discovered

THE HZDR RESEARCH MAGAZINE

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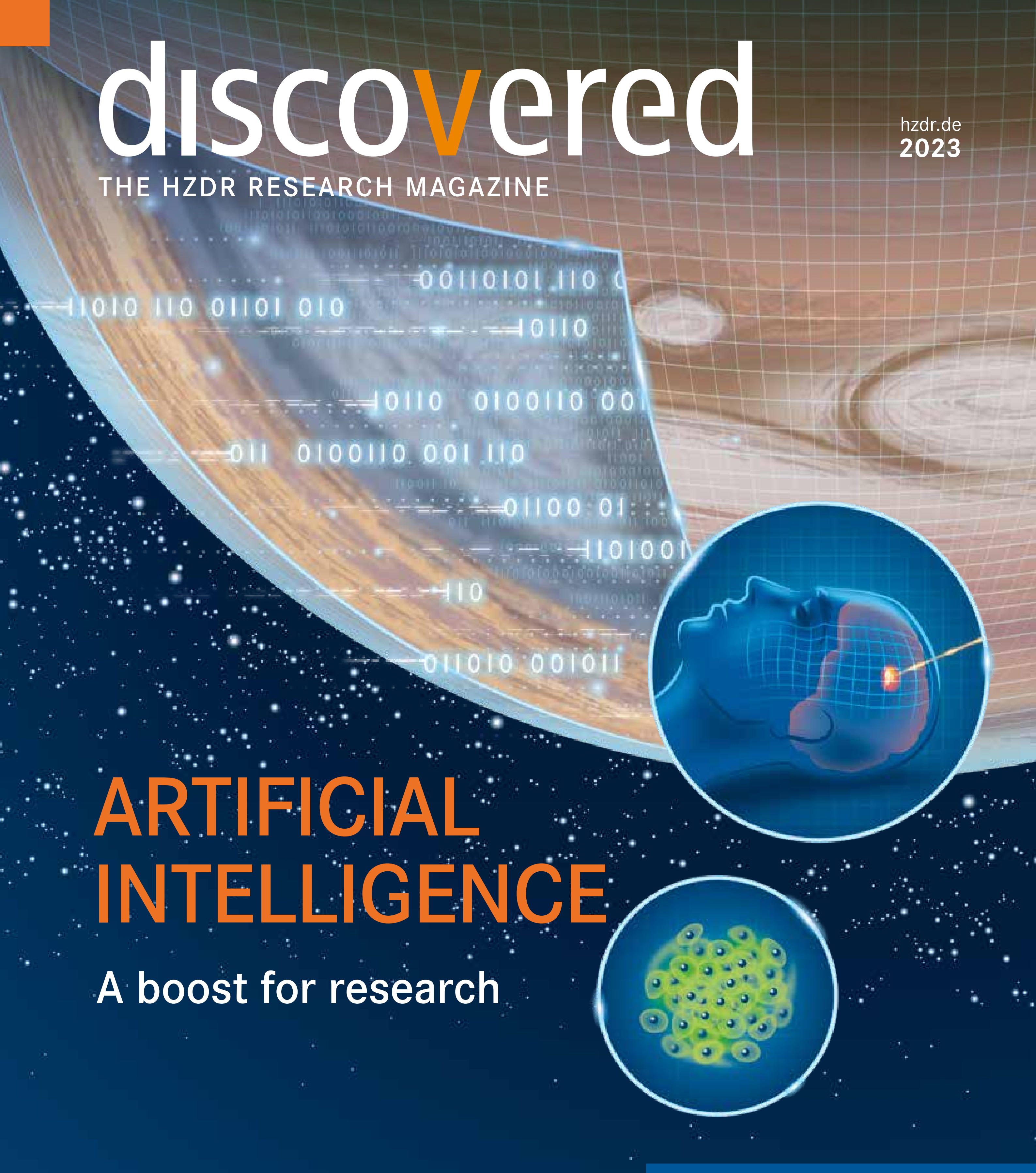
2023



ARTIFICIAL INTELLIGENCE

A boost for research

Where young people are hacking
Playful dive into the world of data

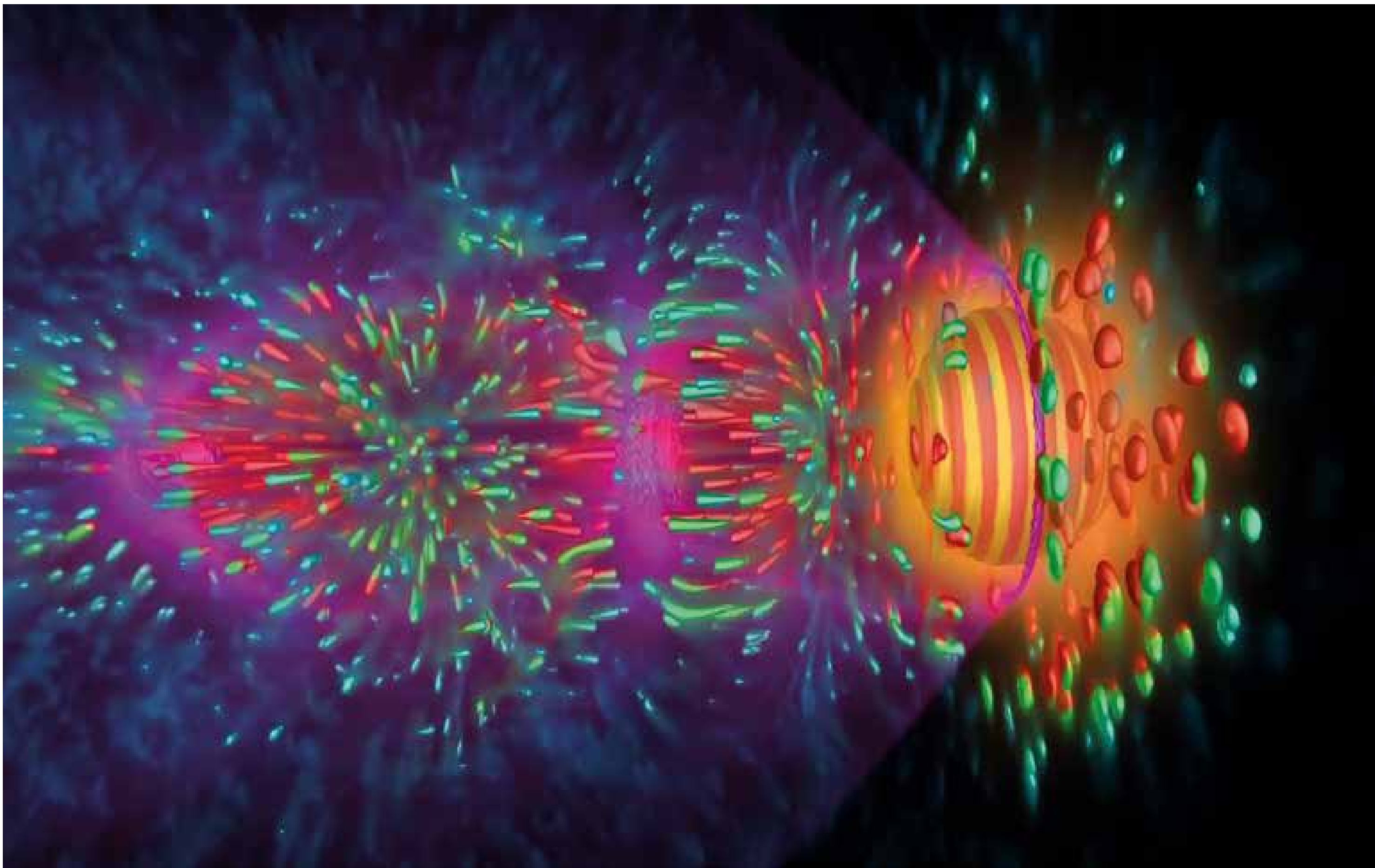
Nobel Prize winner Donna Strickland
On a visit to the "Extreme Lab"

Flowing weightlessly – data treasures from space
Switching off buoyancy for six minutes

HZDR
HELMHOLTZ ZENTRUM
DRESDEN ROSSENDORF

Artwork created by the exascale computer

What happens when an ultrashort and extremely intense laser flash hits the noble gas helium? An explosion as magnificent as a painting! The laser (orange area) creates an exotic state of matter: a plasma of ionized helium atoms. Like a purple wave, the laser drives the electrons from the plasma ahead of it, accelerating the electron pulses (red, green, and blue) to high energies.



Extremely versatile simulation code

The world's most powerful computers are needed to simulate and visualize the acceleration process. And the right tools, such as the HZDR simulation code PIConGPU (Particle-in-Cell on Graphics Processing Unit). Its unique feature: asynchronous data transfer. In other words, the software can process hundreds of billions of macroparticles on a GPU computing cluster in parallel.

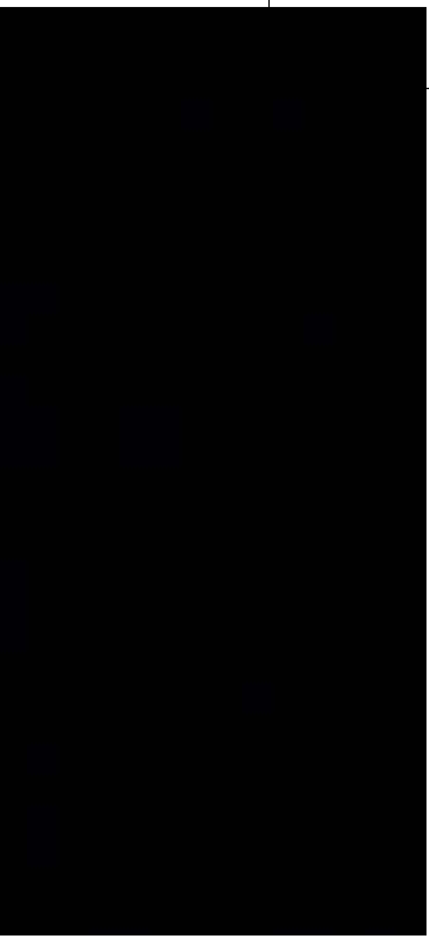
Fastest computer in the world

PIConGPU can be run on graphics cards from all manufacturers. Research groups from the HZDR succeeded in adapting the software to the US American FRONTIER computer at Oak Ridge National Laboratory (ORNL). The exascale system can perform one and a half quintillion floating-point operations per second. With these 1.5 ExaFLOPS, large-scale simulations, which would have been inconceivable just a few years ago, can now be performed.

Data streams captured as images

The artwork also owes its existence to ISAAC, a real-time simulations imaging tool on the FRONTIER supercomputer. ISAAC visualizes the data precisely where it is calculated by PIConGPU: on the graphics cards themselves. For each simulation step, ISAAC can immediately generate an overall image but requires processing a data stream of 22 petabytes per minute to do so. In comparison, the volume of data flowing through the internet in the U.S. is less than ten petabytes per minute.

22
petabytes per minute



Interactive data analysis

The single images strung together result in a continuous film in real-time. Via the Internet, researchers in Dresden can follow what data PIConGPU is currently producing in the USA. They can decide on specific images they would like to see, change the angle of view, zoom in or out, and even interact with the simulation. This allows them to identify relevant data for detailed analysis and long-term storage. (CZ)

↗ **Link to YouTube**

In 2019, the Frontier Center for Accelerated Application Readiness selected eight research projects to accompany the development of the high-performance computer – including the PIConGPU team from the U.S. American University of Delaware in collaboration with HZDR.

1.5
ExaFLOPS

Contact

_CASUS - Center for Advanced Systems Understanding at HZDR, jointly founded by HZDR, Helmholtz Centre for Environmental Research UFZ, Max Planck Institute for Molecular Cell Biology and Genetics, TU Dresden, and University of Wrocław

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Dear Readers,

Based on a keyword list, the text on the left was written first. The AI-supported text generator tool ChatGPT (model 3.5 Turbo) from Open AI was then given the task of composing an editorial based on the list and some partially formulated sentences. The text in the right column, which was produced with minimal effort, breaks off unexpectedly after reaching the specified number of characters.

Neither coincidence nor hype determined the focus of this issue of "discovered." It was rather the widely acclaimed successes CASUS can refer to as an institute for digital, interdisciplinary systems research after a founding and start-up phase of just four years. The fact that another location has to be rented in Görlitz because researchers feel cramped in their current home on the Untermarkt pleases its new director, Thomas Kühne. He regards this as a testimony to the HZDR institute's international appeal.

Artificial intelligence (AI) is changing science as rapidly as every aspect of our lives. Take medicine for a start. At the National Center for Tumor Diseases in Dresden, computer scientist Stefanie Speidel is developing real-time algorithms for the operating theater so that cancer surgery can proceed optimally and medical staff are able to intervene quickly to handle potential complications. Other uses include searching for raw materials in remote areas. Here, scientists are working with machine learning methods to extract valuable information from a wide variety of data sets.

New artificial intelligence tools do accelerate the acquisition of knowledge and help overcome the boundaries between disciplines, but they do not replace humans either in the operating theater or in science.

I wish you an insightful read.

Christine Zimmermann
Department of Communications and
Media Relations at HZDR

The importance of artificial intelligence (AI) and data science in research is steadily increasing. It is therefore no coincidence that the "discovered" is now focusing on this topic. One reason for this is that Prof. Thomas Kühne, an expert in computational science, has taken over as head of the HZDR data institute, the Center for Advanced Systems Understanding (CASUS).

CASUS was founded in Görlitz just four years ago and has already achieved considerable success. The institute has grown strongly and now has to rent another location for its employees. This illustrates the growing influence of AI and data science in research.

One area in which digital transformation has already made great strides is medicine. Here, computer scientist Stefanie Speidel from the National Center for Tumor Diseases Dresden is designing real-time algorithms for the operating room. The use of AI can increase the chances of successful operations and improve patient safety. AI methods also play an important role in the search for raw materials in remote areas. Here, scientists use machine learning methods. This enables a more efficient and accurate search for raw materials, which in turn makes resource extraction and use more sustainable.

It is important to emphasize that while AI methods can cross disciplinary boundaries and accelerate research, they do not replace humans in the operating room or in academia. Human expertise and critical thinking remain un... // Translation by deepl.com

↗ **https://chatgptx.de/**
↗ **https://deepl.com**

Content

Focus

Research

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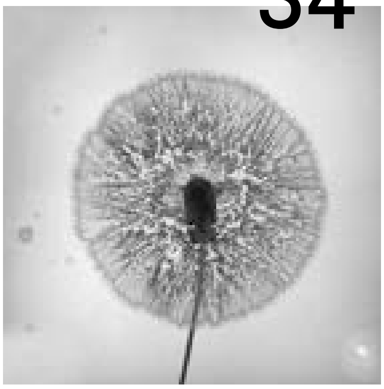
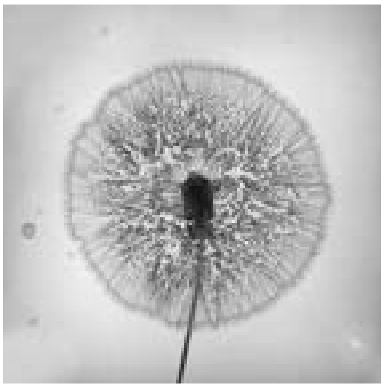
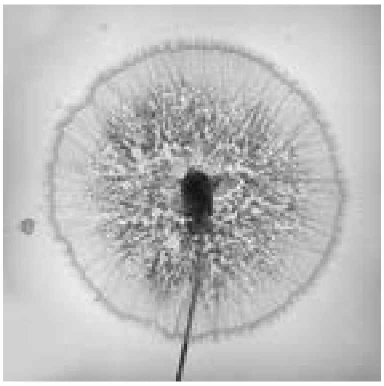






Panorama

Extremely cold and yet liquid

Inside a magnet, the magnetic moments, the spins, "freeze" into well-ordered or glassy structures. However, there are exceptions: Much like water, which simply won't freeze no matter how cold it is, the spins in an exceptionally pure crystal of zirconium, oxygen, and praseodymium remain "liquid." And that even at 20 millikelvin, i.e., one-fiftieth of a degree above absolute zero, as experiments by an international team with participation of the HZDR have shown. The fact that the material remains true to its exotic behavior even when inside a magnetic field is seen by the experts from Japan, the USA, India, and Dresden as proof of the existence of a quantum spin liquid. The new material could serve as a model system for developing highly sensitive quantum sensors, with which, for example, magnetic fields or temperatures can be registered with far greater precision than with conventional sensors.

Publication: N. Tang et al., Nature Physics 2022 (DOI: 10.1038/s41567-022-01816-4)

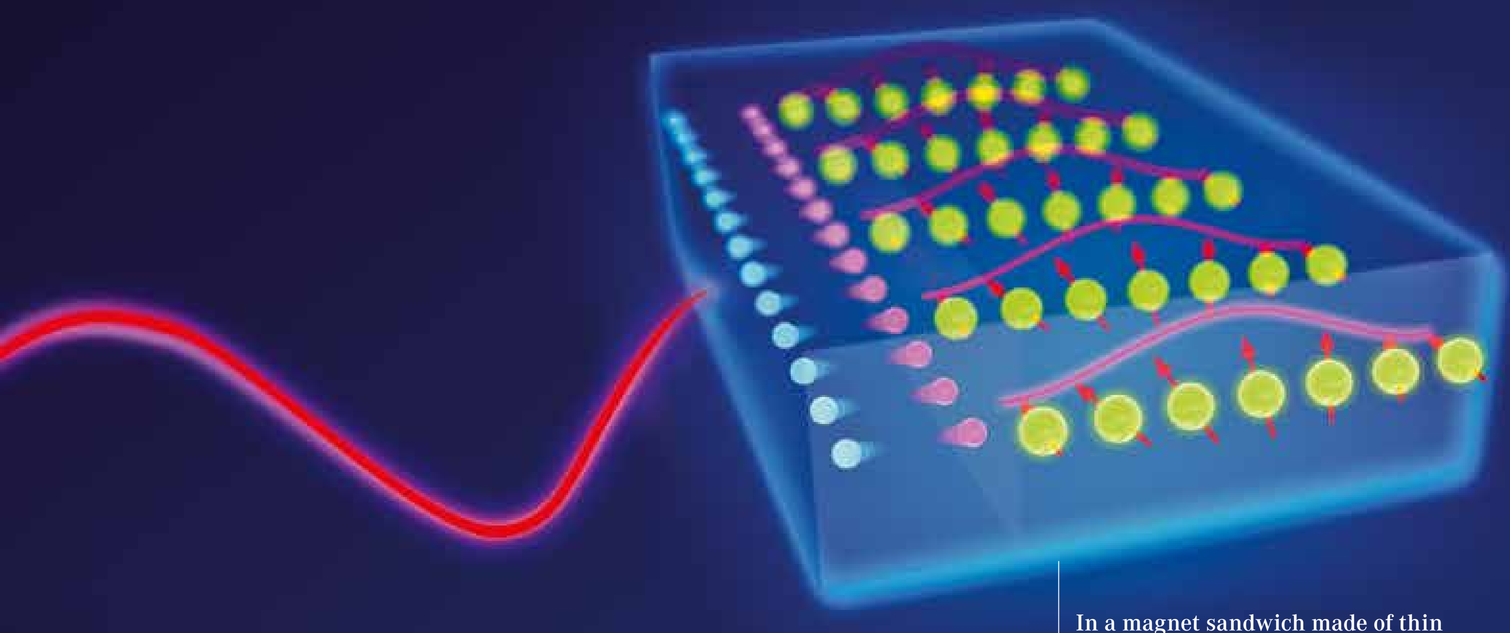
Marriage
between two worlds

Until now, a coupling was considered impossible: Spin and light waves in the terahertz range move too differently. This type of radiation is harmless to humans and is currently used for body scans at many airports. However, terahertz technology is particularly important for novel and ultra-fast data transmission and processing. Spin waves can also be used as information carriers. Their advantage: Since the spin – the magnetic moment of the electrons – remains in its position in the atomic lattice, there are no heat losses due to currents, unlike in common computer chips.

Using a magnet sandwich, an international research team led by the HZDR succeeded in "translating" signals from the world of light into the world of spins. In their experiments, the experts directed intense terahertz pulses onto a nickel-iron alloy previously wrapped in wafer-thin metallic layers of tantalum and platinum. Before they could measure and explain the characteristic oscillations of spin waves, lengthy experiments with different material components and external magnetic fields were necessary.

The greatly simplified result: Terahertz light accelerates free electrons in the heavy metal. Quantum effects now give rise to spin currents, which in turn trigger spin waves at the interfaces between the heavy metal and the ferromagnet. In principle, the new sample system could be easily integrated into circuits.

Publication: R. Salikhov et al., Nature Physics 2023 (DOI: 10.1038/s41567-022-01908-1)



In a magnet sandwich made of thin metal layers, a terahertz light wave (from left) is converted into a spin wave.

Computer scientist Stefanie Speidel regularly exchanges ideas with experts such as Jürgen Weitz, Head and Professor of Surgery at Dresden University Hospital, to ensure that the interaction between man and machine runs smoothly in the operating theater.

AI for cancer surgery

The work in the operating theater is demanding and highly complex. A few millimeters can often determine whether a tumor is completely removed or important nerves and blood vessels are injured. The National Center for Tumor Diseases Dresden (NCT/UCC) is working on intelligent assistance systems that support surgeons during minimally invasive and robot-assisted interventions. The tool: artificial intelligence (AI) algorithms with real-time capability based on data from countless interventions.

_ Text . Frank Grotelüschen

Stefanie Speidel approaches a torso lying motionless on a metal table in her laboratory. She lifts the plastic lid off the rib cage and points to the stomach, spleen, and liver. "It is a phantom; the organs are made of silicone," the Dresden computer science professor describes. "This artificial torso is used to test new AI algorithms for intelligent assistance in cancer surgery."

Then, she points to two robotic arms right next to the dummy. "These are not designed for the operating theater but well suited for our tests." The two robotic arms can insert camera-equipped endoscopes – tube-like surgical devices – into the plastic torso and navigate them with pinpoint accuracy controlled by adaptive algorithms.

Even movement comes into play at the push of a button: "We have installed an extension here that can simulate breathing, for example," says Speidel. "It makes our tests even more realistic."

Targeted camerawork through the body

Speidel's team uses the organ dummy to test AI programs designed to automatically assume camera control during minimally invasive cancer surgeries. During these procedures, an endoscope is inserted through an incision only slightly larger than a keyhole. To enable the surgeons to navigate, a camera is attached to the head of the tube, which provides real-time video images of the inside of the body. So far, the endoscope and camera are operated by medical staff.

Prior to any intervention, the surgeons have to visualize as precisely as possible how the tumor is situated in the tissue and where sensitive blood vessels are located, all based on images taken beforehand. In the future, intelligent systems will also provide valuable assistance in this regard.

"Similar to a navigation system in a car, AI-supported assistance systems will guide the physician to the tumor unerringly and without detours. And in real-time, of course," Speidel reports. "However, decisions are still made by the human being at all times. The computer can only provide support and recommend a certain course of action."

AI assistants guide the way to the tumor

The starting point is CT or MRI scans taken before the intervention. These are used to create a virtual 3D map: It provides three-dimensional images of the tumor and the vascular system, among other things. With the help of this map and the live imagery, the software is intended to recognize which phase of the minimally invasive procedure the surgeon is currently in – and automatically display the appropriate information: Where exactly is the tumor located? Where should the incisions be made? Furthermore, which vessels should not be injured under any circumstances?

Organs in the abdominal cavity present a particular difficulty in this context: due to breathing, heartbeat, and contact with the endoscope, the liver, for example, constantly changes its position and also its shape – which makes automated navigation more complicated. "That is why we need a responsive map that automatically adapts to physical movement," explains Speidel. To accomplish this, the software creates a 3D model of the inside of the body.

The AI algorithms must literally learn how tissue is deformed by breathing and heartbeat – and then transfer this learned ability to a specific intervention. For this to work, the research group needs one thing above all: as much high-quality data as possible to train the algorithms. This is done using video recordings of endoscopic procedures, which often last several hours. Experts then have to screen and mark the data. "This is the only way to train an AI sensibly," Speidel emphasizes.

The data volumes accumulated in the process are considerable: One data set usually consists of 20 to 100 videos of various sizes from a few gigabytes up to 50 gigabytes. The data is stored in the NCT/UCC network and processed in the working group's computer cluster. This comprises 16 high-performance processors and is currently expanded by 30 processors. >

"Similar to a navigation system in a car, AI-supported assistance systems will guide the physician to the tumor unerringly and without detours."

_ Stefanie Speidel, National Center for Tumor Diseases Dresden

Adaptive AI algorithms will enable robot-assisted guidance of surgical cameras in the future.

Medical robots in a real OR environment

The AI assistants are also tested in an experimental operating theater. "In order to allow realistic testing, it is equivalent to a proper operating theater," explains the scientist. She points to a patient table with an operating lamp and a trolley for surgical instruments. Next to it is a latest-generation medical robot – a white machine the size of a person, equipped with four mechanical arms. It is operated from massive consoles, where surgeons gaze intently into eyepieces to precisely control the machine based on the live images from the endoscope.

The training of future surgeons could be another field of application. They train endoscopic procedures on an anatomical model similar to the one used in Speidel's lab. The idea: If the dummy were equipped with a sensor and AI-supported training system, it would analyze and evaluate the users' actions in real-time. This would provide medical trainees with rapid and accurate feedback – AI as a sparring partner.

The AI result should be presented in a way that is intuitively understandable for medical staff and, at the same time, sufficiently accurate. To address this requirement, the computer scientist teamed up with technical design experts at the excellence cluster CeTI, the "Centre for Tactile Internet with Human-in-the-Loop" at TU Dresden. "Dresden as a location is ideal for this kind of project and for our research," enthuses Stefanie Speidel. "There is an excellent university of technology, an outstanding university hospital – and the powerful HZDR, with which we cooperate on imaging, for example."

One of the NCT/UCC supporters – along with Dresden University Medical Center and the Helmholtz-Zentrum Dresden-Rossendorf – is the German Cancer Research Center (DKFZ) in Heidelberg. This comprehensive infrastructure is also helpful for a project that focuses on intervention planning: Speidel's research group is developing an AI app for predicting complications during minimally invasive surgery.

Algorithm calculates complication probability

"Based on image data, lab results, and information about pre-existing conditions, our system is designed to predict whether a patient faces an increased risk of complications," the researcher explains. "This could be, for example, a fistula on the pancreas that forms as a result of the procedure." Other undesirable postoperative effects include bleeding and sutures on the esophagus or intestines reopening after surgery.

"For us, it really is always about supporting the experts in their work and thus reducing their workload."

_ Stefanie Speidel, National Center for Tumor Diseases Dresden

Intelligent help for the surgeon: An assistance system displays the ideal incision line as well as target and risk structures.

Some people are at particularly high risk of such complications. Therefore, the surgical strategy must be adapted to suit them, and they should also be monitored more specifically in the intensive care unit after the surgery. Until now, assessing complication probability has been based on the physician's expertise. "We are trying to quantify this experience and transfer it to software," Speidel explains. "As a result, our app should be able to reliably report whenever there is an increased risk."

Data from multiple clinics

The main challenge for the research team in Dresden is obtaining enough reliable data for the AI training – preferably from several hospitals to allow mapping out a certain variance. The videos of endoscopic interventions form the basis. Experienced surgeons have to screen, classify, and "label" these: Which suture, for example, did not turn out quite right during the hours-long procedure? They also have to identify which features and peculiarities suggest a connection with later complications.

One problem: "In their daily clinical routine, physicians often have little time to label such data," describes Stefanie Speidel. "That is why we try to get by with a few hundred individual images per class and work on strategies to additionally generate synthetic training data that resemble real data." Her team derives the simulated data sets from real image acquisitions to make it work. This also allows rare complication scenarios, for which proper images are simply not available, to be played out.

Does the computer scientist encounter reservations about artificial intelligence or exaggerated expectations? "To some extent, yes," answers Stefanie Speidel. "But then I point out that, after all, you cannot compare an AI with human intelligence."

Instead, her team teaches the adaptive algorithms very specific, narrowly defined tasks. "For us, it really is always about supporting the experts in their work and thus reducing their workload," Speidel emphasizes. "And in the end, the patients will also benefit from it because the medical staff will simply have more time for them."

During the operation, the surgeon receives valuable assistance at the right time via data glasses.

Publications:

M. Carstens et al.: The Dresden surgical anatomy dataset for abdominal organ segmentation in surgical data science. Scientific Data, 2023 (DOI: 10.1038/s41597-022-01719-2)

L. Maier-Hein et al.: Surgical data science – from concepts toward clinical translation. Medical Image Analysis, 2022 (DOI: 10.1016/j.media.2021.102306)

M. Pfeiffer et al.: Learning soft tissue behavior of organs for surgical navigation with convolutional neural networks. International Journal of Computer Assisted Radiology and Surgery, 2019 (DOI: 10.1007/s11548-019-01965-7)

↗ https://www.nct-dresden.de/en

Contact

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Where young people are hacking

Since mid-2021, young people can playfully immerse themselves in the world of data and creatively explore the use of artificial intelligence (AI) at three hackerspace locations in Dresden, Freiberg, and Görlitz. Participation is free of charge and open to anyone between the ages of 12 and 18.

At the "KI-Lab" Dresden, located in the MACHwerk of the Dresden Technical Collections, everything revolves around AI, machine learning, and sustainability. Weekly open lab sessions are complemented by workshops during school vacations. Scientists of the HZDR's AI support team are regularly on-site to support all participants in creating code, programming games, or implementing their own project ideas.

In Görlitz, everyone from newbies to the pros can go on a data journey to explore either their own region or distant worlds. Data professionals from the HZDR and the Görlitz based HZDR institute CASUS – Center for Advanced Systems Understanding provide active support in planning the journey.

The "KI-Lab" in Freiberg offers young people the opportunity to better understand the world through data glasses and to find answers to important questions in the natural sciences. Regardless of whether they like tinkering with hardware, modeling in 3D, or programming in Python, the scientists of the Helmholtz Institute Freiberg for Resource Technology (HIF) of the HZDR welcome all young hackers and their topics.

Saxon Digital Award 2022

The Hackerspaces of the HZDR and the Dresden Technical Collections won 2nd place in the Society category. With the Saxon Digital Award, the Saxon State Ministry of Economics, Labor, and Transport draws attention to the many innovations and solutions in the wake of digitization and honors outstanding contributions. A total of around 100 applications were received. The first place went to the New Work Design Lab of the FHD – University of Applied Sciences Dresden, and third place took the Knowledge Architecture Research Group of the Faculty of Architecture at the TU Dresden. With the 2nd place prize money of 15,000 euros, the HZDR teams intend to make technical upgrades to their AI labs and promote exchange between the young participants across all three sites. *(CZ)*

↗ **https://jugendhackt.org/lab/**

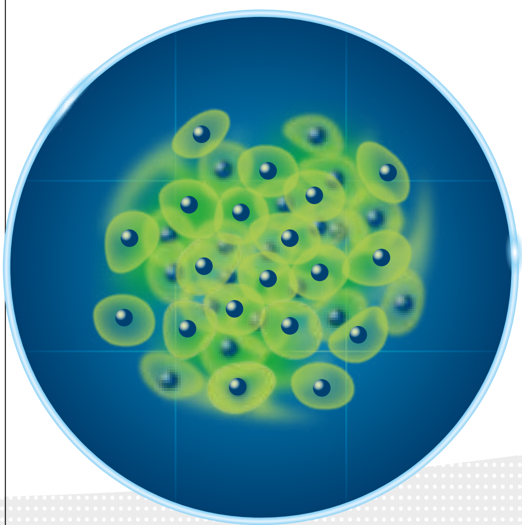
Digital bridges from the smallest to the largest

What happens in the core of planets? How can protons be accelerated in a controlled manner using laser light? And how can the charged particles be directed specifically into the tumor? At HZDR, data scientists and researchers from different disciplines design artificial intelligence models and train them based on cross-thematic and ever-larger data sets. In doing so, they arrive at comprehensive approaches to solutions and, thus, new insights and applications.

_ Text . Christine Zimmermann _ Graphics . Blaurock Markenkommunikation

Materials of the future thanks to faster simulations

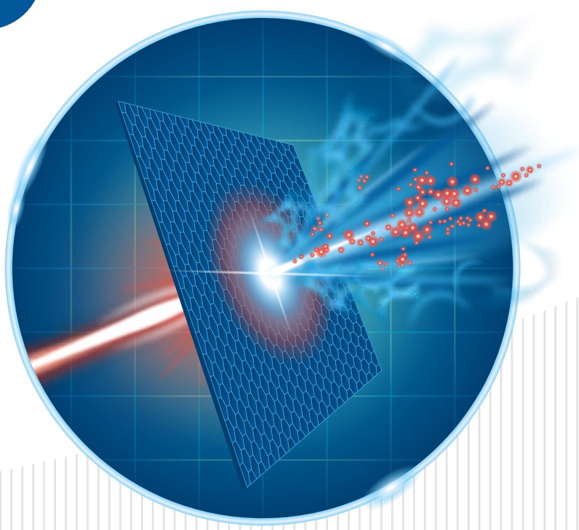
Calculating the properties of every conceivable material combination on a computer instead of carrying out time-consuming experiments in the lab – new information and communication technologies are likely to be the beneficiaries just as the energy transition or drug development. The Materials Learning Algorithms (MALA) software stack makes this possible by combining deep learning methods with physics-based approaches. The starting point: the atoms arranged in space with their respective neighbors. MALA can then be trained to predict the electronic structure of a given material for hundreds of thousands of atoms at an unprecedented speed.



Accelerating particles with light

When a flash of light from a high-power laser hits matter, an explosion is triggered, and a vast number of processes occur virtually simultaneously on different size scales. These processes can neither be measured directly in experiments nor described comprehensively in theory. Therefore, researchers are developing extremely powerful computer simulations and digital twins of the experiments, which can be used, for example, to reconstruct the path of the particles. Their goal is to push laser systems such as DRACO at the HZDR to ever higher intensities and, at the same time, perfectly control the quality of the generated proton pulses.

µm



Predicting extreme states

Thousands of exoplanets have been detected by NASA's Kepler space telescope in distant galaxies. Experts can determine through observation how large such a planet is, whether the temperature on its surface allows life, and what chemical elements it consists of. Many questions – for example, about the internal structure or the existence of a magnetic field – remain unanswered. Data scientists in Görlitz are developing a digital twin based on the available data and different probability assumptions. With their research, they hope to close important knowledge gaps about alien planetary systems.

Brain-inspired computing

Future autonomous driving systems must be able to record data from distance, motion, or speed sensors at lightning speed and analyze it in exact chronological order. Researchers are working with industry partners on hardware capable of processing such analog signals directly in real time and recognizing patterns. For this purpose, they are developing micrometer-sized magnetic disks. Once excited with electrical pulses in the microwave range, waves are generated within the magnet. The quantum particles of these waves, the magnons, can decay into many more magnons. Much like the neurons in the brain, these particles must first overcome an activation threshold.

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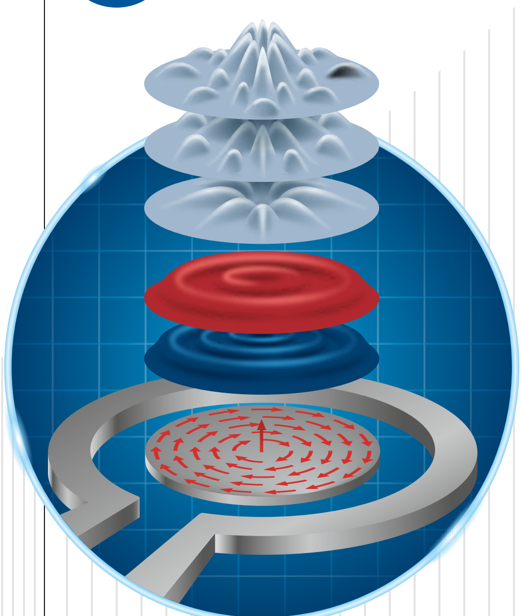
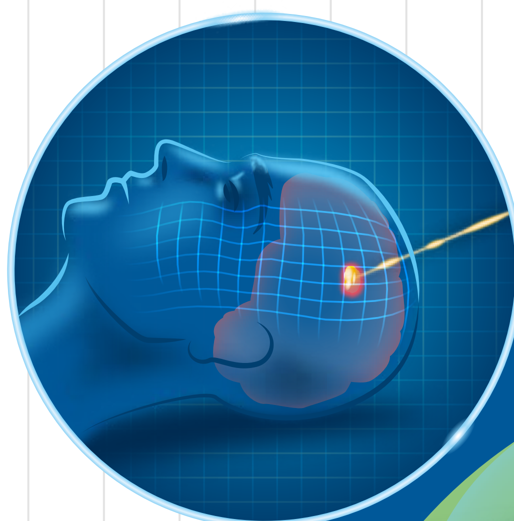
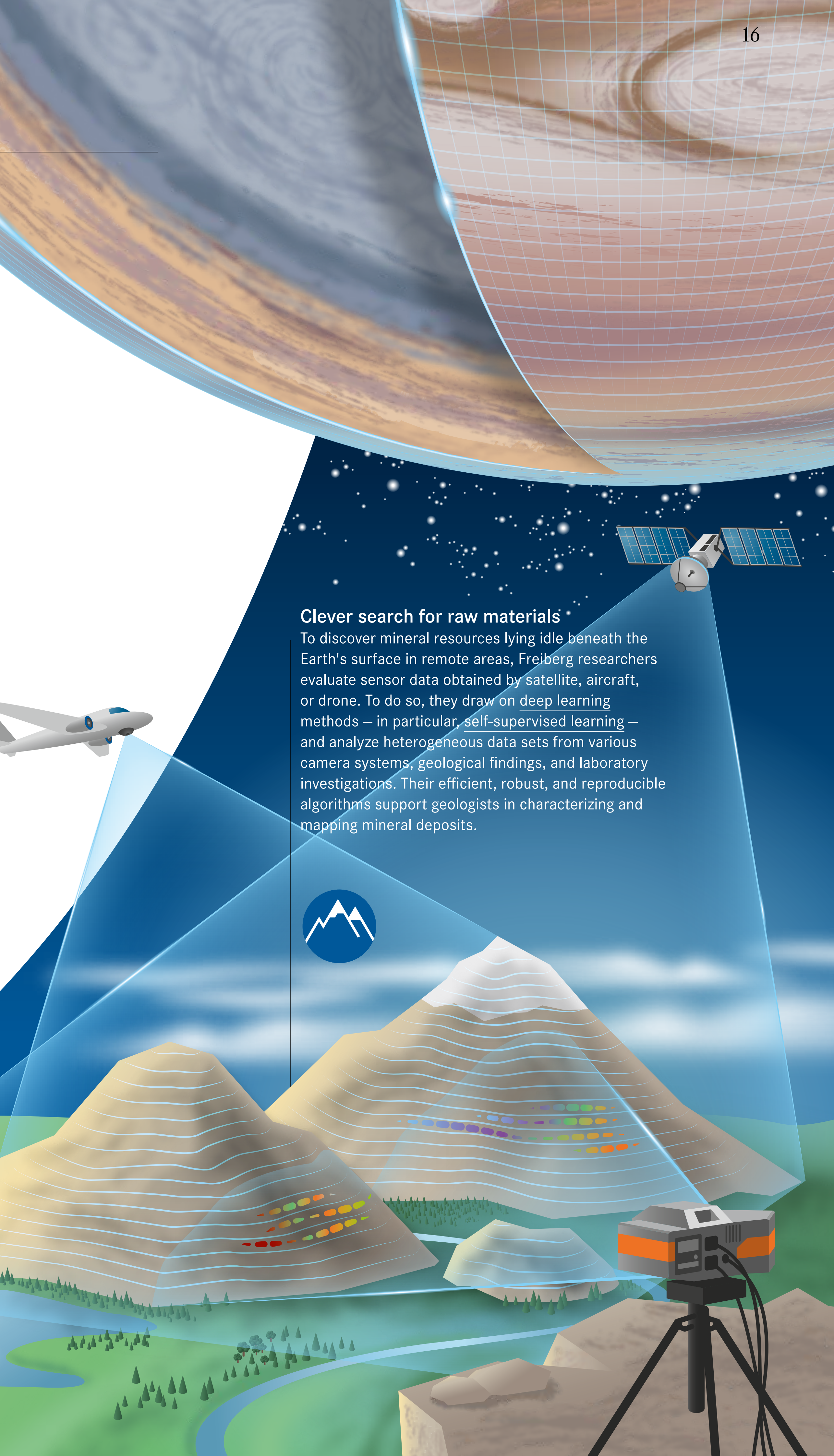


Cancer irradiation with the highest precision

Proton beams destroy tumors very effectively while sparing healthy tissue. However, this relatively new therapy method still lacks precision in responding to regular or irregular motion during treatment or anatomical changes during the course of the therapy, which usually lasts several weeks. Dresden scientists are developing a fully automated feedback loop supported by AI algorithms for continuous treatment monitoring. This allows immediate adjustment of the proton beam to suit changing conditions.





Clever search for raw materials

To discover mineral resources lying idle beneath the Earth's surface in remote areas, Freiberg researchers evaluate sensor data obtained by satellite, aircraft, or drone. To do so, they draw on deep learning methods – in particular, self-supervised learning – and analyze heterogeneous data sets from various camera systems, geological findings, and laboratory investigations. Their efficient, robust, and reproducible algorithms support geologists in characterizing and mapping mineral deposits.

A **digital twin** is a comprehensive digital representation of a complex system from the real world. It can monitor, diagnose, and predict all physical processes within the system. The following elements are linked in a digital twin:

- Data streams from a wide variety of measurements and simulations.
- High-performance computing (HPC) to generate accurate simulation data.
- Mathematical and numerical models of subsystems across time and length scales.
- Data-driven surrogate models and machine learning methods for real-time analysis and prediction.
- Interactive and intelligent visualization methods.

Machine learning (ML) is a branch of artificial intelligence that deals with developing algorithms and statistical models. It allows computers to learn from data without being explicitly programmed to do so. ML focuses on identifying patterns and relationships in data. This enables machines to produce predictions, make decisions, and gain insights.

A subfield of machine learning is **deep learning**, which uses artificial neural networks to solve complex problems. These networks are trained to automatically learn hierarchical representations of data and thereby extract complex patterns and features from the input data. The difference between machine learning and deep learning is that while the former encompasses a broader range of techniques – including decision trees, support vector machines, and clustering algorithms – deep learning refers specifically to using deep neural networks with multiple layers. This allows complex, unstructured, and large data sets to be tapped for text and image recognition, for example.

Self-supervised learning is another branch of machine learning. This virtually autonomous form of learning uses artificial neural networks trained with a simple task. Subsequently, the learning module is able to classify and solve similar but much more complex problems. Self-supervised learning is characterized by the fact that it can act independently of previously annotated data. It is already widely used in image, video, and audio processing.

Improved tumor therapies thanks to adaptive algorithms

X-rays, blood samples, DNA tests – clinics and practices collect enormous amounts of data every day. Hidden within is a treasure trove of valuable information. Artificial intelligence (AI) can link these data and detect hidden patterns. CASUS, the HZDR institute for data-intensive systems research, is creating important foundations for AI algorithms that should noticeably improve the diagnosis and treatment of tumors.

_ **Text** . Frank Grotelüschen

Cancer medicine is, in fact, becoming more effective and can successfully treat more tumors today than in the past. Nevertheless, there is room for improvement, for example, in deciding whether or not to operate on a growth. "In some cases, this is a trade-off between survival probability and quality of life," explains Michael Bussmann, Founding Manager of CASUS, who helped successfully establish the institute.

"Here, AI programs could, for example, provide indications regarding the group allocation for a prostate cancer patient and whether it might be more favorable for members of said group to wait with the intervention." Early tumor detection is also likely to benefit by using machine learning algorithms, which can identify suspicious patterns in a CT scan that remain hidden from the human eye.

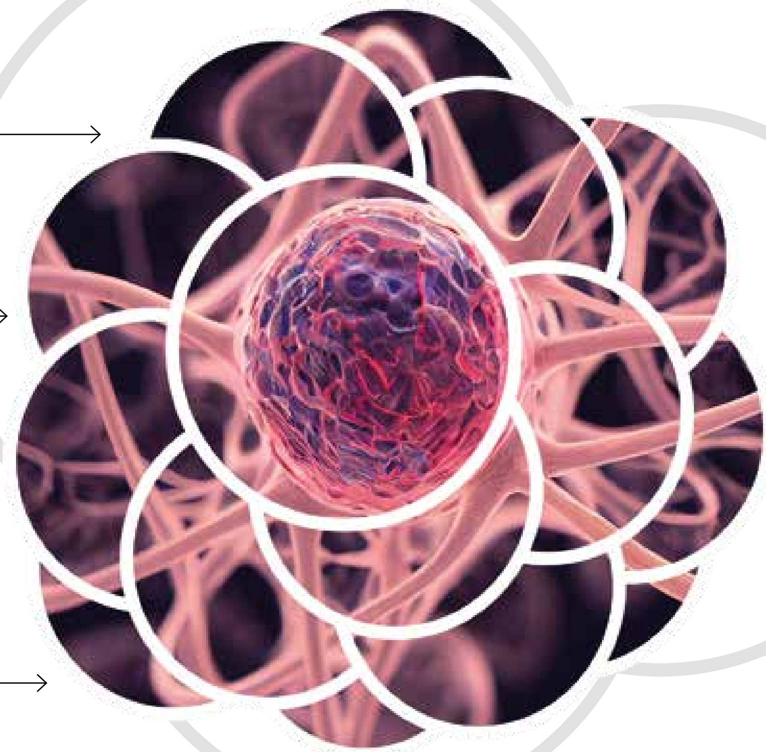
The potential is enormous. That is why several initiatives are dedicated to developing reliable AI systems. CASUS is substantially involved with two major European projects: The PIONEER research consortium is pooling 100 million data sets on prostate cancer research, thereby creating an essential prerequisite for developing new algorithms. Building on this, the OPTIMA (Optimal Treatment for Patients with Solid Tumours) project aims to design AI systems that improve the diagnosis and treatment of prostate, breast, and lung cancer.

Hurdles on the way to AI tools

"Data collection alone reveals our limitations regularly," says Bussmann. "Often, data are available in various formats or are incomplete." Thankfully, a pan-European data standard called OMOP (Observational Medical Outcomes Partnership) is in place. It allows for patient data to be recorded and stored in a standardized form. Nevertheless, it takes a considerable effort to transfer the information, some of which is still handwritten, into this new format.

Equally important is data protection: CT scans and blood levels are considered protected health information, which requires high security standards for transmission and processing. To ensure these standards, researchers work in cooperation with patient organizations and ethics committees.

One of the concepts: If a new algorithm is to be trained with MRI images, the clinic does not send the images to the research center, but the algorithm is send to the clinic



instead, where it is tested and optimized. Thus, all data remain safely on the hospital server. In addition, they are to be intelligently anonymized to retain as much research-relevant information as possible.

The algorithms the OPTIMA team plans to develop are intended to support the treating staff in hospitals. Currently in testing are, for example, programs based on biopsy data that can analyze the progression status of a prostate tumor. Another goal: AI assistants that help to find the best possible treatments and provide information on the most successful therapy methods used in similar cases at other hospitals.

"Such AI tools are by no means intended to make decisions for physicians, but rather to offer valuable assistance and additional information," Michael Bussmann emphasizes. "In which cases, for example, might it make sense to deviate from a familiar treatment regimen?"

For staff and patients alike, any results of the AI system should be easily comprehensible. The software should provide information about the data used or present similarly situated cases of illness. "We will only create acceptance for this valuable tool if we manage to explain the AI decisions in clear and simple terms," Bussmann says. "That's a challenge we hope to master with appropriate interfaces and training."

Experts are currently in the process of expanding the existing database for prostate tumors by adding data on breast and lung cancer. OPTIMA is scheduled to continue until 2026. It is hoped that the first field-tested AI algorithms will be operational by the end of the project. And with SOLACE another EU project with HZDR participation started in April 2023. It is dedicated to collecting and analyzing medical data for lung cancer screening.

↗ **https://prostate-pioneer.eu**
↗ **https://www.imi.europa.eu**

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Looking into the sun with AI glasses

Tobias Dornheim is banking on random numbers. And on artificial intelligence. That's how he wants to provide research with tools to unravel the secrets of solar fire and ultracold matter.

_Text . Kai Dürfeld

What exactly does the inside of our sun look like? What temperatures exist there? And what about the pressure? Research teams at large-scale research facilities around the globe are trying to understand the universe a little better. And, in the process, solve the riddles surrounding nuclear fusion to perhaps provide us with a clean and inexhaustible energy source on Earth. Igniting such a solar fire is already possible – if only for the briefest moments. "Warm dense matter" is the technical term for this state. But how does one exactly learn about the prevailing conditions at the center of such an experiment? "I can't just stick a thermometer in there," says Tobias Dornheim, smiling mischievously.

Since 2019, the young quantum physicist has been working at CASUS, the institute for digital interdisciplinary systems research at the HZDR in Görlitz. Off the record, he is already being treated as a shooting star. At just 32 years of age, he has already received one of the coveted grants from the European Research Council (ERC). "I want to invest the roughly 1.5 million euros over the next five years to make the path integral Monte Carlo method significantly more efficient," Dornheim explains. He says this as if it were the most ordinary thing in the world and adds: " Monte Carlo simply means doing something with random numbers. We are working with Markov Chain Monte Carlo, to be specific." His computer models are all about estimated values and error margins. Put simply, in their simulations, he and his team have the computer guess a large number of random values and from there statistically approximate the actual value.

"I think quantum mechanics is just cool"

Tobias Dornheim considers his daily math work to be quite alright. But his heart really beats for theoretical physics. Quantum physics, to be exact. His love for it began in school. "Back in high school in Schleswig-Holstein, I majored in physics. And the thing that really interested me, that sort of got me hooked, was quantum mechanics," he says with a twinkle in his eye. "I find the concept of probabilistic wave functions fascinating. And I've stuck with quantum mechanics to this day."

After finishing college and earning his doctorate, he was drawn away from the coast directly to Lusatia. "I just applied unsolicited because I knew: A lot of people here are working on warm dense matter," he recalls. "And I had already done research on it for my dissertation." As it would soon turn out, his initiative was a stroke of luck because he was talking to Michael Bussmann, who was in the process of setting up CASUS. And in this new center, there was to be a group working on matter under extreme conditions. "So he tried to recruit me for this group." The decision was not hard for Tobias Dornheim, and a short time later, he was the first scientific employee at the CASUS institute.

His theoretical models and simulations have now been complemented by concrete applications. His group is collaborating with researchers at the National Ignition Facility (NIF) in Livermore, California, who recently ignited another solar fire in the lab. When asked about the matter, Tobias Dornheim is in his element. He explains, "To determine the

Warm dense matter

Neither solid, liquid, nor plasma: Warm dense matter has properties of all three aggregation states. The attribute "warm" denotes temperatures between 5,000 and some 100 million degrees Celsius. The pressure is also gigantic. It can be a solid million times higher than the atmospheric pressure at the Earth's surface. Warm dense matter can be found inside the gas giants Jupiter and Saturn, within stars, and now also in research laboratories. It can be created – at least for a very brief moment – by firing short laser pulses of very high energy at a piece of metal. Unlocking its secrets, so it is hoped, would expand our understanding of the universe, and bring us one step closer to nuclear fusion.

Physicist Tobias Dornheim is fascinated by the properties of warm dense matter, which is found in planetary interiors and for brief moments in the laboratory such as the international research center European XFEL.

samples' temperatures during the experiments, you shoot an X-ray laser flash at it. It penetrates the sample and is scattered. The scattering intensity of the laser is measured, and we use our calculations to draw conclusions about the actual conditions that prevailed in the sample."

Exciting physics at absolute zero

Dornheim can distinguish significant readings from random noise with his models, formulas, and algorithms. But that consumes computing power, which increases exponentially due to quantum statistics as temperatures to be measured fall. "That's one of our biggest problems," he says. "We certainly cannot study the metallic hydrogen phenomenon this way. And even some regions within planets are very problematic because the temperatures are so low that it would take almost forever to calculate them with path integral Monte Carlo."

His idea was, therefore, to combine this method with machine learning. He is sure that the bottleneck can be overcome with this approach. If so, the path would be clear to calculate and simulate not only warm dense matter. "We would also like to apply our methods to ultracold atoms," he says. "They have extremely exciting physics to offer and are also quite important as we seek to improve our understanding of the world."

Publications:

T. Dornheim et al.: Electronic density response of warm dense matter. Physics of Plasmas, 2023 (DOI: 10.1063/5.0138955)

T. Dornheim et al.: Accurate temperature diagnostics for matter under extreme conditions. Nature Communications, 2022 (DOI: 10.1038/s41467-022-35578-7)

M. Böhme et al.: Static electronic density response of warm dense hydrogen: ab initio path integral Monte Carlo simulations. Physical Review Letters, 2022 (DOI: 10.1103/PhysRevLett.129.066402) ⅃

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"We are shifting the paradigm."

_ Questions . Kai Dürfeld

Thomas Kühne has been director of the Center for Advanced Systems Understanding (CASUS) since May 2023. The computer scientist and professor of computational systems science is an expert in developing computational methods for research fields as diverse as chemistry, biophysics, and materials science. In this interview, the 43-year-old tells us where he wants to lead the HZDR institute in the future, about the role of sustainability in this process, and why CASUS is the ideal place for up-and-coming researchers.

Professor Kühne, what new areas of research have you brought to Görlitz?

On the one hand, of course, my own research topic. My research group simulates the behavior of materials at the atomic level. The research in this context usually goes hand in hand with experimental work done at our partner institutions. Based on our simulations, we can explain experimentally obtained results and make specific suggestions for further investigations. Moreover, sustainable applications such as new catalysts, the reduction of CO_2 emissions, and the green production of synthetic fuels are particularly close to my heart.

CASUS is currently not associated with the topic of sustainability. What are you planning?

The current structure of our institute is very much shaped by our five founding partners. Consequently, our topics are very heterogeneous and range from elementary processes of plasma formation to optimal cancer treatment to complex processes in the Earth system. Here, for example, we are looking for solutions to effectively protect animal species threatened with extinction. What unites CASUS thematically are the methods of data-driven science and artificial intelligence, which we further develop and redevelop to address such highly complex systems. In addition to the existing methodological bracket, I would

also like to gradually create an externally perceptible thematic umbrella. Considering the expertise already available and my areas of focus, the topic of sustainable systems science suggests itself for this purpose.

What does that specifically mean?

As the Center for Advanced Systems Understanding, we are increasingly involved with sustainable applications. Take catalysts, for example. They are a key element in creating a clean future and in making a wide variety of processes more efficient. And that saves energy and raw materials. Now, the customary method of finding new catalysts is trial and error. Research teams, therefore, pore over the literature, synthesize a possible material combination, and finally test whether the material produces the desired effect. We are turning this approach upside down by combining artificial intelligence with material databases. This not only allows known materials to be examined for their suitability as catalysts. The computer also learns what constitutes a potential catalyst and then suggests completely new materials that no one has ever produced before. In other words, we do not use our computer simulations to explain what happened in an experiment. We use them as a prediction that can be experimentally verified afterward. Another example is processes under extreme conditions, such as high pressures and temperatures. These conditions are found inside of stars, for example. Although this may not sound very application-oriented at first, it is the basis for nuclear fusion research, and we are actively involved in trying to tap a sustainable energy source for the future.

But sustainability can also affect research itself.

Exactly, that's where we are active as well. We are committed to open science principles and make our methods and software available to the scientific community. The exciting thing is to see whether a method might also work for a completely different area of application, one that was not even thought of during its development. However, this would not happen without CASUS because researchers usually develop their methods specifically for their questions. They rarely exchange ideas beyond their institute or even across disciplinary boundaries. With us, on the other hand, such exchange takes place very promptly.

You have already mentioned your research partners. Who are currently the most important?

The HZDR, to which we belong as an institute, is very important. Because our colleagues in Dresden can, for example, synthesize the materials we have predicted and analyze them with their large-scale research facilities. Our other founding partners also play an active role. Like the University of Wrocław, with which we established the Scultetus Center. Through this meeting place, we intend to promote exchange between young talents from Germany, Poland, and the Czech Republic. Moreover, we would like to strengthen our involvement in the scientific community of Dresden. In addition to the TU Dresden, this includes primarily the Max Planck Institutes, with which we already cooperate well. Görlitz also has interesting research facilities – for example, the Hydrogen Lab of the Fraunhofer Society, which is currently being established. Here, we can help find catalyst materials for electrocatalysis. We also intend to support the German Center for Astrophysics DZA, particularly in analyzing data readings.

That sounds like an exciting research environment. In your opinion, what is the most compelling argument to draw scientific talent to CASUS in Görlitz?

Our unique selling point, so to speak, is our mode of operation. Usually, computational research takes place at institutes specialized in one field of application. We are shifting the paradigm and focusing on the methods instead. Their development is highly prioritized, particularly among our junior research groups, and the application areas are very diverse. That is why we have a large number of specialists working under one roof who might otherwise be spread across half a dozen different institutes. This creates entirely new synergy effects and allows us to tackle questions far too large to be addressed by a single institute or data science group within a conventional institute. That is definitely a great incentive to join us.

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Particle accelerators, planets and digital twins

_ In conversation . Attila Cangi and Anna Willmann _ Questions . Gabriele Schönherr

What do planets have to do with particle accelerators? Why does a data scientist need to communicate effectively? And where is data science headed? Two data scientists from the HZDR report on how artificial intelligence (AI) and machine learning (ML) are transforming everyday research.

Profile Anna Willmann

- Ph.D. Student at Institute of Radiation Physics and Helmholtz AI Local Unit Group: "Artificial Intelligence for Future Photon Sciences"
- Age: 27
- Background: B.Sc. in Applied Mathematics; M.Sc. in Computer Science
- Data Scientist, because she has been fascinated by working with (physical) data since her first work on simulations in fluid dynamics, while at the same time being able to do research on new AI methods
- Current Research Projects: development of a digital twin for free-electron lasers (see also graphic on page 41)

Profile Attila Cangi

- CASUS department head (acting): "Matter under Extreme Conditions"
- Age: 40
- Background: M.Sc. in Physics; Ph.D. in Chemistry; former Staff Scientist at Sandia National Laboratories, Albuquerque, USA
- Data Scientist, because he has been absolutely convinced of the potential of AI since attending an interdisciplinary AI workshop in 2011; returned from the U.S. to join CASUS
- Current Research Projects: new AI model for the electronic structure of matter; digital twin for the interior of a planet

What exactly does a data scientist do?

Cangi: Basically, there is no difference between us and many other scientists. We investigate open questions and use data as a tool for that purpose. The distinctive feature is that we often work with enormous quantities of unstructured data. The challenge is to structure them with digital methods and extract information from them.

Willmann: I would like to add that this job also has a highly communicative and interdisciplinary side. In fact, it often is quite the opposite of the general belief that we spend all our time alone in a dark room behind the computer. There is a fair amount of exchange about the data going on.

What are the methods we are talking about? And what do they mean for research and everyday life?

Cangi: We develop digital solutions for complex systems: through mathematical models, on high-performance computers and, above all, with the help of artificial intelligence and machine learning. At CASUS, the Center for Advanced Systems Understanding at HZDR, we work in an exceptionally interdisciplinary manner with very low barriers between the various groups, even though we belong to very different research areas: from matter under extreme conditions to systems biology and Earth sciences to digital health and autonomous systems.

"And that is precisely the beauty of it: We can transfer the methods from one problem to the other."

_ Attila Cangi, HZDR

Willmann: Whether in medicine, physics, industry, or commerce, we collect vast amounts of data everywhere. But humankind is simply incapable of grasping such a multidimensional data space. Artificial intelligence, however, can. That means we can use AI to identify trends in very large databases that would otherwise remain undetected; for example, doctors could learn from medical data in good time whether patients belong to an at-risk group or not.

What intrigues you personally most about data science?

Willmann: As developers, we can gain fascinating insights with the help of AI: For example, physicists at our institute collect a lot of data from particle accelerators about processes that are impossible to observe directly. But through our work, we can still understand in detail what exactly happened to the particles in the accelerator.

Cangi: Another aspect that fascinates me is automation and acceleration. With AI, we can make simulation methods significantly faster. In my case, it is about the electronic structure of matter. With conventional methods, simulations on supercomputers are limited to a few thousand atoms at most. With the AI method we are developing, simulations can be done with hundreds of thousands to millions of atoms.

What are you using artificial intelligence for in your current research?

Cangi: We use AI to find out how matter behaves under extreme conditions. Such conditions occur in planets and neutron stars but are also relevant for new methods of energy generation through nuclear fusion and for the development of innovative materials. Thanks to AI, we can now describe the complete electronic structure of matter under these extreme conditions – a complex probability cloud of electrons, so to speak.

Once we can describe the electronic structure, we know all the material properties. We know whether a material is electrically conductive or an insulator, whether it is strong and durable like diamond or suitable for technological applications like photovoltaics. Therefore, we can also accelerate the development of new materials by digitally exploring numerous material combinations. In the lab, we would then only have to produce the most promising candidates.

Willmann: At our institute, physicists are currently developing a compact free-electron laser so powerful that it could image every single atom of a protein structure. This is an enormously important topic for medicine. For such experiments, however, you have to be able to control and direct the system very well. Usually, you trace the path of the accelerated electrons, for example, by letting them fly through foils, where they leave a trail. But in the process, the particles are destroyed, and the experiment stops. We are, therefore, developing a digital twin for indirect diagnostics. This is a virtual experiment where we can reconstruct the trajectory of the particles throughout the entire experiment.

What does such a digital twin provide?

Willmann: In the experiment, many details cannot be foreseen and explained with equations. Given an identical input, this will lead to a different output. Ordinary simulations, therefore, often produce different results than the actual experiments. This is where AI comes in: Through a sort of black box process, it can also provide the expected output variation. Now, we can tell how stable an experiment is and whether we should improve it.

Cangi: In general terms, a digital twin is a comprehensive digital representation of a real process: it could be an experiment, a process, or a whole other issue. Using AI, we merge completely different simulations into a common digital setting. This allows the digital twin to respond to the user. It can provide me with an immediate answer to the question of what will happen if I change certain parameters. In my department, we are currently working on developing a digital twin for the interior of a planet.

How do your approaches differ?

Cangi: Actually, only in our research objective. And that is precisely the beauty of it: We can transfer the methods from one problem to the other. That's what machine learning and data science are all about. Even though one problem is about a planet and the other is about a laser, Anna and I can exchange ideas about our digital twins and learn from each other.

Willmann: This is the very reason why the "Helmholtz AI Local Units" were established: We support the use of machine learning in research and its adaptation to different problems. Machine learning is a research field that is developing incredibly quickly. New things are being created all the time. That's why research groups exist within the "Local Units": We not only use the methods, but we also research new methods.

What are the current trends? What is in store for the future?

Willmann: One trend is "streaming learning." Traditional machine learning requires a lot of storage space for files that the system initially trains with. It would be much more efficient to have a model that constantly learns new things via streaming. But there are still many problems, like the so-called "Catastrophic Forgetting." This is where the model forgets what it learned at some point in the past – much like a human. We are working on methods to make such models resistant to forgetting without requiring enormous buffer memory.

Cangi: Artificial intelligence is becoming more reliable and autonomous. This is already evident in the public domain, with examples like ChatGPT and other language models. Anyone who has tried ChatGPT is usually fascinated and amazed by how independently AI can operate. In research, experiments and simulations are coming much closer together. The question is: Will there be a general AI that possesses even more capabilities and creativity? How far this will go, only time will tell.

Certain steps can be automated very well. However, as a researcher, I must still have a conceptual framework and make a careful selection of data and methods to thoroughly comprehend the scientific results and employ AI responsibly. In Germany, the academic world is driving progress, taking a more cautious approach to data and methods compared to profit-driven companies. I see promising opportunities to develop guidelines for dealing with large volumes of data and AI, thus implementing AI in a socially responsible manner.

Publication:

L. Fiedler et al.: Predicting electronic structures at any length scale with machine learning. npj Computational Materials, 2023 (DOI: 10.1038/s41524-023-01070-z)

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Indispensable for today's and tomorrow's technologies

Europium is used in lamps, counterfeit-proof banknotes, and sensors. It is one of the most thoroughly researched rare earth elements (REE). Nevertheless, a large meta-study from the HZDR reveals considerable knowledge gaps. With the help of reliable data, europium could be mined and recycled in a more environmentally friendly way and with greater efficiency in the future.

_ **Text** . Antonia Rötger

Some of the information in the literature on europium was so contradictory that chemist Norbert Jordan wanted to verify it through experiments in his own laboratory – with some astonishing results.

Rare earth elements such as lanthanum, praseodymium or europium can be found in every cell phone. While often only in tiny quantities, there are billions of devices. Wind turbines, batteries, catalytic converters, and many other high-tech devices also require several different elements from the rare earths group. They are considered critical raw materials because of their particularly complex extraction process. In nature, they do not occur in elemental form, but are firmly bound to minerals such as monazite or bastnasite – but in the lowest concentrations. In order to extract the individual rare earths from the mined ore and separate them from each other, enormous amounts of rock are moved, ground, and treated with toxic chemicals and highly concentrated acids, which leaves the mining areas permanently polluted.

Enormous losses from mining to production

The coveted europium – like all rare earth elements – comes primarily from China and Brazil, although there are also deposits in the U.S., Australia, and some European countries. "At every stage, from mining to processing, production of components to recycling of rare earths, we have enormous losses that we really cannot afford anymore. Mining, in particular, often destroys landscapes and the environment extensively," knows Vinzenz Brendler, head of the Department of Thermodynamics of Actinides at HZDR's Institute of Resource Ecology.

The processes involved in ore beneficiation, further processing, and reprocessing can only be made more efficient and compatible based on sound and reliable data regarding the chemical behavior of these elements. Data expert Brendler and his colleague Norbert Jordan have therefore designed a major study on europium and enlisted the support of partners: experts from the Paul Scherrer Institute (PSI) in Switzerland and from repository safety research in Sweden. Their results are now available in a structured database and accessible to everyone.

Europium: known for its luminescence

Discovered in 1901, europium is, along with americium, the only element named after a continent. With a density of 5.24 grams per cubic centimeter, it is a lightweight among the heavy metals. It has a silvery sheen but tarnishes immediately upon contact with air and is highly reactive. In aqueous solutions or with acids, it can react to form complex compounds. At temperatures above 150 degrees Celsius, it spontaneously ignites. Its physical properties make europium particularly valuable, in fact, for some applications, even indispensable: It glows intensely red when exposed to light of a particular wavelength.

In the past, europium was used in the red pixels of cathode screens for color televisions; today, it makes light-emitting diodes glow, is needed for medical imaging processes, and its fluorescence makes banknotes counterfeit-proof. For this purpose, it is incorporated into host lattices made of metallic or semiconducting elements and, depending on the environment, can also glow in colors other than red. Europium is also used as an additive in catalysts, magnets, alloys, and glass – or as a strong neutron absorber in the control rods for nuclear reactors.

The annual global production volume is around 400 metric tons of europium oxide. This seems small compared to production quantities of other raw materials, but since bastnasite is composed of only 0.1 percent of the element, large amounts of overburden containing environmentally harmful components are produced.

"Many believe that the chemical and thermodynamic properties of europium are very well known, but this is not the case, even though more publications on europium exist than on any other rare earth element," explains Norbert Jordan. For example, more than 50 publications on the behavior of europium with sulfate in aqueous solution can be found. After a thorough review, however, only the data from eight of these papers proved to be reliable.

120 years of publications evaluated

More than ten years ago, Jordan had already begun to question results from older publications on europium critically. Since then, he has continued to work on this topic in a small team, but more or less on the side. Only when he succeeded in acquiring funding did the europium project gain momentum. Now Jordan and Brendler, together with their cooperation partners, have reviewed all major publications – no less than 350 references with 1,430 values – from scientifically recognized journals published between 1901 and 2021.

"Publication culture has changed a lot during this large timespan; moreover, we also included publications in Russian and Chinese and evaluated them with the help of native-speaking colleagues," Jordan explains. About half of all the data come from 1960 to 1980. "For the more recent publications, we often contacted the research groups if something was unclear to us," the chemist continues. At the same time, he emphasizes the quality of some of the publications, which illustrate in detail how the results were obtained.

But that was not always the case: "Sometimes it took us days to understand a paper because important information was missing. Other times, the results presented were unlikely or contradictory." In some cases, Jordan repeated the experiments in his own lab. "For example, the results on the complexation of europium with phosphate that we found in the literature were incorrect. We therefore obtained accurate data in the lab that can now be used to improve processes," Jordan reports. In the presence of chloride in aqueous solutions, europium also behaves quite differently – it does not react as strongly as claimed, but on the contrary, rather weakly.

Computer simulation instead of trial and error

The new findings on the chemical and physical behavior of europium in different environments are much needed. Until now, many technological processes for extracting and processing europium have been based on estimates and experience. With reliable data, chemical reactions could be simulated in advance on a computer. This would help developing more environmentally friendly methods or improve e-waste recycling processes – for less mining and a viable circular economy.

"We started with europium because we had extensive research data on it. However, such a database would also be necessary for the other elements in the rare earth group," emphasizes Brendler. His colleague Jordan hopes the new findings will also motivate other research groups to generate

No less than 350 publications on europium were put to the test before Norbert Jordan, together with data expert Vinzenz Brendler (left), was able to transfer the verified results into a database accessible to everyone.

robust thermodynamic data on rare earth elements. "Now we know how to set up such a database, and the Computational Science Department at HZDR helped us with this," Jordan looks back.

There are 17 rare earth elements in total – a lot of work for the experts from Dresden. It should be helpful that a deeper understanding of the chemistry of europium can be transferred to a large extent to other rare earth elements and also to the chemistry of the trivalent, radioactive actinides in spent fuel rods of nuclear power plants.

Publication:

N. Jordan et al.: A critical review of the solution chemistry, solubility, and thermodynamics of europium: Recent advances on the Eu^{3+} aqua ion and the Eu(III) aqueous complexes and solid phases with the sulphate, chloride, and phosphate inorganic ligands. Coordination Chemistry Reviews, 2022 (DOI: 10.1016/j.ccr.2022.214608)

"At every stage, from mining to processing, production of components to recycling of rare earths, we have enormous losses that we really cannot afford anymore."

_ Vinzenz Brendler, HZDR

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Nobel Prize winner Donna Strickland on a visit

High-power lasers owe their existence to the pioneering research of Donna Strickland. She received the 2018 Nobel Prize in Physics jointly with Gérard Mourou "for their method of generating high-intensity ultrashort optical pulses." The principle is called Chirped Pulse Amplification (CPA) and is based on stretching laser pulses in time before amplifying them, and then recompressing them again.

"CPA technique has set in motion a revolution in the field of laser optics," physicist Toma Toncian knows. His workplace is in Schenefeld in the metropolitan region of Hamburg, more precisely: at the European XFEL, the world's most powerful X-ray laser. The HZDR operates two high-power lasers through the Helmholtz International Beamline for Extreme Fields (HIBEF) user consortium at this location. As department head, Toncian is responsible for the operation and maintenance of the HIBEF facilities for the HZDR. Naturally, he could not miss the Nobel laureate's visit on February 10, 2023.

"His" lasers at the European XFEL's High Energy Density (HED) platform promise insights into the structure of materials and into extremely fast processes. This will enable researchers worldwide to gain new insights into stars, planets, plasma clouds, quantum systems, and versatile materials. *(CZ)*

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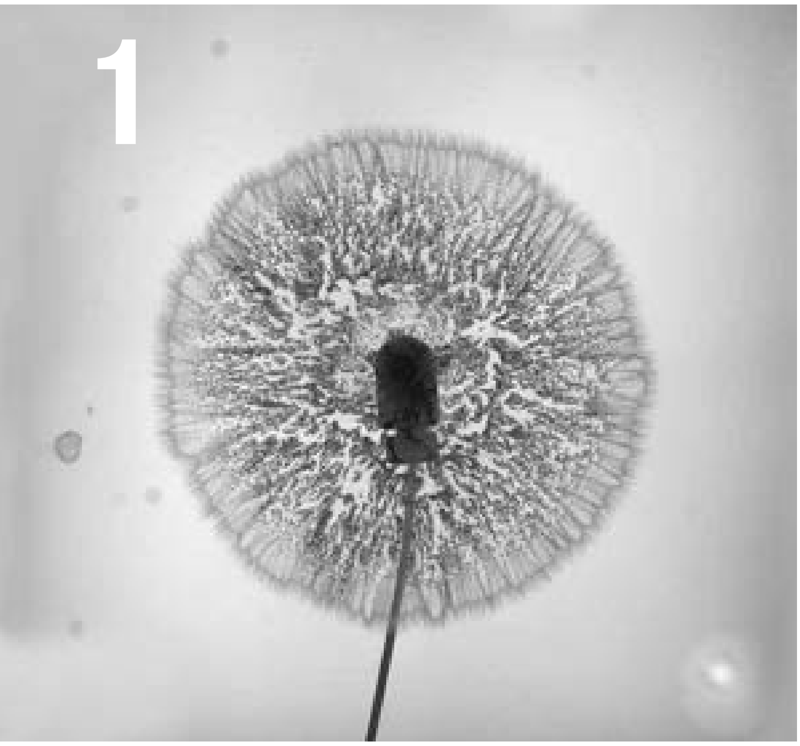
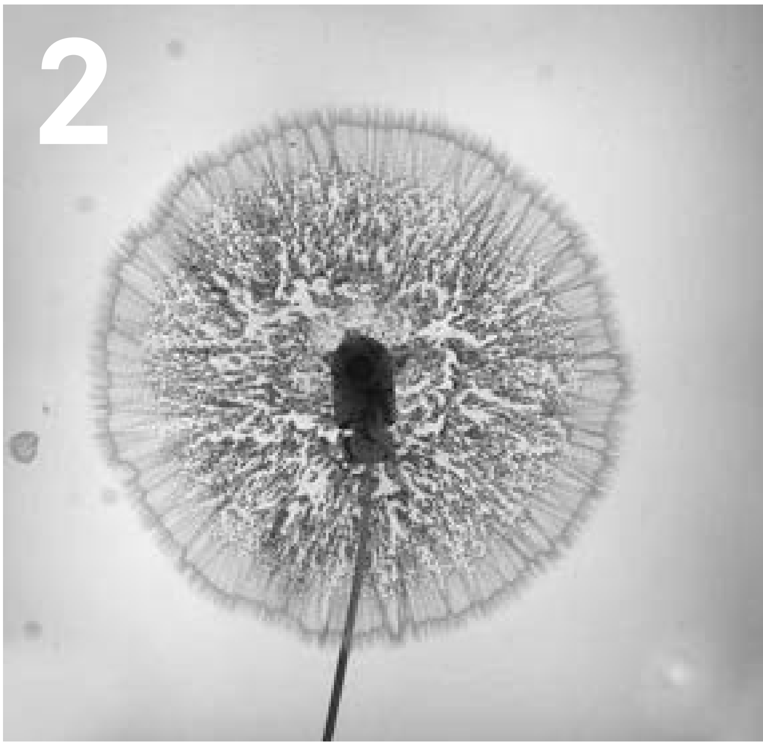
Helmholtz International Beamline for Extreme Fields (HIBEF) at the European XFEL in Schenefeld

The Nobel laureate surrounded by physicists from the HZDR and the English partner institutions at the international HIBEF user consortium. From left: Thomas Cowan, Thomas Butcher from the Science and Technology Facilities Council (STFC), Donna Strickland, Toma Toncian, Ulrich Schramm, Justin Wark from Oxford University.





Flowing weightlessly – data treasures from space

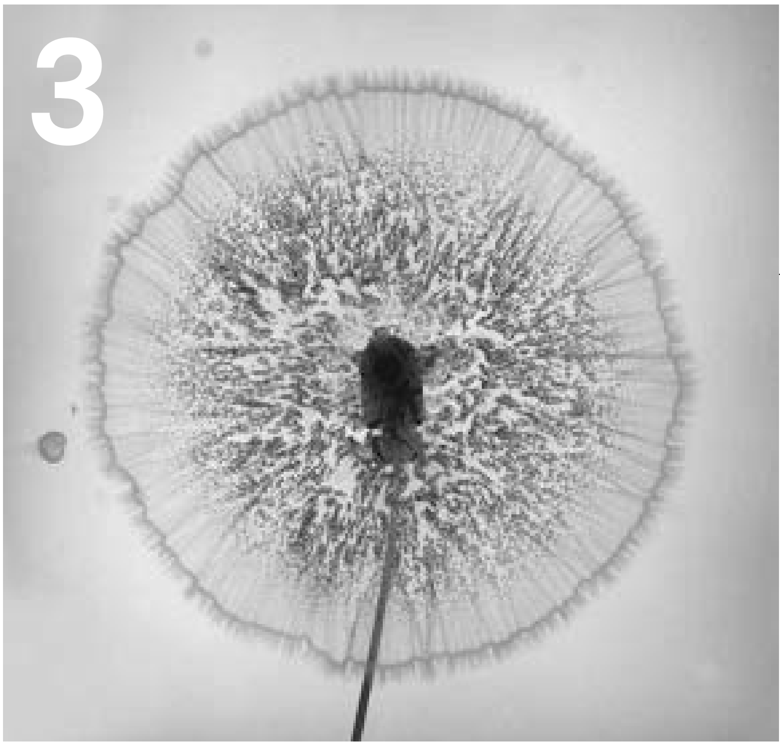
It is ever-present on Earth: Gravity shapes our environment and its physics, chemistry, and biology. Karin Schwarzenberger and her team want to find out how gravity affects the mixing of two dynamically flowing liquids. For the comparison to weightlessness, they even launched an experiment into space aboard a rocket. Their findings are expected to help improve environmental technologies.

_ **Text** . Gabriele Schönherr

The engineers and researchers have been waiting several years for this moment: It is October 1, 2022, 07:26 a.m. local time, when the TEXUS-57 sounding rocket – a cooperative project between Airbus, the European Space Agency (ESA) and the German Space Administration (DLR) – finally lifts off from the launch pad at the Esrange Space Center in Sweden with four experiment modules on board. A moment of relief for the entire team. At least for a short while. Whether the experiment in space is a success will only be known weeks later, after the data has been evaluated. Many things can go wrong, Karin Schwarzenberger knows: "The experiment can be damaged during launch. The rocket can have a hard landing, or it can crash into a lake – in northern Sweden, twenty percent of the area is covered with water or swamps. If you are unlucky, all the data is gone." She knows the risks and hurdles of space exploration very well. But she also understands its profound research value.

Knowledge for planet Earth

At HZDR and TU Dresden, the engineer researches transport processes at interfaces, for example, between two liquids. New findings in this field could help improve environmentally relevant technologies, such as CO_2 storage or soil remediation. "In soil remediation, one often works with active ingredient solutions introduced into soils under pressure to bind pollutants or solidify the soil. In the case of CO_2 sequestration, a carbonate-rich solution is injected into alkaline soil, where it encounters a solution of alkaline ions



The reaction front between two liquids forms complex flow patterns.

Launch of the TEXUS-57 sounding rocket on October 1, 2022, with the Dresden experimental module on board.

that mineralize the CO_2," Schwarzenberger explains. Central to both methods is the reaction of two liquids as one flows into the other – dynamic reaction fronts with complex flow patterns form in the process.

Calculating such reaction fronts in scientific models, including the complete flow dynamics, is currently still very complex and time-consuming. Therefore, Schwarzenberger and her team are investigating whether certain scenarios can be handled with simpler models. Excluding influencing factors can reduce the computational effort tremendously. One such factor is buoyancy in liquids since it has little influence on porous media, such as soil materials. "Put simply, this is because the individual pores in the material are so small that surface effects on the walls and flow pressure dominate what happens," says Schwarzenberger.

Turning off gravity

This is where gravity enters the picture, as it is the physical cause of buoyancy. Cooperation partners of the HZDR team at the Université Libre de Bruxelles have already developed respectively simplified theoretical models. They describe the injection flow, the chemical reaction of two liquids, and their diffusion, i.e., the random self-motion of the molecules. However, they do not take gravity into account.

"If we use the models of our colleagues in Brussels, the reaction front can be calculated on a normal PC. With the effects of gravity taken into account, high-performance computers are needed to solve the complete flow equations in direct numerical simulations," Schwarzenberger notes. "The crux: Even the simpler models without buoyancy must first be validated. Experimentally, this is much easier to do in weightlessness than in porous media. Microgravity basically switches off all the buoyancy force, and we can observe effects that are otherwise overshadowed by the gravity on Earth," the scientist explains.

"The crux: Even the simpler models without buoyancy must first be validated."

_ Karin Schwarzenberger, HZDR and TU Dresden

In the first step, this was achieved by a parabolic flight campaign. The state of weightlessness is reached several times, at least briefly, during the free fall of the aircraft: the research group had 22 seconds per parabola. "We replicated the flows using a simplified setup, the so-called Hele-Shaw cells. Each of these cells consists of two planar acrylic glass plates stacked parallel to each other with a very narrow gap in between, into which two different liquids are injected one after the other. A two-dimensional flow pattern develops as a result," Schwarzenberger describes the experiments.

By comparing the experimental data obtained in weightlessness with the simplified models, the researchers were able to validate some of the theoretical predictions. But not all of them because the 22-second intervals of weightlessness were not long enough for the diffusion process to take place. Time scales also change in microgravity. In the absence of buoyancy, the same process may suddenly take longer than on Earth. "Therefore, the parabolic flights were just a first step, and the rocket flights a huge opportunity," the engineer emphasizes. In 2016, the group presented the first technical design of an experimental module for the European sounding rocket program. Three years later, the flight ticket was granted.

Six years of preparation for a six-minute experiment

The space mission placed new demands on the hardware set-up once again. During the rocket's launch and landing, enormous forces affect the experiment, and space is extremely limited. Moreover, once launched, experimenters can no longer intervene, so every centimeter and every second had to be meticulously planned. On board the rocket, three cameras were recording the reaction fronts live. Reassuringly, for the first time a "digital downlink" was provided for this mission. The team could have saved at least a few images if something had gone wrong during the landing.

Since the beginning of 2020, the researchers and engineers met regularly with their development partner, Airbus, in Bremen for testing. Then, unexpected circumstances unfolded: the Corona pandemic, a major fire at the launch pad, and eventually, in February 2022, one day after the first test countdown, the launch was cancelled due to the war in Ukraine. Finally, in October 2022, the delayed launch took place. Six years of preparation for thirteen minutes of flight time and six minutes of weightlessness. Was that worth it? "Six minutes is really long. Rocket experiments are far superior to parabolic flights in this respect," says Schwarzenberger.

Data evaluation with a twist – and a happy ending

With the new data from the rocket experiment, the research group was now also able to compare the influence of diffusion on the reaction fronts with the predictions of the models – but only after months of evaluation. "In the experimental data, we always have interfering effects, such as small bubbles in the flow, especially under the extreme conditions on parabolic flights and in the rocket. We then have to remove part of the data from the analysis again," explains Yorgos Stergiou. The chemical engineer joined the project for his doctoral thesis and was present on board during the parabolic flights. "That was so awesome, but it takes you a while to get your mind back on the data afterwards," he recalls.

The data from the rocket experiment still held a unique challenge. Unnoticed, a wrong component had been installed in the experiment, and some data seemed to be unusable as a result. Only after extensive investigation could the team breathe a sigh of relief: the experimental results were reliable and matched the theoretical models.

"In the experimental data, we always have interfering effects, such as small bubbles in the flow, especially under the extreme conditions on parabolic flights and in the rocket."

_ Yorgos Stergiou, HZDR

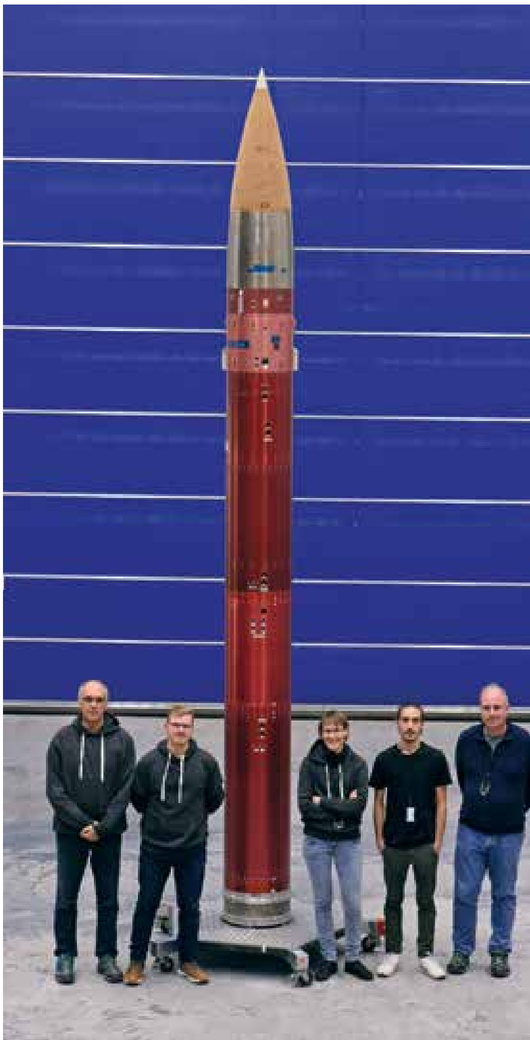
Airbus was responsible for the technical implementation of the experiment module. Two different liquids are injected one after the other into the individual cells made of closely stacked acrylic glass plates. Three cameras capture the resulting reaction fronts.

The experiments confirmed: The further the reaction front between the two liquids moves away from the injection point into the cells, the more important diffusion becomes. Close to the injection point, the flow is very swift, and the reaction front is influenced mainly by wall friction and is effectively extended. Towards the outer region, the flow velocity decreases quickly. As a result, the diffusion movement of the molecules gains influence and now mixes the liquids at the reaction front more thoroughly.

Since then, the team in Brussels has been working intensively on the data. "The work is very promising. We have already been able to show that the model, which takes wall friction into account via a simple parabolic velocity profile, matches our rocket experiment well. Therefore, this model should also apply to reaction fronts in small pores," Schwarzenberger summarizes the results so far. "Taking measurements in real porous media is extremely difficult; without the conditions of weightlessness, we would not have been able to figure this out experimentally via our Hele-Shaw cells."

Rocket experiments

The planning and realization of the experiments took place within the framework of the CHYPI-FLOWER ESA Topical Team selected by the European Space Agency; CHYPI stands for “chemo-hydrodynamic patterns and instabilities”. In this collaborative effort, several international research teams are pooling experiments, data, and theoretical models on the chemistry and physics of hydrodynamic patterns and instabilities. In doing so, they are considering applications in space and on Earth.



Ready to go: After six years of preparation, the Dresden group and its partners are looking forward to the launch. Their module: the third from the bottom.

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WINNERS

Coveted ERC grants

Physicist **Larysa Baraban** receives a Consolidator Grant from the European Research Council (ERC), which will provide her and her team with nearly two million euros to digitize tumor characteristics. Her "ImmunoChip" platform is designed to determine whether and how a patient responds to immunotherapy. For this purpose, Baraban is developing bio-nanosensors whose data can be used to determine cancer immunity and strategically plan and track treatment.

Larysa Baraban optimizes immunotherapies against cancer

Tobias Dornheim calculates quantum properties

Tobias Dornheim wants to use machine learning methods to answer fundamental questions about hydrogen and heavier elements and thus contribute to materials research, astrophysical models, and nuclear fusion (see article on pages 20 - 21). With a Starting Grant from the European Research Council (ERC), he now has around one and a half million euros over a period of five years at his disposal.

↗ https://erc.europa.eu/funding

Award-winning battery research

Anna Vanderbruggen receives the CHANGE Award from the European Institute of Innovation and Technology (EIT) for her innovative method of graphite recycling. In her doctoral thesis, she succeeded in separating the fine powder from crushed lithium-ion batteries into two valuable products, enabling efficient and highly selective recycling of both graphite and metals. Vanderbruggen is a graduate of EIT's Emerald master's program and was nominated for the award by EIT RawMaterials, Europe's largest raw materials network.

↗ https://eit.europa.eu/

Anna Vanderbruggen and Bernd Schäfer (CEO and Managing Director EIT RawMaterials)

CONVENED

Networking in the border triangle

"Building Bridges for the Next Generations" – that was the title of the tri-national science conference held at the International Congress Center Dresden (ICD) on May 16 and 17. It provided a platform for young researchers, especially from Saxony, Poland, and the Czech Republic, to engage in dialogue with stakeholders from politics, business, and society. The conference was organized by the HZDR on behalf of the Free State of Saxony.

↗ **https://building-bridges-conference.eu/**

PLANNED

New NCT sites

Diagnostics, therapy, research, and patient care under one roof: That is the recipe for success of the National Center for Tumor Diseases (NCT), which bases its activities on long-term cooperation between the German Cancer Research Center (DKFZ) in Heidelberg and selected oncology centers at universities and research institutions throughout Germany.

Back in 2015, the green light was given for the first partner site of the Heidelberg NCT: the NCT/UCC Dresden with its partners University Hospital Carl Gustav Carus Dresden and Carl Gustav Carus Faculty of Medicine at TU Dresden as well as the HZDR. In February of this year, the Federal Ministry of Education and Research (BMBF) has now confirmed four new sites:

- NCT Berlin
- NCT West: Cologne/Essen
- NCT SouthWest: Tübingen/Stuttgart-Ulm
- NCT WERA: Würzburg with partners in Erlangen, Regensburg, and Augsburg

↗ **www.dkfz.de**
↗ **www.nct-dresden.de**

The NCT building on the grounds of Dresden's University Hospital was already scheduled to open in 2020.

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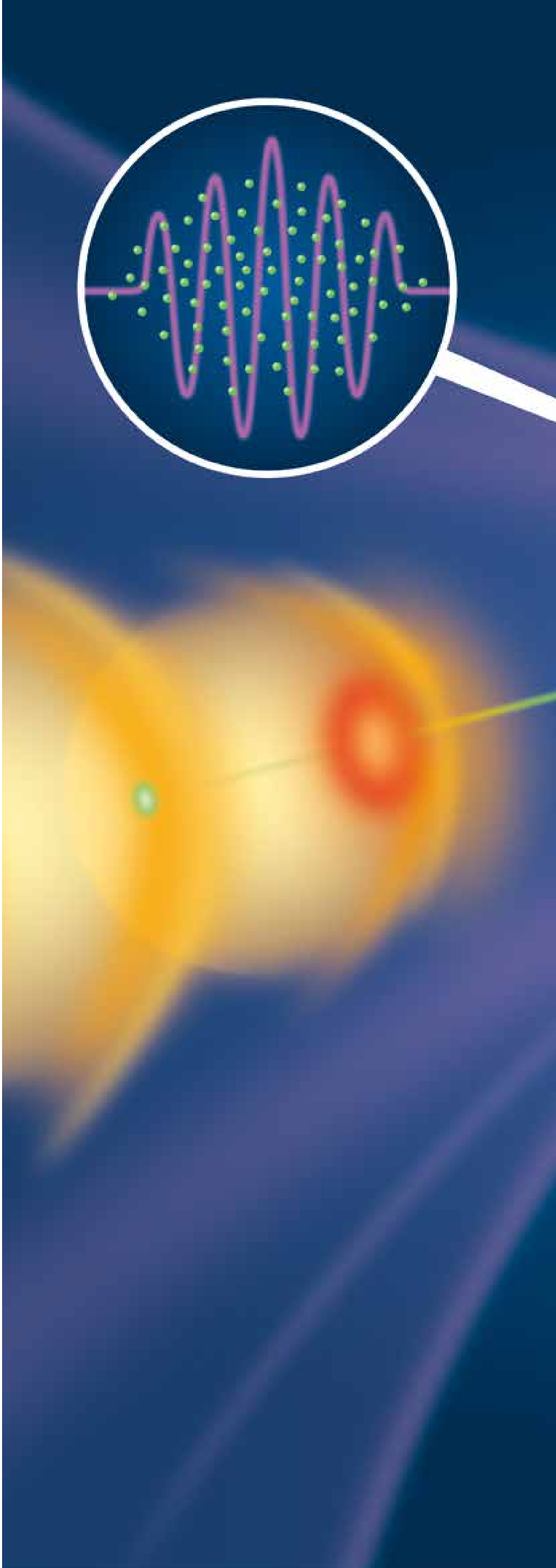

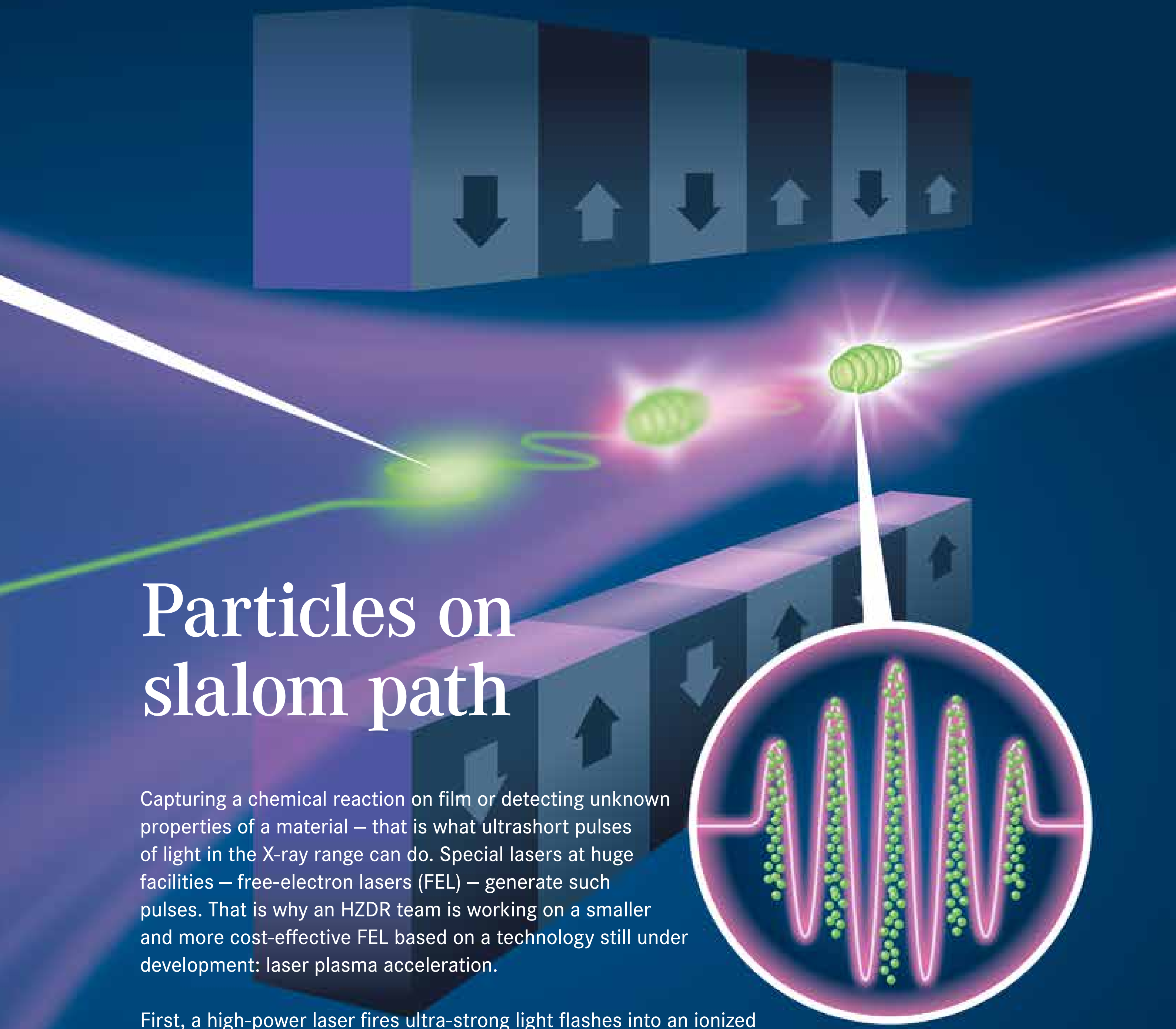

Particles on slalom path

Capturing a chemical reaction on film or detecting unknown properties of a material – that is what ultrashort pulses of light in the X-ray range can do. Special lasers at huge facilities – free-electron lasers (FEL) – generate such pulses. That is why an HZDR team is working on a smaller and more cost-effective FEL based on a technology still under development: laser plasma acceleration.

First, a high-power laser fires ultra-strong light flashes into an ionized gas, i.e., into a plasma (yellow-red). An alternating electric field is created, similar to the wake of a ship. This wave accelerates the electrons in the plasma. The particles, now bundled into bunches (green), fly on into the so-called "undulator", where an arrangement of alternating magnets forces them onto a slalom path. In the process, the particles emit light at every turn. Only when the electrons interact with the light in a perfect way, the desired laser pulses are generated.

In cooperation with the French synchrotron SOLEIL, the HZDR experts have succeeded for the first time in generating a well-controllable laser light in the ultraviolet (UV) range via plasma acceleration. Their next goal: accelerating the electrons to much higher energies in order to produce the type of high-intensity X-ray flashes demanded in research.

Publication: M. Labat et al., Nature Photonics 2023 (DOI: 10.1038/s41566-022-01104-w)

International Conference **Building Bridges for the Next Generations**

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