the hydrogen atom, but the computational effort increases exponentially for many-particle systems. For this reason, researchers resort to approximations even with just a few atoms. Yet it is not always certain that the approximations are close enough to reality.

Then Läuchli brings out the crowbar. "Brute force" is the term for the method he uses to subdue the Schrödinger equation for up to 50 particles, with raw computing power. Then 20,000 processor cores with several terabytes of RAM can work together on such a problem simultaneously, for several weeks. Even the supercomputer in Lugano is then temporarily off-limits to other users. Läuchli: "Sometimes the brute force method is important to test whether or not our approximations are really valid."

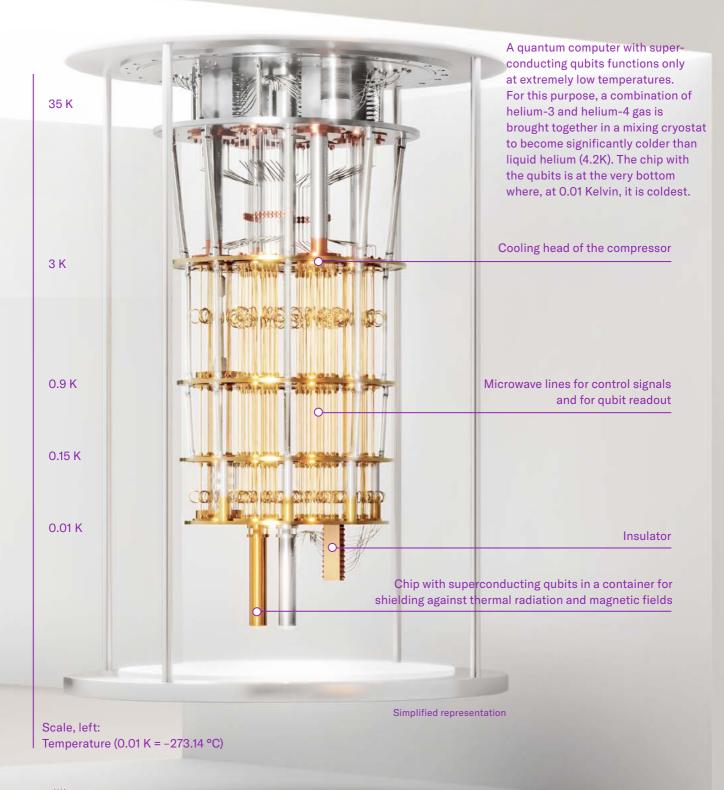
Naturally, not every work group can use the computer spontaneously. Each team needs to submit an application of up to 20 pages to the SNSC in Lugano, which is evaluated according to the scientific knowledge to be gained and the efficiency of the algorithms. The use of the computer cluster Merlin at PSI is less bureaucratic. However, anyone who has consumed a lot of computing time there will be downgraded and will have to get in line again, farther back in the queue.

Laboratory head Andreas Läuchli investigates, among other things, how energy levels or magnetic moments behave in so-called many-particle systems. In this enormously complex task, a quantum computer could serve him well.

Andreas Läuchli has great expectations for the Quantum Computing Hub (QCH), which was established at PSI in 2021 (see article on page 18). "Perhaps in the future we will be able to map physics problems that cannot be calculated on classical computers onto quantum computers." The Hub would also benefit from this cooperation because quantum computers are based on the physical principles that Läuchli and his team are investigating. Andreas Läuchli: "SCD and QCH working together – I see great potential there."

Step by step – or all at once

The quantum computer is opening up new possibilities in computer technology. Because its qubits are interconnected and simultaneously assume many different states, it can perform computational tasks that classical computers can never solve.

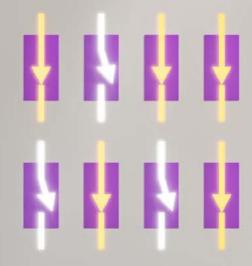


DATA IN NEW DIMENSIONS

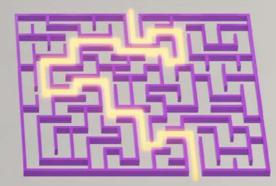
Classical computer



Each bit can only assume one of two states at a time: 0 or 1 – like a light bulb that is switched on or off.



Besides that, the bits are independent and do not affect each other.

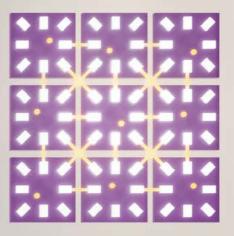


As a result, a classical computer can only perform one calculation at a time. To find the way through a labyrinth, it must try out all possibilities, one after another.

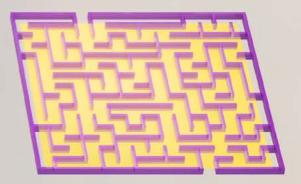
Quantum computer



Each qubit can assume any number of states at any time – like a light bulb whose brightness and colour tone are continuously variable.



Qubits (here, in ion traps on a microchip) are entangled, so they influence each other.



As a result, the quantum computer can carry out many calculations simultaneously – for example, trying out all possible paths through a labyrinth in parallel. In the end, you get an answer. Each calculation must be repeated several times, however, so that the probable best path emerges from the statistics of the answers.

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Solving the unsolvable

PSI and ETH Zurich have co-founded the Quantum Computing Hub, where top researchers work together on concepts for quantum computers. One day these machines should comfortably outperform conventional computers in certain computing tasks.

Text: Bernd Müller

Kirsten Moselund and Cornelius Hempel will be conducting research at PSI on how a functioning quantum computer could be implemented. If you were to make a list of the world's leading researchers in quantum computing, Jonathan Home and Andreas Wallraff would be close to the top. These two physics professors from ETH Zurich are masters of their field – yet they are not alone: in recent years, quantum research expertise in Switzerland has developed to a level comparable with much larger nations. There are also numerous young companies developing quantum technologies, such as Zurich Instruments and ID Quantique.

All good, right? Not quite. "Quantum technology has taken a big step towards practical application," says Gabriel Aeppli, head of the Photon Science Division at PSI. "For that, it now requires experts with capabilities that go far beyond what even a renowned university like ETH Zurich can provide – above all, engineers who can translate research results into functioning prototypes." And this is where PSI comes into play. "A national laboratory like PSI unites all the skills needed for this scale-up," says Aeppli. This means the transition from a basic experiment to a technology that can, in the foreseeable future, solve real – and eventually also commercial – problems.

For years, PSI has been proving it can do this at large research facilities such as the Swiss Light Source SLS and the X-ray free-electron laser SwissFEL, where technologies are needed that can't just be procured anywhere. As a national laboratory, PSI benefits from the fact that experienced experts can work on complex challenges over a longer period of time. This is not the case with a research team at a university. "We have many talented scientists, but they have to leave the team after a few years, mostly after their doctorate," says Jonathan Home. Therefore the kind of scale-up that PSI can accomplish would not be possible at ETH Zurich.

ETH Zurich and PSI recognised that the two institutions perfectly complement each other in the development of quantum computers. That's why they jointly established the Quantum Computing Hub. Organisationally, this research institution is assigned to Gabriel Aeppli's Photon Science Division and, within it, to the Laboratory for Nano and Quantum Technologies. The Quantum Computing Hub is housed on the PSI campus near Villigen, where a building has been upgraded for quantum research. Researchers there are pursuing different approaches to realising a quantum computer.

On the basement level, the team of Jonathan Home, Professor of Experimental Quantum Information, is now building quantum circuits based on ion traps. On the upper floor, Professor of Solid State Physics Andreas Wallraff is engaged with the same questions. However, he and his team are using ultracold superconducting components. Two more research teams are set to join this year, exploring other concepts for building quantum computers. From the current 20 researchers, the Hub is set to grow to 100 in five years. In addition, a clean room with nanofabrication facilities is being built close to PSI in the new Park Innovaare, where the researchers will produce their own qubits, the basis of every quantum computer.

Kirsten Moselund, who since February 2022 has headed the Laboratory for Nano and Quantum Technologies at PSI and thus the Quantum Computing Hub as well, is charged with organising this growth. A professor of Electronics and Microtechnology at EPF Lausanne, Moselund previously worked at IBM Research Zurich, located in Rüschlikon. There she conducted research on nanophotonics. "In the new hub, we are bringing together quantum technologies and a strong technology platform," says Moselund. A real race has broken out for quantum computers, similar to the race for the first manned moon landing. Moselund sees the hub as being in an excellent starting position: "ETH Zurich and PSI complement each other very well. And with large research facilities such as SLS and SwissFEL, we have opportunities that others do not have, for example when we want to investigate defects in materials for future quantum chips."

"Switzerland needs a strong presence in quantum technologies."

Kirsten Moselund, Head of the Laboratory for Nano and Quantum Technologies

No universal and fault-tolerant quantum computers are commercially available yet. Devices such as those being developed by IBM and Google currently have just over a hundred qubits. Because each qubit can not only assume the states zero and one, but any arbitrary combination of states, and because the qubits are "entangled" with one another, a few dozen qubits can already process problems that would be too complex for microprocessors with billions of transistors. In the quantum computers demonstrated so far, however, only a few qubits are ever entangled at the same time, which limits actual computing power.

"Already today researchers are having fun with quantum computers," says Cornelius Hempel, head of the Ion Trap Quantum Computing Group at PSI. There are questions in physics that can be solved with just fifty gubits. At ETH Zurich, Home's team uses electromagnetic fields to confine groups of atoms in an ion trap and, by manipulating them with laser light, to have them interact and carry out logical arithmetic operations (see also graphic on page 16). PSI is planning microchips with dozens of ion traps between which ions can be pushed back and forth and which, together, form a larger quantum chip. Laser light fed into the chip via fine optical fibres manipulates the atoms, changing their energetic states, while electric fields move them back and forth. Identical by nature, atoms are perfect qubits - the challenge lies in controlling them.

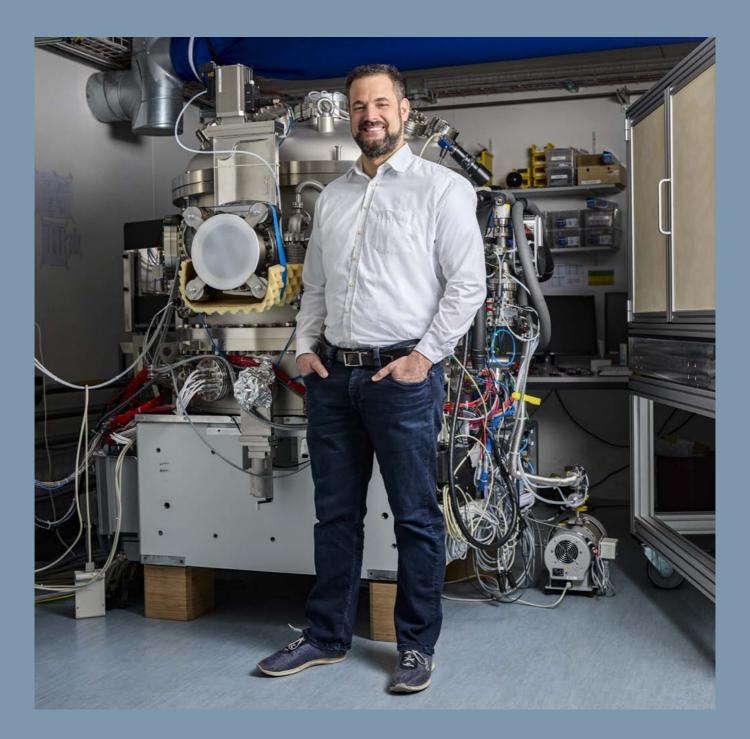
For practical applications in industry, this is still uninteresting. For example, nitrogenase is an enzyme that bacteria use to fix nitrogen from the air, which acts as a natural fertiliser for plants. Today, as a hundred years ago, artificial fertiliser is produced using the Haber-Bosch process, which requires a great deal of energy. Knowing how the enzyme works and being able to replicate it would be a breakthrough for the global food supply. But this puzzle cannot be solved even with supercomputers. However, a quantum computer with a thousand error-free qubits could model the enzyme in just a million calculations.

The emphasis here is on "error-free" operation, because gubits currently calculate with an error rate of one percent, which is far too high. For comparison: a transistor only miscalculates once in 10²⁷ (a number with 27 zeros) arithmetic operations. Logical qubits offer a way out of this impasse. These consist of several physical gubits and can detect and eliminate errors. Error correction has already been demonstrated on a small scale in the Wallraff and Home laboratories. And error correction is getting better with the use of larger and larger systems. For the nitrogenase problem, some estimates predict it would take about a thousand physical qubits for one fail-safe logical qubit, which means the number of gubits in the computer would need to be about a million.

So how to get from the 127 physical qubits recently demonstrated by IBM in one chip to a million qubits? That appears to be just a matter of scaling up fabrication. Unfortunately, there is currently no way to build larger and more complex systems without introducing more errors into the system. In this respect, all reports of success, such as those regularly disseminated by Google, IBM and Amazon, should be treated with caution. These are bugprone devices not yet ready to take direct advantage of more qubits. A desktop quantum computer that solves real problems will not exist in the next ten years, maybe ever. But the researchers are confident that commercial quantum computers are possible. Such a computer with millions of qubits would operate in a data centre alongside traditional supercomputers.

It is still not at all clear which qubit concept will prevail. In addition to superconducting qubits and ion traps, researchers around the world are still working on half a dozen other ideas – which will also be pursued at the Quantum Computing Hub, assuming there are promising concepts for their implementation. There may also be completely new options, speculates Cornelius Hempel. For example: "Who knows – maybe our colleagues at SLS or SwissFEL will find a new material from which we can build much better qubits."

For Kirsten Moselund, there is no alternative to the Quantum Computing Hub. "Switzerland needs a strong presence in quantum technologies," the engineer insists. Commercial quantum computers, which Google, Amazon and others will probably make accessible as a cloud service at some point, are a black box that you're not meant to look inside. Moselund: "To be able to use quantum computers sensibly, we need to know what's happening under the hood. And that's what we offer at PSI." ◆



Circuit diagram of the brain

The interconnections of nerve cells in the brain are formed on the basis of experience and learning processes. It remains unclear what the pattern of connections looks like. Neuroscientist Adrian Wanner wants to use the X-ray light of the Swiss Light Source SLS to investigate neuronal structures down to their finest ramifications. Among the questions he will pursue is how neurons process information. The insights gained concerning the way the brain works will make medical therapies for neurodegenerative diseases possible.

Hercules and batteries, X-rayed

For ancient artefacts and modern technologies alike, examination methods that leave the object completely intact are required. For this, researchers at PSI use elementary particles called muons and are developing a new experimental method that is useful for archaeology and can also answer questions relevant to battery development.

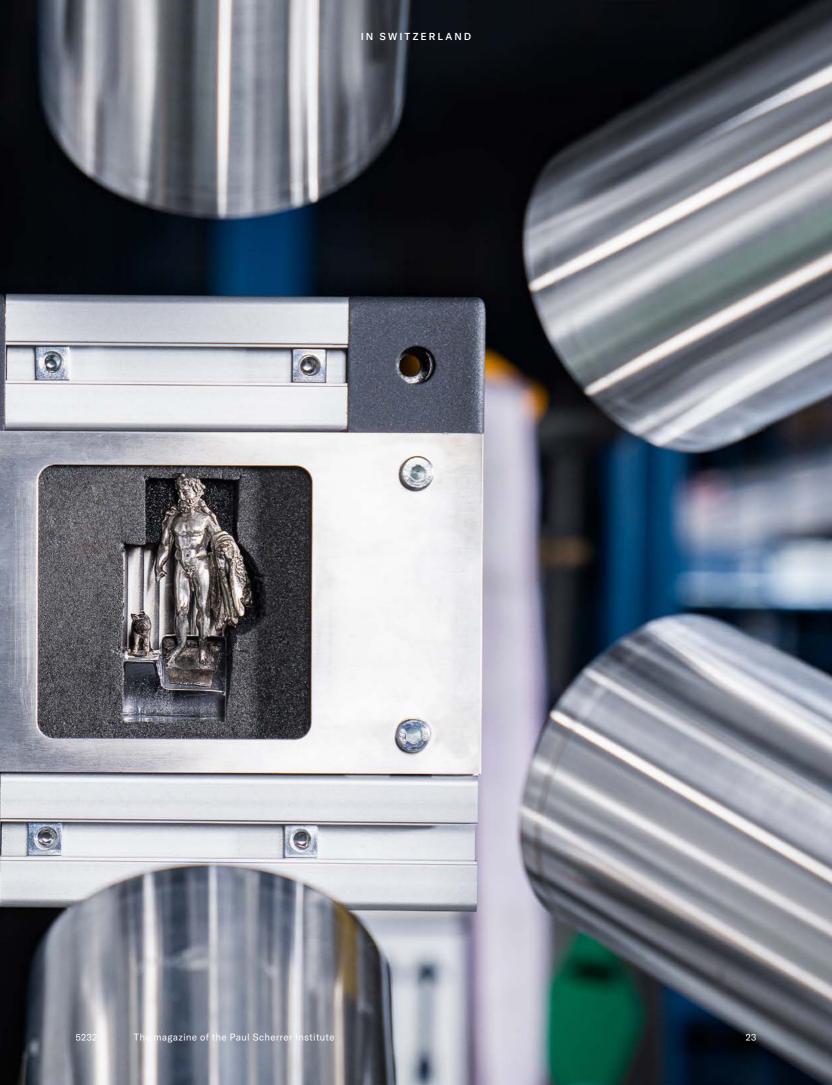
Text: Barbara Vonarburg

Padded in cut-to-fit foam: A six-centimetre-tall silver statuette of the Greek hero Hercules, accompanied by a mythological boar, waits to

IN SWITZERLAND

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be examined with muons.



By hand, two researchers are putting the final touches on preparations to transport a measuring instrument. For security, the apparatus – developed and assembled by a research group at PSI over the past ten months – is framed by a set of rods roughly two and a half metres high. "This instrument will enable us to non-invasively determine the chemical composition of a sample," explains Lars Gerchow, who was responsible for designing it. For this, the researchers will need special elementary particles called muons.

Gerchow, his colleague Sayani Biswas, and others lending a helping hand are in the large hall housing PSI's muon source. Muons are naturally occurring elementary particles that are pervasive as part of cosmic radiation. "On average, a muon rains down on us every second," the physicist explains. Nevertheless, at PSI these particles are generated artificially with the help of a large accelerator.

The measuring instrument is ready to be moved to its intended place – a delicate task that requires an indoor crane. The crane operator receives instructions from the ground by radio, and then the instrument is hoisted aloft.

Gold and silver from a Roman settlement

In the control room, from which the physicists will monitor the muon experiment, archaeologist Isabel Megatli is making the final preparations for her mission. She has brought precious gold and silver objects that were excavated in Augusta Raurica, one of the most important Roman sites in Switzerland, around ten kilometres east of Basel. Especially lovely are two figurines from the second century CE, representations of Roman deities from a household shrine. Hercules with a lion's skin over his arm, just six centimetres tall, is accompanied by a mythological boar that the researchers have nicknamed "the little pig". Minerva wears a richly pleated robe and an extravagant helmet.

The statuettes were cast from silver and partially gilded. "We want to know which silver alloy was used," Megatli says. "With previous methods, we could only investigate the outermost hundredths of a millimetre, but often this surface has been adulterated over the course of centuries." With muons, in contrast, it is possible to look inside several millimetres deep.

Megatli has also brought along several ancient pieces of jewellery that were found as grave goods. "The metal casters of antiquity all had their own strict recipes," the archaeologist explains. "If two objects have the same alloy, it is also likely that they were made in the same workshop." Through further examinations, the researchers can sometimes even

"We were able to show that Minerva and Hercules are made of a high-quality silver alloy."

Isabel Megatli, research associate at the Roman settlement of Augusta Raurica.

determine which mine was the source of the metal ores used. "And we can also expose counterfeiters," Megatli says, "as aluminium, for example, has only been processed since the 19th century."

Fingerprint of the elements

Physicist Sayani Biswas explains how the experiment will work. "We have a sample, and we send negatively charged muons to it." An atom in the sample captures a muon. Now, in place of an electron, a muon is orbiting the atom's nucleus. At first it is in an excited state, and then it falls stepwise to its ground state. In the process, X-rays are emitted. The energy of this radiation is characteristic for the type of atom: in other words, the element that has captured the muon. Biswas, who is responsible for the data processing and analysis, points to a previously recorded curve that has sharp peaks, a socalled spectrum. Each element has a specific pattern of such lines in the spectrum – like a fingerprint.

In the hall, the measuring instrument has now been delivered with the utmost care to its destination. Several specialists are now attaching six large X-ray detectors to the rods.

Alex Amato, interim head of the Research with Neutrons and Muons Division at PSI, is also lending a hand. He initiated the project, which is a joint effort of PSI, the Roman settlement of Augusta Raurica, Empa, and the Natural History Museum of Bern, with financial support from the Swiss National Science Foundation, which is providing nearly one and a half million Swiss francs within the framework of the Sinergia Programme. "Thirty years ago, researchers at PSI were already trying to use muons to determine the elementary composition of materials deep inside, but at that time the particle beam was not sufficiently intense," the research leader explains. "Today we're twenty times better. And our instruments are a thousand times more powerful than our colleagues' in the UK and Japan who are performing similar experiments."



The Sinergia description also states: "This project aims to make Switzerland one of the leading locations worldwide in non-destructive element analysis." And huge demand is expected from industry, culture, and academic fields.

But the researchers are still at the beginning – gathered in the control room before a row of computer monitors. Now there is no human activity in the experiment area, but only the statuettes of Hercules and Minerva, awaiting examination. They stand in foam holders cut to fit and placed in metal frames, which in turn have been positioned on a rail in front of the detectors. In the control room, Lars Gerchow gives the command: "We can start the beam." With that, the measurements begin, and will continue around the clock.

Batteries in the muon beam

Two days later, the researchers place a completely different object in the muon beam: a lithium-ion battery. "We want to find out how the battery ages through use," explains Ryo Asakura, a researcher at Empa in Dübendorf. For this he has brought both a new and a used battery to PSI – little flat packs that look like the batteries in smartphones. "The cathode of these batteries contains nickel, manganese, and cobalt," Asakura explains. Over time, these metals shed from the cathode – which contributes to the ageing of this type of battery. The measurements with the muons should make this process visible. Later, the researchers would like to trace what happens to the lithium in the battery. The results should help to improve both the energy density and the safety of lithium-ion batteries.

After a week, the measurements on the ancient objects as well as the batteries have been completed. "With the battery, we see nice lines for nickel, manganese, and cobalt in the spectrum," says Sayani Biswas with satisfaction. In the coming weeks, Ryo Asakura will repeatedly charge and discharge the batteries at Empa so that, during a second measurement period, the changes following this ageing process can be observed.

The spikes show two silver isotopes

In the measurement data on the samples from Augusta Raurica, Sayani Biswas points to several overlapping peaks: "Here you can see two different silver isotopes," that is, minimally different types of silver atoms. The relationship between these isotopes can help archaeologist Isabel Megatli determine the origin of the silver. She is already enthusiastic about the preliminary results: "We were able to show that Minerva and Hercules are made of a high-quality silver alloy."

The next measurement period is planned to start in two months. Then, besides other antique pieces and the lithium-ion batteries, a Bronze Age arrowhead that may have been made from meteorite material will be examined. "To answer this question, too, our non-destructive method is perfectly suited," says Lars Gerchow. ◆

Latest PSI research news

1 New, better coronavirus rapid test

Researchers at the Paul Scherrer Institute PSI and the University of Basel have developed a rapid test for Covid-19. Its novel functional principle allows reliable and quantifiable conclusions about a Covid-19 disease and its course. But it can also detect Covid variants or other pathogens such as influenza. Unlike antigen tests, it does not directly detect components of the virus, but rather the antibodies that the immune system produces in response to the infection. Among other things, it makes use of very narrow tubes, so-called capillaries, in which beads with antibodies docked to them get stuck at specific points. The test promises significantly more information and is just as inexpensive, quick, and easy to use as previous antibody tests. Before it can go into widespread use, however, it must still undergo further testing and optimisation.

Further information: http://psi.ch/en/node/49630

29 blood samples were checked using the new kit.

Z minutes is all it should take to perform the test once optimised.

100 times thinner than a human hair: the width of the test capillaries at their narrowest point.

2 Simulant material could aid in Fukushima clean-up

Researchers from the Paul Scherrer Institute PSI, in a project led by scientists from the University of Sheffield, have developed a new simulation of the most dangerous radioactive debris from the damaged nuclear power plant in Fukushima, Japan. Using what is known about the materials used in the Fukushima reactors - the fuel, cladding, and concrete, for example - a recipe for the fuel debris was developed. The researchers heated these materials to the extremely high temperatures experienced during the accident, thereby creating a low-radioactivity version that should correspond to the actual fuel element debris. For the first time, almost 11 years after the disaster, authorities can learn more about the chemical composition and mechanical properties of the debris and develop safe strategies for its disposal, using the simulant material. The researchers used the Swiss Light Source SLS for their investigations. Their study could give an enormous boost to the clean-up effort.

Further information: http://psi.ch/en/node/49916

3 More insight into the sense of sight

PSI researchers have shed light on an important component of the eye. This concerns a protein in the rod cells of the retina that enable us to see in half-light. Acting as an ion channel in the cell membrane, the protein is responsible for relaying the optical signal from the eye to the brain. The ion channel acts as a gatekeeper controlling whether specific particles are allowed to the interior of the receptor cell. It is embedded in the fat-rich shell - the cell membrane - of the rod cells. In darkness, the jon channel, and thus the gate to the cell, is completely open. But when light hits the eye, it triggers a cascade of processes in the rod cells. This ultimately causes the gate to close, with the result that positively charged particles, such as calcium ions, can no longer enter the cell. This electrochemical signal continues via the nerve cells into the brain's visual cortex, where a visual impression - such as a flash of light - is created. People in whom the molecule doesn't work properly due to a hereditary disease go blind. The researchers have now deciphered the three-dimensional structure of the protein, paving the way for innovative medical treatments.

Further information: http://psi.ch/en/node/49360

4 Manure and slurry are underused energy resources

Barely any of Switzerland's solid and liquid animal manure is used to generate energy. Yet fermentation of manure and slurry has the potential to replace fossil fuels and make agriculture more climate-friendly. A publication by energy researchers from institutions including the Swiss Federal Institute for Forest. Snow and Landscape Research WSL and PSI aims to help government and industry professionals better exploit this valuable resource. The study gives numerous tips for improvement. Technical innovations in their process could make biogas plants more cost-effective. Pre-treatments with microorganisms boost the energy yield, as does separating the solid and liquid components of animal waste. Also, the largely unused waste heat from the plants contains yet more energy. Taken together, these factors could make investments in anaerobic digestion plants more attractive to farmers. So-called hydrothermal processes are an attractive alternative to the fermentation of manure and slurry, since the biomass can be converted largely without transformation losses. This could benefit the power supply nationwide.

Further information: http://psi.ch/en/node/49910

Art at PSI

Works of art can inspire us with their beauty, make us think, or simply amuse us. They invite us to forget the routine of everyday life for a few moments and look, as if through a window, into another world. On these pages we display a selection of artworks at PSI that invite you to engage with them.

Text: Christian Heid

Crystalline Growth

Gerda Steiner & Jörg Lenzlinger, 2008

Yellow, orange, red, brown, light and dark green, light and dark blue – in all these colours, these motley crystals appear to virtually hover in the redesigned Visitor Centre. New shapes and colours emerge where the spherical, coral-like, and needleshaped crystal forms meet. Staged by the artist duo Steiner/Lenzlinger, the crystals grow out of a saturated salt solution through the gradual evaporation of water; the shapes and colours that emerge in the process are determined by the different substances in the solution. Crystals also find use at PSI in materials research and biology.



DOUBLE-TRUNKER "our mammoth"

Bruno Weber, 2003

Painter, graphic artist, sculptor, inventor, carpenter, mason, house painter, plasterer and architect: the Dietikon-based artist Bruno Weber is as versatile as his collected works are unique. The roughly two-metre-high "double trunker" in front of the PSI auditorium aptly demonstrates that his works are close to the art movement of fantastic realism, in which fabulous creatures and dream figures play a definitive role and which, in Weber's case, is characterised by a closeness to nature. The relationship between the "double trunker" and "our mammoth" is easy to guess.

Spiral

Cornélia Patthey, 2016

With its three-metre diameter, this mirrored spiral by the Lausanne-based artist Cornélia Patthey is an imposing artwork in the entrance hall of the X-ray free-electron laser SwissFEL. It welcomes visitors to the large research facility, which itself stretches over seven hundred and forty metres in length. The observer's gaze is led into two infinities: inward, into the infinitesimal; outward, into the interminably large. With this visual contradiction, the spiral stands for something all-encompassing, something eternal, daring us to address questions of how and why – questions that bring creative artists and researchers closer together.

"CYCLUS"

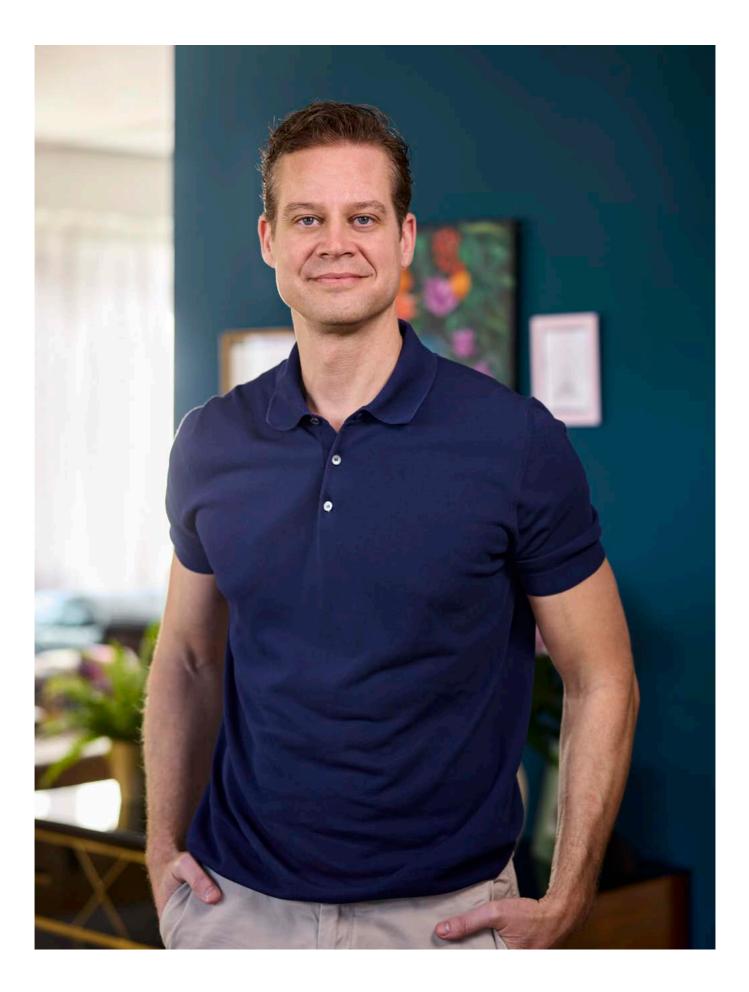
Beni Schweizer, 1983/84

The gleaming golden-coloured rods of this installation in the stairway of the auditorium immediately capture the eye. It doesn't matter whether you're going down to the basement or up to the first floor, on your way you must circle around the artwork by autodidact Beni Schweizer, which fills the clear space in the middle of the stairwell. To orbit: the Latin word cyclus means orbit, and the Latin inscription – in capital letters and with inverted commas – points insistently to another, ancient concept of time that was strongly influenced by the constantly recurring cycle of nature and the heavenly bodies.

Recumbent figure

Roman Signer, 1998 Walter A. Bechtler-Stiftung

This work of art is located not far from the Aare River, which flows through the middle of PSI: installed under the heels of the black rubber boots are spray nozzles that produce jets of water that turn on and off. The mechanism that the two boots are fastened to has some play in it, so that movement, standstill, and a mixture of both are possible. The Appenzell-based artist Roman Signer designed it all in such a way that standstill and movement occur unpredictably. Thus the "recumbent figure" above the asphalt possesses an unpredictable life of its own.



Seizing opportunities

IN PERSON

As a doctoral candidate at PSI, Philipp Kraft built a novel X-ray detector. Today he is taking part in the modernisation of a financial institution's test centre. Doing the job from home works well, he says, but it also has pitfalls.

Text: Barbara Vonarburg

"Architect in the test centre" is Philipp Kraft's job title at PostFinance, the financial services subsidiary of Swiss Post. That does not mean he is a construction professional in the conventional sense, but rather that Kraft deals with information technologies. "As IT architect, I plan and support projects for improvement, optimisation and modernisation in general within the test centre," explains the 44-year-old physicist, who did his doctoral research at PSI. "I work out visions, objectives and roadmaps for future IT development, and I represent the test centre with respect to overarching issues of IT across the enterprise."

The test centre is an essential part of every banking. "This department determines whether or not a new software programme or update will be released," Kraft explains. So, for example, it must be guaranteed that information about the opening of a new account will be stored correctly in the archive, or that everything associated with a payment arrives in the right place and gets booked. "We carry out the system tests," Kraft says, adding: "Currently we are in a transitional phase." Previously, an applications team prepared new software, had it checked out in the test centre and, if everything was in order, switched to the new version twice a year. "These days everyone is agile," Kraft says. That means software is made available continuously, and a rapid rollout is the ultimate goal. "Unfortunately, we are still relatively far from that," says the IT architect. Although there are now four release dates per year, much more automation and quality assurance will be needed as early as possible in the development process. "This is currently one of my main issues."

Kraft started work at PostFinance in August 2020, in the midst of the Covid-19 crisis, and therefore is not in the office at the company headquarters in Bern, but rather at home in an environment that, at first glance, does not appear to fit the austere world of finance at all. The interior design of the house is very original, with many colourful pictures and comical hunting trophies from an old storeroom on the walls. "My wife is responsible for that," Kraft explains. "Painting is her hobby, and she has an artistic flair. I'm responsible for technical things like the robotic vacuum cleaner and automatic controls for the lamps and rolling shutters." Scratching posts also reveal the existence of two four-legged housemates, and soon Gaston the cat actually makes an appearance. The big cat with silky fur and blue eyes welcomes visitors and follows what's happening with interest.

Working from home generally functions well, Kraft explains, although so far he has only seen profile pictures of some of his co-workers. But there are situations in which physical presence would be better, for example during appraisal interviews, when things aren't running smoothly, or when you'd like to use an improvised visual aid to help explain something. "On the computer, you struggle with the technology, whereas otherwise you can sketch it on paper or a whiteboard instead," he says.

Studying physics in spite of doubts

In his younger days, Kraft could hardly have imagined that he would one day work in a bank. He actually wanted to start an apprenticeship as an electronics technician or an assistant in a physics laboratory. "But looking into it, I noticed that it wasn't the lab assistant but rather the physicist who had the really cool job," he says. He then completed high school, but after graduating, he again had doubts as to where his path would lead: "Back then I was playing saxophone in a band and was thinking about becoming a musician." His music teacher suggested that he play music eight hours a day for three days during the holidays. The young saxophonist followed this advice and decided: "That's enough." On his mother's advice, he signed up for career counselling. "Because of intelligence tests, and others, I was advised against studying physics," Kraft says. "The psychologist thought I would have to work day and night just to complete my studies." What was no doubt meant to deter him actually spurred him on instead. He registered as a physics student at ETH Zurich and succeeded.

He wanted to do his diploma thesis in the field of particle physics, to get to the bottom of the origin of the universe. He went to the Paul Scherrer Institute to apply in person. But the team leaders in particle physics at PSI had no free places. "I was advised to go down the corridor where another group was using the same technologies," Kraft says. "I was extremely lucky." That's because the highly motivated group that gave him a friendly welcome was in the midst of developing novel detectors for the Swiss Light Source SLS - an undertaking that ultimately proved so successful that it spawned the spin-off company Dectris. Today Dectris is world leader in sales of the X-ray detector called Pilatus and others, for use in synchrotron facilities. Silicon sensors convert X-ray photons into electrical charges, which can be recorded and processed electronically. In this way, the individual photons can be counted.

A drastic diagnosis

Kraft seized the opportunity to work in this group as a graduate student. For his thesis, he was allowed to study the new and eagerly awaited readout chip, and he helped to fix an error on it. He liked working in the team so much that he stayed at PSI for his doctoral thesis. While the first Pilatus detectors were being used to study protein crystals, Kraft was tasked with building a smaller detector for what is known as small-angle X-ray scattering, which can be used to image nanostructures of a wide variety of materials. The doctoral candidate was working on software for the detector, writing automation scripts for experiments and doing data analysis when he got cancer at the age of 28. "The diagnosis was completely unexpected and life-changing," Kraft says. He had to undergo chemotherapy and was on 100 percent sick leave. "But at home in my little apartment, I felt the walls closing in on me," he recalls. So he went back to PSI, where he had company, and worked whenever he could. In this way he was still able to successfully complete his doctoral thesis.

He presented his results at a conference in Berkeley, California, and thought about continuing his research on the West Coast of the USA, but once he was home, he rejected the idea. "Shortly before, I had fallen head over heels in love, and the woman of my dreams – she still is – preferred to stay in Switzerland," he says. This newly won happiness was something he didn't want to risk losing. He accepted an offer from the IT firm Supercomputing Systems (SCS), and he worked for this firm in Zurich for seven and a half years before moving to the Kistler Group, headquartered in Winterthur, which specialises in measurement technology. At SCS he had worked as a software developer and later as a project leader for a variety of customers, for example on the development of an intelligent gate sensor and on a new instrument for determining blood groups.

At Kistler Kraft, he served as head of product development and as a software project leader in the areas of roads and traffic, biomechanics, and cutting force measurement. The main focus was on the use of existing sensors. "For example, we integrated various force sensors into a sprint starting block, and for that we developed the readout electronics as well as the software for readout and analysis," Kraft says. The software development was done in Slovakia. "At the beginning, that was very exciting," he recalls. But the problems with the software engineers' new and then highly praised "agile" approach to development quickly became clear: it made planning more difficult. If new requirements arose after an initial development phase, the architecture had to grow with them. "But if you start building a garden shed and then try to convert it into a multifamily home, the foundation simply isn't going to be good enough," Kraft explains.

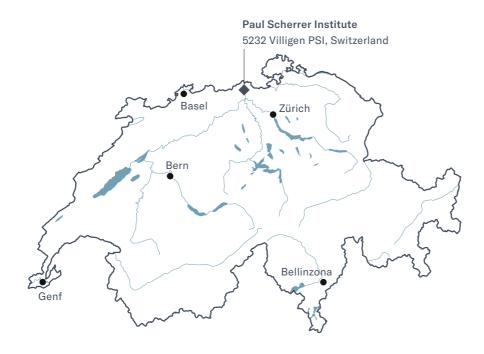
Kraft continued his education in software topics through courses and extensive reading in specialist literature. Now he's applying his knowledge at PostFinance. To balance the mental work, he likes to do sports. "I begin every day at six o'clock with a fitness training session before I start work at eight," he says. He and his wife enjoy travelling, mainly in southern Europe, though a recent trip inspired by the television series "Death in Paradise" - in which a British detective inspector solves tricky cases in the tropical environment of the Caribbean - took them to Guadeloupe. "The landscape really was as beautiful as in the film," he recalls. He has fond memories of PSI. He was particularly impressed by the international environment and the people in his team."I was the carefree youngster, while my colleagues had families, but we still got on well together: "It was a memorable time." 🔶



"Because of intelligence tests, and others, I was advised against studying physics."

Philipp Kraft, software specialist at PostFinance

From our base in Aargau we conduct research for Switzerland as part of a global collaboration.



5232 is Switzerland's prime address for experiments on large research facilities. The Paul Scherrer Institute PSI even has its own postcode, a distinction that seems justified for an institute that extends over 342,000 square metres, has its own bridge across the River Aare, and has around 2,200 employees – more people than in most of the surrounding villages.

PSI is situated on both banks of the River Aare in the canton of Aargau, in the municipal areas of Villigen and Würenlingen. Its main areas of research are in the natural sciences and engineering. Funded by the federal government, it belongs to the domain of the Swiss Federal Institute of Technology (ETH Domain), which also includes ETH Zurich, EPFL Lausanne, and the research institutes Eawag (Swiss Federal Institute of Aquatic Science and Technology), Empa (Swiss Federal Laboratories for Materials Science and Technology) and WSL (Swiss Federal Institute for Forest, Snow, and Landscape Research).

Complex large research facilities

Switzerland's federal government has given PSI the mandate to develop, build, and operate large, complex research facilities. These are the only such facilities within Switzerland, and some are the only ones in the world.

Running experiments at our large research facilities enables many scientists from the most diverse disciplines to gain fundamental insights for their work. The construction and operation of these kinds of facilities involve so much time, effort, and cost that comparable meaurement equipment is not available to academic and industrial research groups at their own institutions. That is why we keep our facilities open to all researchers worldwide.

To obtain a time slot to use the experimental stations, however, both Swiss and foreign scientists first have to apply to PSI. Selection committees comprising experts from all over the world assess the scientific quality of these applications and recommend to PSI which candidates should be given measurement time. Even though there are around 40 measuring stations where experiments can be carried out at the same time, there is never enough capacity for all of the proposals submitted – around onehalf to two thirds have to be rejected.

Around 1,900 experiments are performed every year at PSI's large research facilities. Time slots are free of charge

5

large research facilities that are unique in Switzerland

800

scientific articles a year based on the experiments performed at PSI's large research facilities

5,000

visits every year from scientists from across the globe who perform experiments at our large research facilities for all researchers working in academia. In a special process, users from private industry can buy time to carry out proprietary research and use the PSI facilities for their own applied research. For this, PSI offers special research and development services.

PSI operates five large research facilities in total where the internal processes of materials, biomolecules, and technical devices can be explored on the nanometre scale. Here scientists use different beams to "illuminate" the samples they want to investigate in their experiments. The beams available for this range from particles (neutrons or muons) to intense X-ray light from a synchrotron or X-ray laser source. The different types of beams allow a wide variety of material properties to be studied at PSI. The high complexity and cost of the facilities is due to the massive size of the accelerators needed to generate the different beams.

Three main areas of research

However, PSI not only acts as a service provider for researchers, but also carries out an ambitious research programme of its own. The findings produced by PSI scientists help us to understand the world better, and also lay the foundation for developing new types of equipment and medical treatments.

At the same time, our own research is an important prerequisite for the success of our user service programme for the large research facilities. Only researchers personally involved in current scientific developments in the fields external researchers are working in can support them in their investigations and further refine the facilities to ensure they continue to meet the needs of cutting-edge research in the future.

PSI has three main areas of research. In the area of Matter and Materials, scientists study the internal structure of different materials. These results contribute towards a better understanding of processes occurring in nature and provide starting points in the development of new materials for technical and medical applications.

In the Energy and Environment area, activities focus on the development of

new technologies to facilitate the creation of a sustainable and secure supply of energy, as well as an uncontaminated environment.

In the Human Health area, researchers search for the causes of illnesses and explore potential treatment methods. Their fundamental research activities also include the elucidation of generic processes in living organisms. In addition to research activities, PSI operates Switzerland's sole facility for the treatment of specific malignant tumours using protons. This particularly sensitive procedure allows tumours to be destroyed in a targeted manner, leaving the surrounding tissue largely undamaged.

The brains behind the machines

The work at PSI's large research facilities is challenging. Our researchers, engineers, and professionals are highly specialised experts. It is important for us to foster this expertise. So we want our employees to pass on their knowledge to the next generation, who will then put it to use in a variety of professional positions, not just at PSI. Around a quarter of our staff are therefore apprentices, doctoral students, or postdocs.

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Editorial team

Monika Blétry, Monika Gimmel, Martina Gröschl, Christian Heid, Dr. Laura Hennemann, Sebastian Jutzi (resp.), Dr. Mirjam van Daalen

Translation Patrick Regan

Editor Graeme High

Design and Art Direction Studio HübnerBraun

Photos

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Coming up in the next issue

With its Energy Strategy 2050, Switzerland has committed to gradually phase out nuclear energy while simultaneously increasing energy efficiency and expanding energy production from renewable sources. In addition, the country wants to achieve net-zero greenhouse gas emissions by 2050. But what if it encounters a technical failure, or political or economic shocks? Researchers from various institutions, under the leadership of the Paul Scherrer Institute PSI, are investigating how the energy supply in Switzerland can be made as sustainable and trouble-free as possible over the coming decades. In doing so, they examine selected events that could affect the Swiss energy system of the future and consider how the supply could be designed to make it as resilient, adaptable and sustainable as possible.

