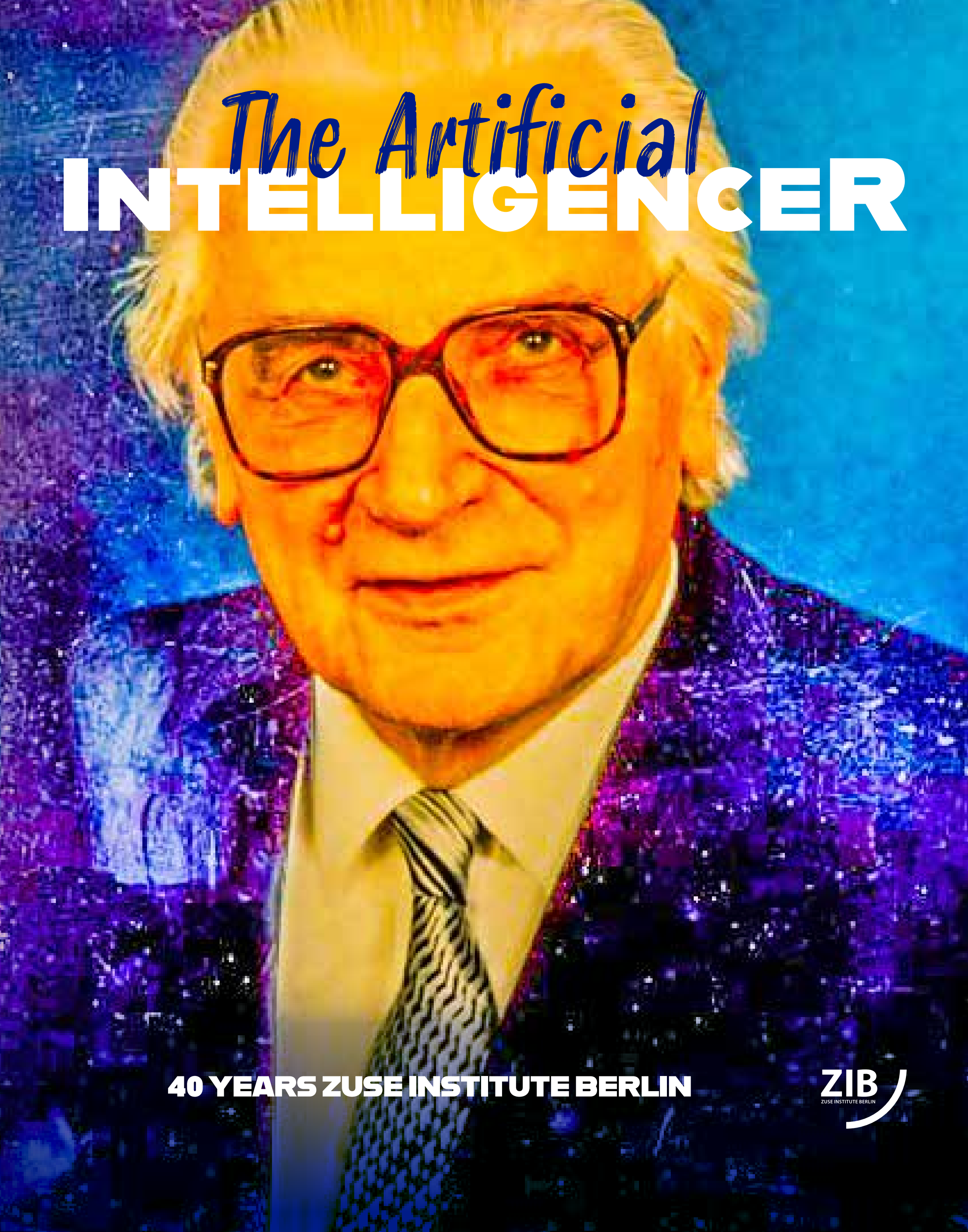
The Artificial INTELLIGENCER



40 YEARS ZUSE INSTITUTE BERLIN

ZIB
ZUSE INSTITUTE BERLIN

Welcome

The Zuse Institute Berlin (ZIB) Celebrates Its 40th Anniversary!

For four decades, ZIB has been synonymous with cutting-edge research in applied mathematics and data-intensive high-performance computing. Our mission is to develop knowledge and technologies through innovative research that enrich and improve life across all societal domains.

ZIB is nothing without the people who drive it: 300 employees, predominantly researchers from diverse disciplines, along with numerous dedicated professionals providing high-quality scientific services for Berlin and Germany.

On the following pages, you will find examples of our work. Whether it's artificial intelligence, more efficient energy, sustainable transportation systems, or revolutionary medical technologies, our blend of mathematics and high-performance computing helps shape the future.

We hope you enjoy reading!

Your Members of ZIB

ZIB IN NUMBERS

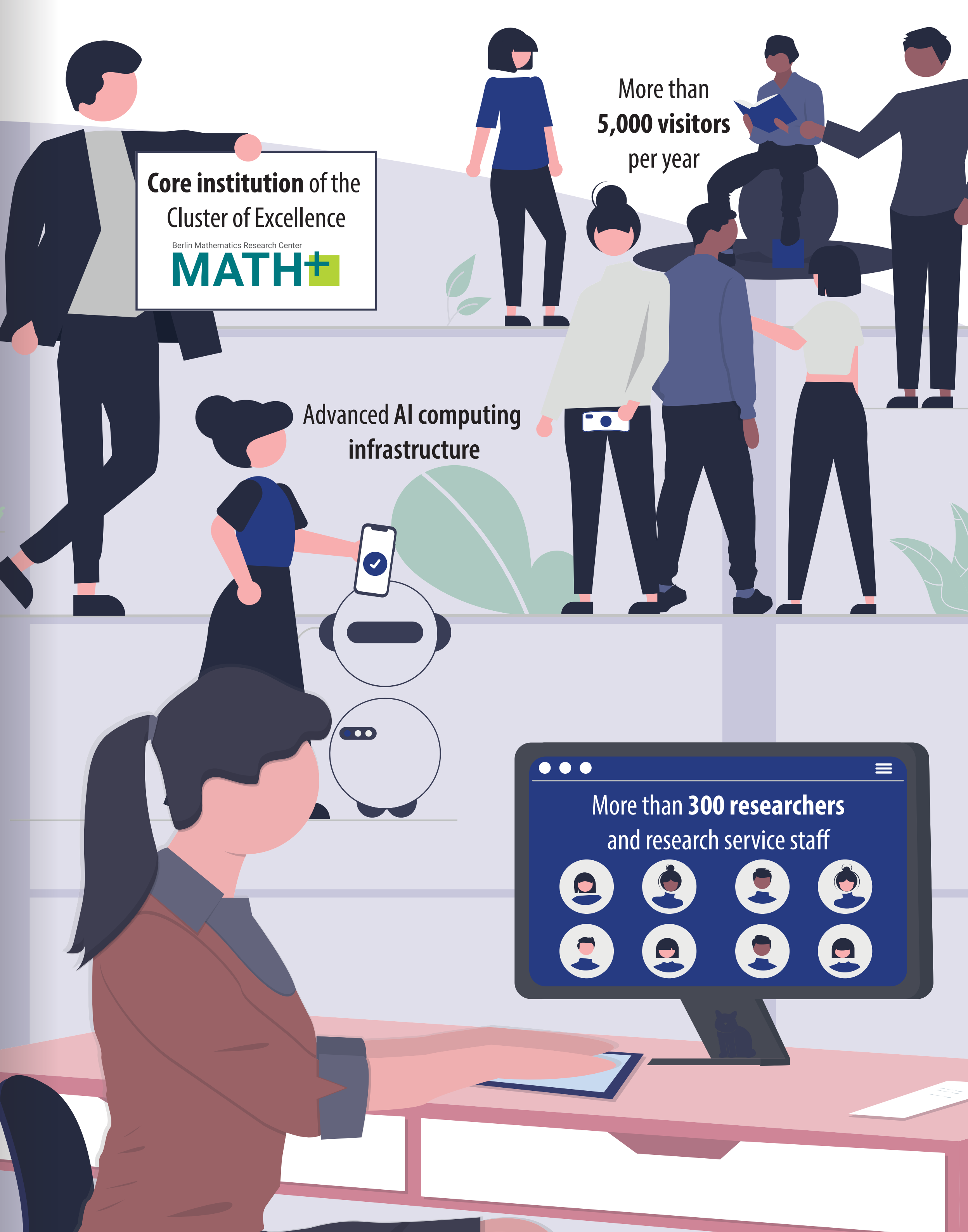
Home of the largest mathematics-centered public-private partnership, the Research Campus MODAL, with more than **30 industry partners**

Over **100 research projects**

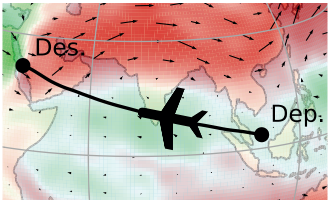
Home of Berlin's high-speed **research data exchange network** with up to 400 Gbit/s

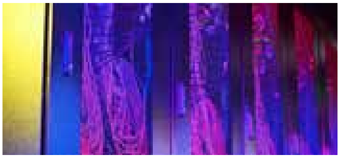
Data storage with more than **200 Pbytes** capacity

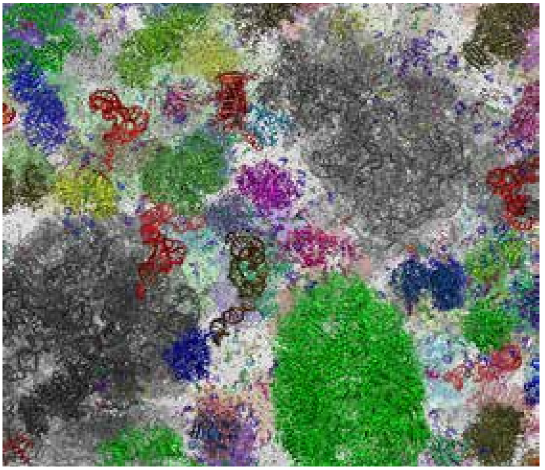
Supercomputer with 120,000 CPU kernels, allowing almost **10,000,000,000,000,000** operations per second

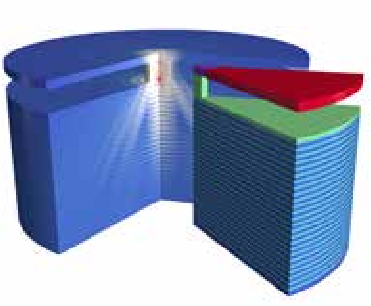

Core institution of the
Cluster of Excellence
Berlin Mathematics Research Center
MATH+
More than
5,000 visitors
per year
Advanced AI computing
infrastructure
More than 300 researchers
and research service staff

CONTENTS // SHOWROOM









Toward Sustainable Public Transport

In the evolving landscape of public transportation, achieving efficiency, sustainability, and cost-effectiveness is paramount. With over 8 billion passengers annually, Germany's public transport system faces unique challenges. The strategic application of advanced mathematical methodologies has emerged as a pivotal tool in redefining the operational capabilities of buses, trains, and even airplanes. Together with our industrial partners, we optimize vehicle scheduling, manage fleet operations, and pioneer sustainable solutions. Our innovative mathematical methods not only address the challenges of urban expansion and environmental concerns but also highlight the transformative impact of research in shaping a smarter transportation future.

As cities grow and evolve, their transportation systems must also adapt to meet new demands. In collaboration with Berlin's public transport operator BVG, we took on the task of enhancing public transport efficiency through advanced vehicle scheduling optimization. Imagine the city's network of roads and stops as a colorful map, where each color represents different travel times between various destinations, illustrating not just the physical distance but also the efficiency of routes from one point to another. We developed a so-called Lagrangian pricing method that can optimize this map, finding the quickest routes while considering passenger flows and costs. Based on this map, our method finds optimal schedules for all involved vehicles and can tackle massive problem sizes with hundreds of millions of possible connections and dozens of vehicle types. The result of this partnership is a high-performance scheduling system, which is today used by half of Germany's public transport providers, saving time, money, and reducing emissions.

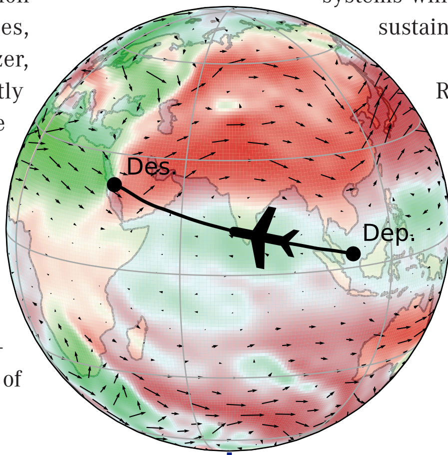
Expanding beyond urban transportation networks, efficiently scheduling long-distance trains involves not only finding optimal schedules but also dealing

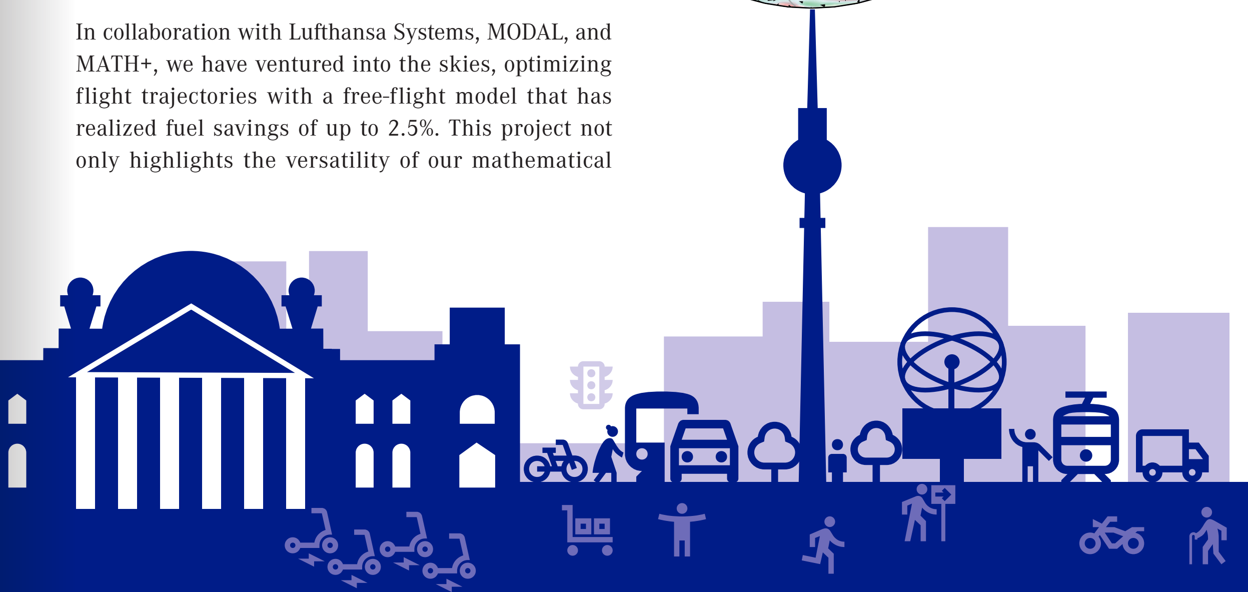
with the challenge of forming specific train compositions, as individual units can vary in type and orientation. In close collaboration with Deutsche Bahn (DB), the Research Campus MODAL, and the MATH+ Cluster of Excellence, we have pioneered a groundbreaking approach dubbed the “hyperflow model,” which is revolutionizing train scheduling. Similar to a skilled conductor leading a symphony of trains, the hyperflow model orchestrates the movement of travelers and goods throughout the train network, ensuring minimal delays. This results in gigantic optimization problems with several hundred million variables, which our newly developed coarse-to-fine optimizer, tailored for this specific problem class, efficiently solves. This new method can dynamically adjust the level of detail during computation to achieve the best combination of efficiency and accuracy. As a result, our new approach allows the entire German ICE fleet for a standard week to be scheduled on a modest computing cluster. Moreover, our technology seamlessly integrates into scheduling systems such as DB’s, contributing to annual savings exceeding 70 million euros and reductions of 34,000 tons of CO_2 emissions.

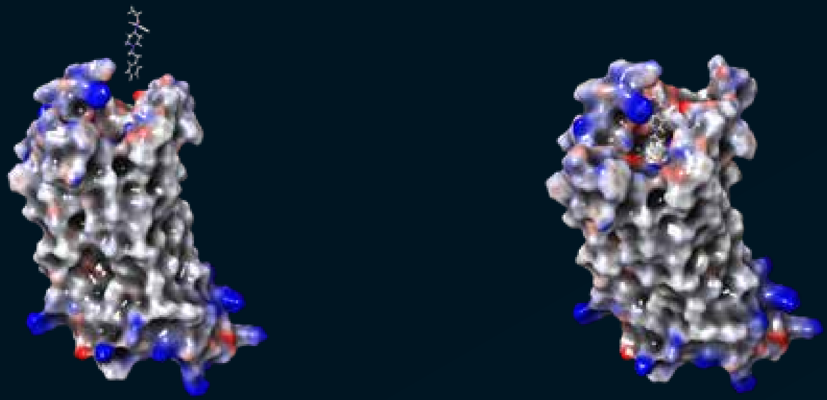
In collaboration with Lufthansa Systems, MODAL, and MATH+, we have ventured into the skies, optimizing flight trajectories with a free-flight model that has realized fuel savings of up to 2.5%. This project not only highlights the versatility of our mathematical methodologies but also underscores our commitment to environmental stewardship across all modes of transportation.

ZIB is developing sophisticated algorithms capable of optimizing transportation across various modes, including buses, trams, trains, and airplanes. This initiative exemplifies our dedication to advancing modern mobility and highlights our innovative strategies to directly address the complexities of current transportation systems while prioritizing sustainability.

Ralf Borndörfer





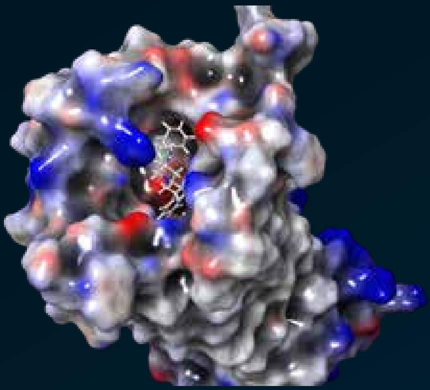


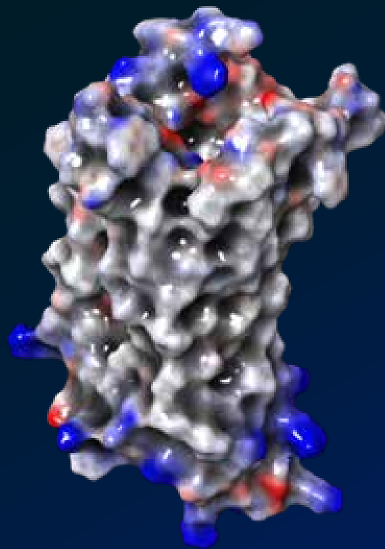
BETTER DRUGS FOR SEVERE DISEASES

Pain therapy is one of the most important areas of health care with 12–15 million patients with chronic pain, including 5 million with severe pain, in Germany alone. Worldwide, more than 100 million patients take opioid-based medications, despite the significant side effects, including death. These numbers are rising and can lead to a societal crisis, as the current "opioid epidemic" in the USA with several hundred thousand deaths shows.

Our goal was to develop new drugs that produce the desired effect (relief of severe pain) but not the undesirable side effects (e.g. respiratory distress, addiction, cardiac arrest). When developing drugs, we try to find a small molecule called a "ligand" that can bind to a specific target molecule on the surface of our cells and, by binding, induce the desired effect, in this case pain relief. The problem is that most ligand molecules bind not only where the effect is needed (in diseased, e.g. inflamed, tissue), but also where they cause side effects (e.g. in healthy tissue in the brain). Diseased and healthy tissue differ by the chemical environment of the affected cells in our body. Therefore, the idea was to find ligands that only bind to the cell surface where needed – in the chemical environment characteristic of the disease. This represents a new paradigm of drug design that was proposed only a few years ago jointly by ZIB researchers and physicians from the Charité University Hospital.

This team succeeded in finding a ligand molecule that actually binds only in inflamed tissue and not in healthy tissue. The development was achieved without laboratory or animal experiments, but by using ZIB's supercomputer. To do this, we had to solve a serious problem: the calculations needed to understand whether a ligand binds better in inflamed than in healthy tissue require an enormous amount of computing time on the supercomputer; the power consumption alone would cost millions of euros and produce thousands of tons of CO_2. Together with other mathematicians from the MATH+ Cluster of Excellence, we overcame this obstacle. We succeeded in developing new mathematical techniques to perform the calculations in an intelligent and very efficient way, reducing the computing time to days and the electricity consumption and CO_2 production to less than a thousandth. The new drug candidate has been patented and medical experiments





have shown that it does indeed relieve severe pain and also works solely in inflamed tissue as calculated. Clinical trials are currently being conducted in collaboration with Queen's University Canada to see if it really does have no or very mild side effects. Inspired by this success, we are now working to use the new mathematical techniques and the novel drug design paradigm to develop other nonaddictive drugs. Not only for pain relief, but also for other serious diseases such as cancer or cardiovascular disease. To this end, our team, in collaboration with Harvard University, has developed a highly automated software platform that is able to search for new drugs in huge libraries of billions of candidate molecules on supercomputers. With success: new drug candidates have already been found and are currently being chemically produced and tested in detail.

In the future, we want to go much further than this approach. We are working on a way to use artificial intelligence to suggest new chemical substances with "drug-like" structures. In this way, we can find substances that are completely new and have never been considered as drug candidates. Initial results are very promising.

Marcus Weber,
Konstantin Fackeldey,
and Christof Schütte

The four images show the mu-opioid receptor, a molecule our cells use for pain reception. Also depicted is a small drug molecule that is entering the receptor in the left-most picture, is embedded in its binding pocket in the second and third images, and is exiting from the receptor in the right-most image.

WORLD-RECORD SOLAR CELLS

Perovskite-silicon tandem solar cell with world-record efficiency.

Image courtesy of L. Zimmermann and J. Beckedahl (Helmholtz Zentrum Berlin)

Our society is facing tremendous changes related to climate change. In order to reduce CO_2 emissions from energy production, we need to exploit sustainable sources of energy. Moreover, an independent energy supply has become a geopolitical topic of highest importance. A cornerstone of any sustainable energy network is solar energy accessed through photovoltaic devices. Consequently, any improvement in photovoltaic cell efficiency can save enormous amounts of emitted CO_2. Further, solar fuel devices allow solar energy to be converted into usable fuels. These can be stored and then distributed through existing networks. The research and development of such renewable-energy processes therefore has a major impact on our future society.

In our collaboration with the Helmholtz Center Berlin for Energy and Materials (HZB) and the MATH+ Cluster of Excellence we investigate methods for simulating solar cells of the next generation, so-called perovskite–silicon tandem cells. In this collaboration we succeeded in developing cells with an efficiency of nearly 30%. The design value could also be achieved in the experimental realization and constitutes a world record in efficiency.

In particular, this type of solar cell consists of various layers of different materials and of thicknesses of a few tens to a few hundreds of nanometers. A nanometer is one millionth of a millimeter. Some of these layers additionally contain regular patterns with a periodicity of a few hundreds of nanometers. The purpose of the various layers is to absorb different parts of the solar spectrum. This means that energy from blue light is harvested in a different material layer than energy from red light. The additional nanopatterns efficiently trap the radiation in these layers. The role of ZIB in the collaboration is to develop and apply simulation tools which allow the best setting of the various layer thicknesses and further geometrical parameters of the nanopatterns to be found. Such a project consists of a chain of various tools: an accurate model of light–matter interactions in the illuminated solar cell, an accurate computational method in order to solve the model, and an efficient and reliable optimization method in order to find the best model parameters.

As mathematics is transferable to different fields, we are also using these methods for other renewable-energy-related projects. For the solar cell a major challenge is to couple the light from the sun to the microscopic layers in the cell. However, for energy-efficient light-emitting diodes (LEDs), the challenge is just the opposite: the light needs to be effectively coupled out from the semiconductor layers of the LED. Both application cases have in common that nanostructures can do the trick – and that the same modeling, simulation, and optimization methods can find the most efficient structures.

In further projects we are investigating how quantum effects on metal surfaces can help in photocatalysis and thereby allow for the synthetization of storable energy forms, so-called solar fuels. Also here, optimized nanostructures can greatly enhance the efficiency of the processes. We believe that in these fields, we can use our numerical and mathematical tools to create a great impact both on science and on future society.

Sven Burger

40 YEARS OF EXCELLENCE IN HIGH-PERFORMANCE COMPUTING

What do such diverse fields as climate modeling, renewable energy, artificial intelligence, and precision medicine have in common? They all rely on high-performance computing (HPC), the art of innovative research with the help of super-powerful computers. Today, HPC systems are similar to tens of thousands of individual computers (computing nodes) with superfast processors connected by a special data network so that they can work together to solve one single problem, often being a million times more potent than a standard laptop.

Here at ZIB we have been operating HPC systems for science for 40 years. Presently, we manage the HPC system “Lise,” with a total computing capacity of approximately 10 petaflops per second. To put this into perspective, this implies that within a single second, our system can perform calculations equivalent to what the entire global population of 8 billion individuals would take 2 years to achieve, working around the clock.

Since 2021, ZIB is part of the National High-Performance Computing Alliance (NHR) that has been built to pool top-level HPC resources and expertise for German science. In addition to building and operating HPC systems, the focus is on helping scientists and engineers to run HPC workloads as well as on optimizing energy efficiency by decreasing energy consumption while increasing computing power.

Recently, artificial intelligence (AI) and big data have revolutionized the HPC world. Machine learning, for example, the art of training AI based on lots of data, requires enormous computing power, which can only be provided by sophisticated computer architectures based on accelerators like GPUs, a high-performance communication network, and sophisticated memory and storage, all working together to deliver the best performance regarding computing power as well as energy efficiency. At ZIB, we not only work hard to make our HPC system fit for AI and unleash the potential of AI technologies, but also consider their transparency and societal implications, in particular in critical applications.

Our HPC system holds immense potential for researchers. We actively assist our users in unlocking this potential through scientific consulting services and also open up new horizons for computational research: ZIB researchers are leveraging the system to drive innovation and address research challenges. Examples include advancements in renewable energy, sustainable mobility, cutting-edge drug design, and enhancing the reliability and security of artificial intelligence.

HPC is currently more accessible and valuable than it has ever been. At ZIB, we are working with many other scientists in Berlin, in Germany, and all around the world to harness its capabilities to address the pressing challenges that our society encounters.

Thomas Steinke

MATHEMATICS FOR THE

In the face of one of the most pressing challenges of our time – the transition to sustainable, fossil-free energy systems – Germany continues to emit greenhouse gases amounting to 750 million tons of CO_2-equivalent. The energy sector alone is responsible for a third of this. Just 50% of the generated electricity comes from renewable sources, while the situation is more precarious for heat generation with only 17%. Technological, economic, political, and societal solutions are needed for transforming the system.

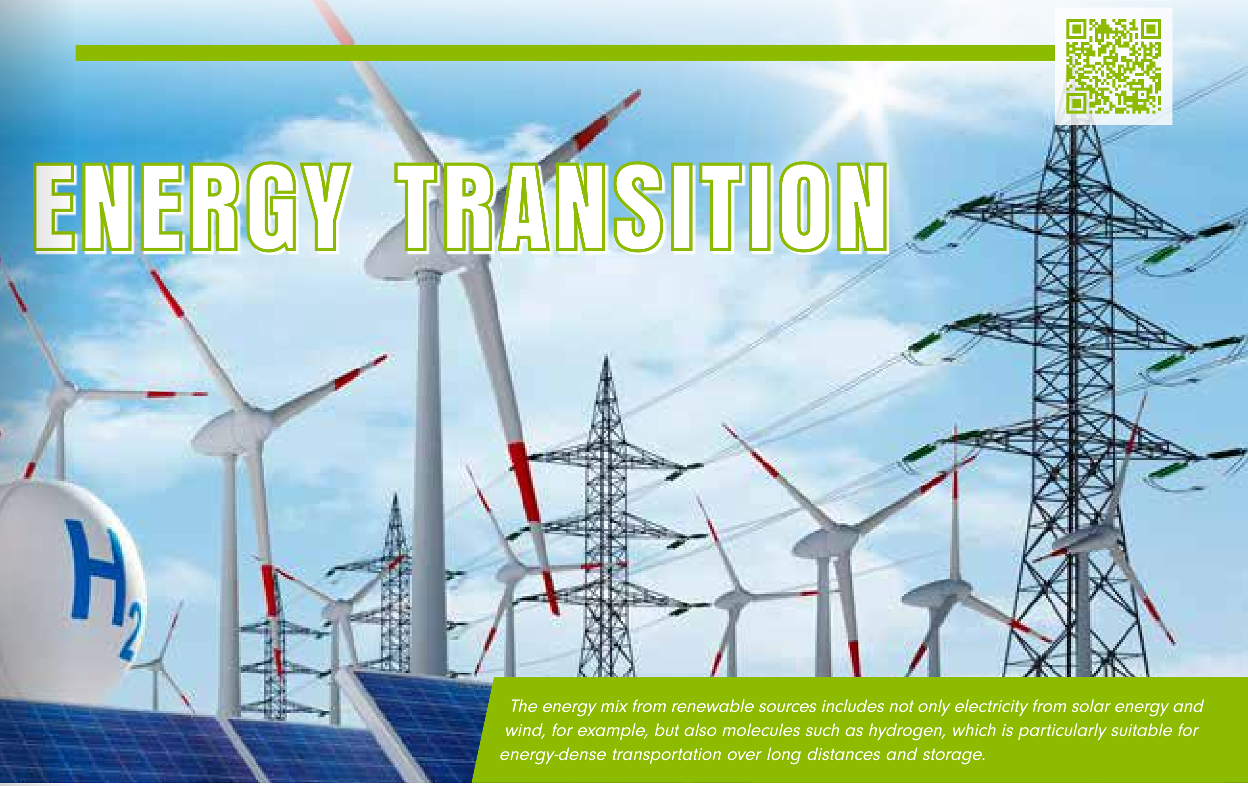
Our focus is on supporting politics and industry in their transformation efforts for the benefit of society. In doing so, we need to analyze the variety of potential solutions and identify the most promising ways to accelerate the transformation process. Our methods for finding such solutions are based on mathematics and artificial intelligence and identify optimal transformation pathways for multi-sector energy systems from a single neighborhood to the whole of Europe.

In the past, the primary focus in planning and operating energy systems has solely been on economic goals, such as minimizing costs while maximizing revenues. However, the ongoing transformation necessitates a shift toward incorporating ecological objectives, like reducing CO_2 emissions, and societal considerations, such as minimizing public opposition, simultaneously.

This results in an optimization problem with multiple conflicting targets. For example, the team of the Research Campus MODAL at ZIB has introduced a novel method for determining optimal wind farm locations where the desired solutions provide an optimal compromise between the federal targets for wind energy expansion, the availability of potential grid connection points, and the categorization for interventions in the landscape.

Another example is the optimal investment planning for the Berlin district heating network, which is considered one of the most complex in Western Europe. The objective was to consider CO_2 emissions in addition to economic costs. The

ENERGY TRANSITION



The energy mix from renewable sources includes not only electricity from solar energy and wind, for example, but also molecules such as hydrogen, which is particularly suitable for energy-dense transportation over long distances and storage.

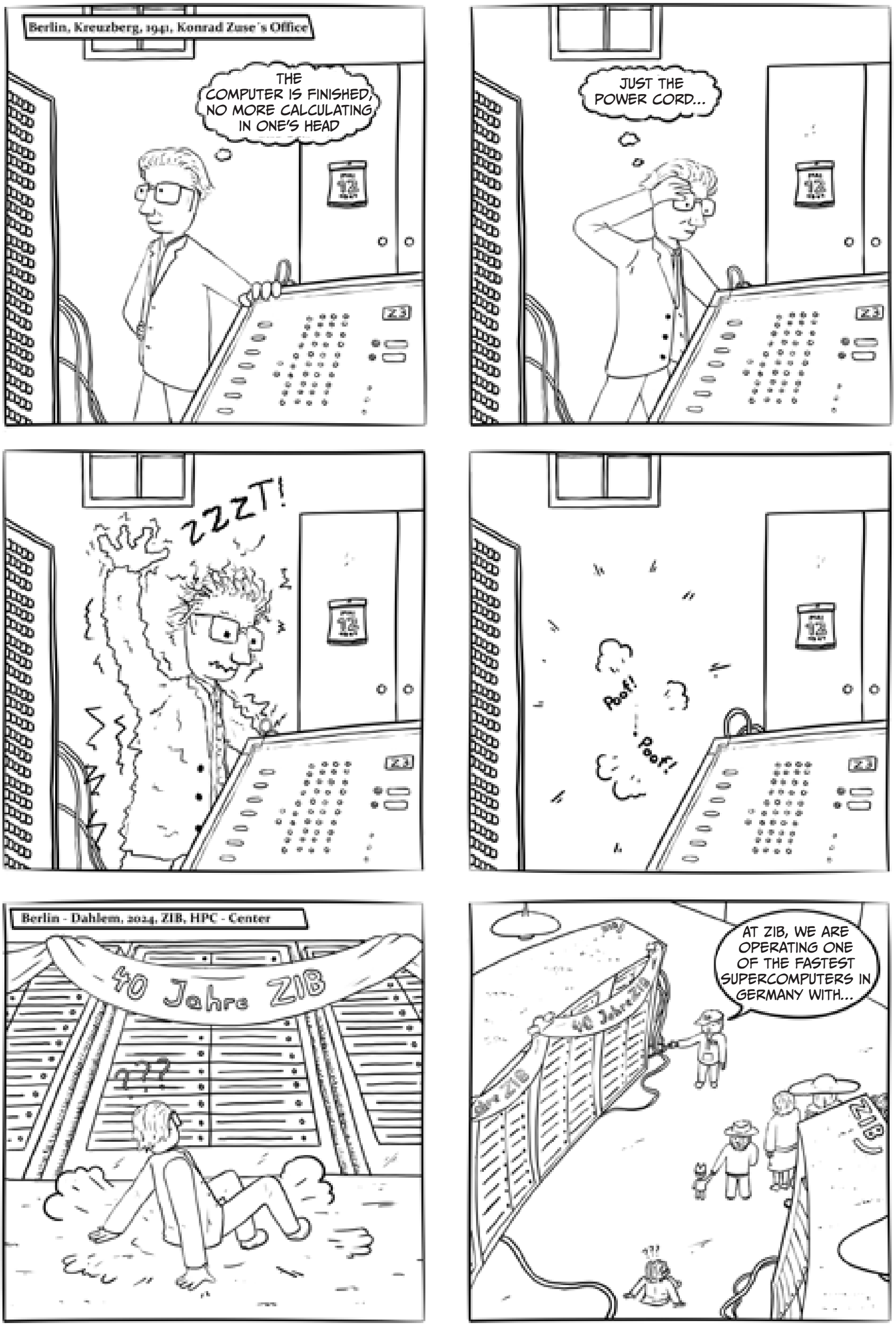
predominant challenge facing this network lies in its existing centralized structure, characterized by a limited number of large fossil-fired power plants and a scarcity of small combined heat and power plants. The transformative strategy entails a shift toward decentralization, incorporating a greater number of smaller production units. Examples include large heat pumps harnessing industrial and wastewater heat, and geothermal reservoirs. The redesigned system promises enhanced flexibility in unit use during operations. However, this requires multi-objective optimization to identify the optimal tradeoff between economic and ecological goals. We devised new methodologies to address such problems, involving millions of variables. The solutions minimize costs and CO_2 emissions while maximizing efficiency.

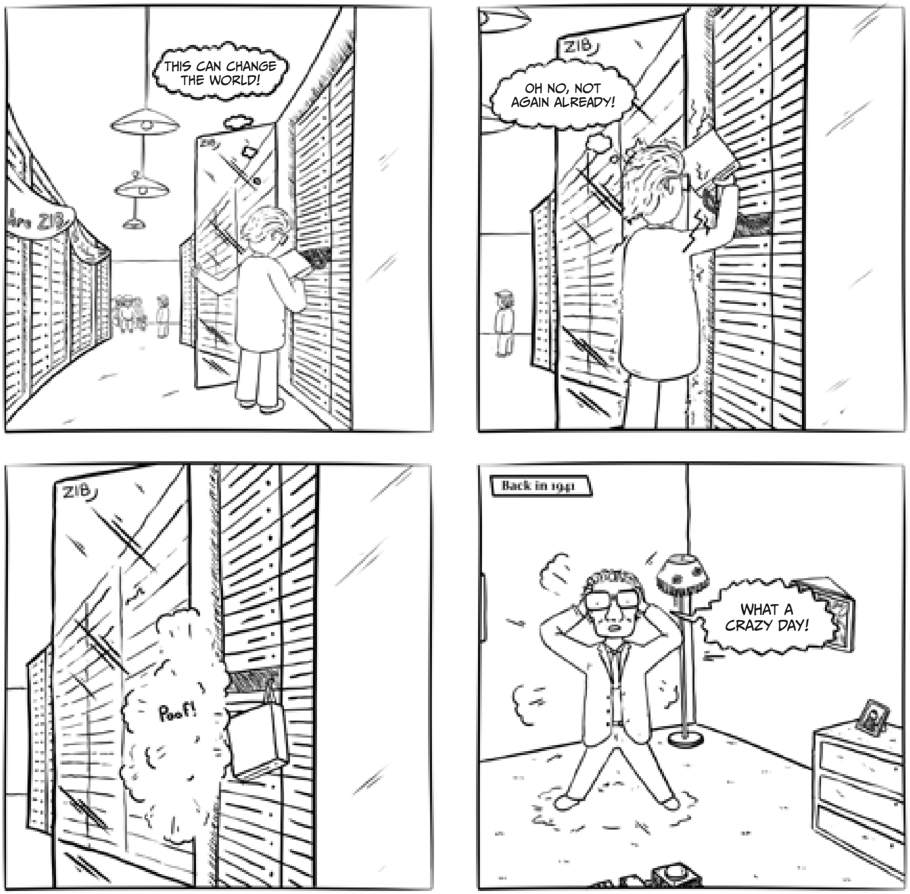
Furthermore, methods developed at ZIB, together with MODAL and the MATH+ Cluster of Excellence, allow the dynamical behavior of large energy networks to be predicted in order to steer them optimally, especially regarding the cotransport of green hydrogen. For example, one of the largest gas transmission system operators employs them to forecast the expected hourly gas flows in a large part of Germany. These methods will now be extended to the entire German natural gas market area.

In the future, we want to extend our methods to large consumers and their energy processes. This will enable us to optimize not only energy generation and its transport including large consumers. This holistic optimization allows the costs to be fairly distributed between producers and consumers, based on the advanced mathematical methods we are developing in close cooperation with industry and research partners.

Janina Zittel, and Thorsten Koch

TIME TRAVEL


Berlin, Kreuzberg, 1941, Konrad Zuse´s Office
THE COMPUTER IS FINISHED, NO MORE CALCULATING IN ONE'S HEAD
Z3
JUST THE POWER CORD...
ZZZT!
Poof!
Poof!
Berlin - Dahlem, 2024, ZIB, HPC - Center
40 Jahre ZIB
???
AT ZIB, WE ARE OPERATING ONE OF THE FASTEST SUPERCOMPUTERS IN GERMANY WITH...
ZIB


THIS CAN CHANGE THE WORLD!
OH NO, NOT AGAIN ALREADY!
ZIB
Poof!
Back in 1941
WHAT A CRAZY DAY!


THIS IS GOING TO BE BIG!!!

BETTER HEALTH CARE

At the beginning of the 21st century, a doctor's understanding of a patient's health was largely limited to the data gathered from physical exams, basic lab tests, and the patient's own recounting of symptoms. Now, two decades later, the approach to understanding patient health has undergone significant evolution. Today, it is possible to routinely gather comprehensive information about an individual's biological characteristics at the molecular level. This includes extensive genetic profiling and measuring the levels of thousands of proteins and metabolites that are critical to physiological functions. Additionally, advanced wearable devices provide continuous monitoring of vital signs and physical activity, offering real-time insights into an individual's health status.

In collaboration with our partners at Charité, we have developed innovative, data-driven technologies that allow physicians to make more informed decisions leveraging this wealth of newly accessible data. A key aspect of our efforts has been in the area of biomedical big data analysis. Through our innovative methods, even a single drop of blood becomes a treasure trove of gigabytes of information. Such data is invaluable for detecting subtle variances in protein levels that may signal the early stages of a disease, or identifying discrepancies in the microbial populations within our bodies, thus permitting the early recognition of complex health conditions. The technologies we have developed over the last years for interpreting this molecular-level data have been pivotal in identifying early markers of diseases, which can often be detected long before traditional symptoms manifest.

Leveraging our expertise in managing and interpreting large datasets, we

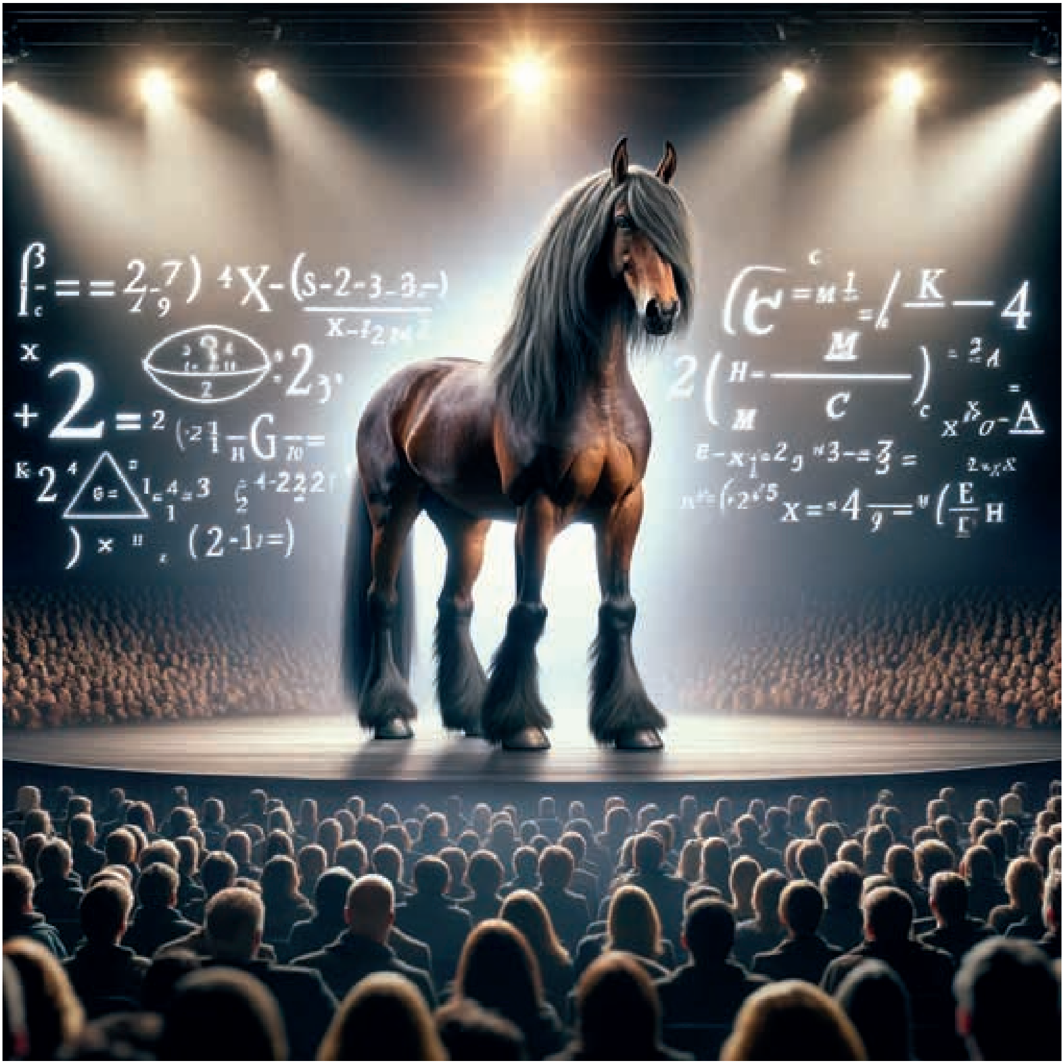
WITH BIG DATA

have expanded our focus to include the integration of data from wearable health-tracking devices, thereby significantly enhancing the scope of patient care. Together with partners from industry, we have developed new advanced methods that allow detailed analysis of large-scale ECG data coming from implanted biomonitors. These devices continuously monitor heart activity, allowing us to detect early signs of cardiovascular disease. Our new method not only exemplifies our commitment to preventive health care but also demonstrates how this technology is used to continuously monitor the health conditions of more than 100,000 patients and provide early warnings before more serious symptoms develop.

Another cornerstone of our efforts to refine diagnostic precision and treatment efficacy lies in the advanced realm of medical imaging. A key development in this area has been our work on algorithms for analyzing large medical imaging datasets that are created during routine examinations. Our new methods help improve 3D anatomy reconstruction and can aid in the diagnosis and treatment planning of conditions like osteoarthritis.

In conclusion, our recent advancements in developing innovative ways for medical data analysis are crucial steps toward personalized, predictive, and precise health care, empowered by big data. This progress illustrates a shift from merely treating diseases to predicting and preventing them, ensuring health care is customized for each individual's unique biological profile. Our commitment to utilizing big data is paving the way for a future where health care is not only reactive but proactive, significantly improving health outcomes for all.

MAKING POWERFUL AI LESS OPAQUE



AI-generated illustration of the horse Clever Hans, with math-like formulae hallucinated by AI.

Deep learning methods excel in various domains, yielding substantial economic benefits and practical implications. From powering self-driving cars and enabling protein folding solutions in drug development to driving recommendation algorithms in major social networks, these methods demonstrate remarkable versatility. Large Language Models like ChatGPT are notable examples, processing vast amounts of data with increasing efficiency. However, their widespread application brings to light a critical issue: the opaque, "black-box" nature of these models. This lack of transparency, particularly in parameter-dense and highly complex neural networks, poses significant challenges in sensitive areas such as medical diagnosis and autonomous driving, where clear and understandable reasoning is crucial for trust and reliability.

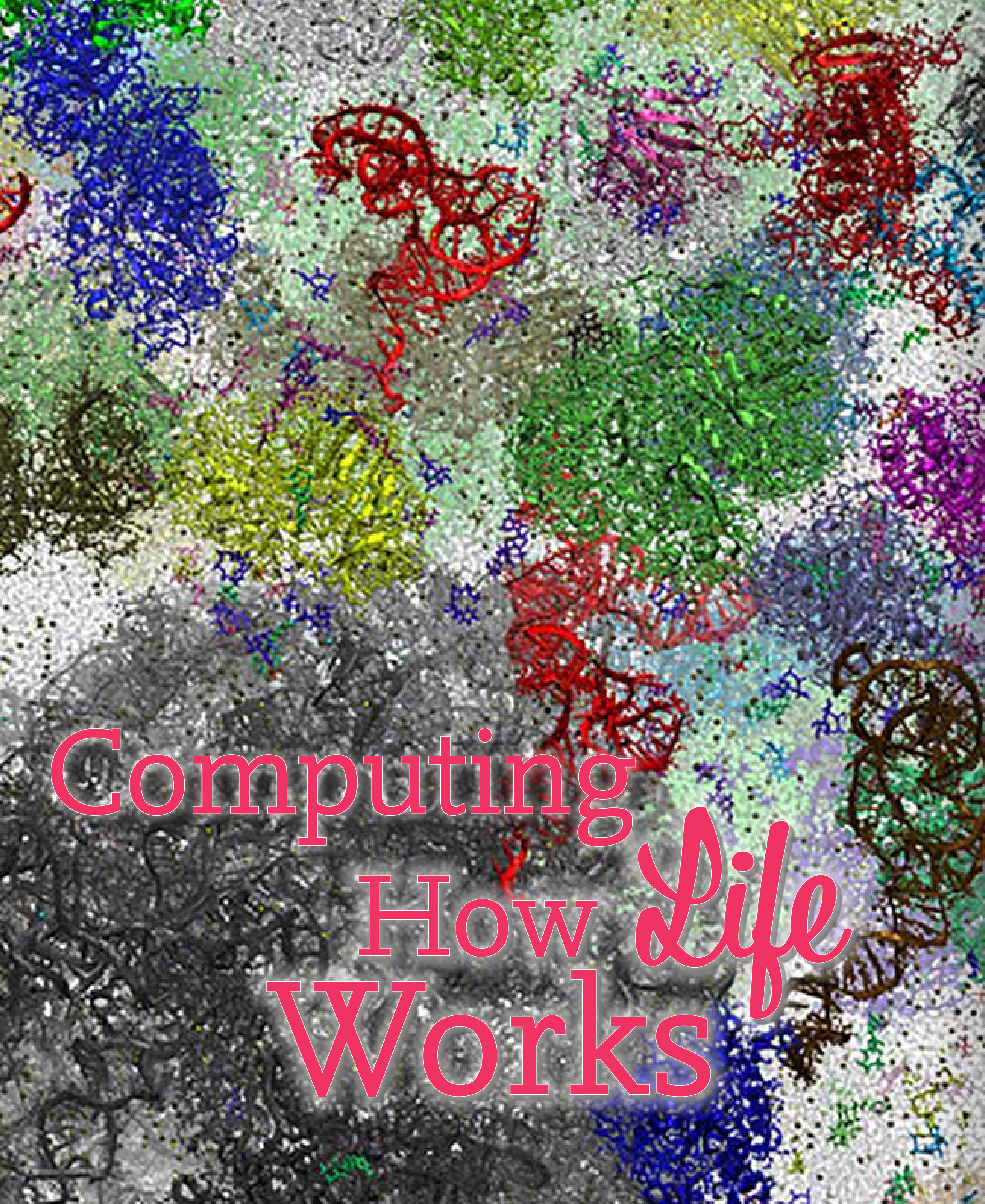
To more clearly illustrate the point let us consider the Clever Hans phenomenon, which provides a fascinating glimpse into the complexities of interpreting animal behavior and, by extension, the challenges in understanding how artificial intelligence systems make decisions. Hans was a horse that lived in Germany at the turn of the 20th century, and he became famous for his supposed ability to perform arithmetic and other intellectual tasks. His owner, Wilhelm von Osten, a phrenologist and retired math teacher from Berlin, believed Hans could understand German and respond to questions by tapping his hoof. For instance, if asked a simple math question, Hans would tap his hoof the correct number of times to indicate the answer.

It turned out that Hans was not actually performing calculations or understanding language. Instead, the horse was incredibly sensitive to subtle, involuntary cues in the body language of his trainer and the audience around him. For example, when the correct number of taps was reached, the trainer's posture and expressions would – however slightly – change, indicating to Hans that he should stop tapping.

This discovery highlighted that it was not the intellectual prowess of the horse at play but a nuanced form of communication based on visual cues that the human observers were giving off without realizing it; a side channel. In the context of AI, the Clever Hans phenomenon underscores the necessity for explainability. Just as Hans' apparent intelligence was actually a reflection of human cues, AI systems might "learn" from data in ways that reflect underlying biases or patterns invisible to their developers. Without a clear understanding of how and why AI algorithms arrive at their decisions, we risk misinterpreting their capabilities and relying on their judgments in situations where they might not be valid or fair.

At ZIB, we have been working on Explainable Artificial Intelligence (XAI) in order to make neural networks transparent and understandable, with the goal of ensuring that these AI systems are not only effective but also adhere to ethical and social standards. In the future we aim to extend our research to both text and learned feature spaces with the aim of deepening the understanding of interpretability across different modalities and data types. This is particularly important in the evolving AI regulatory landscape, such as the European Union's AI law, where interpretability of AI systems plays a crucial role.

Shpresim Sadiku, Sebastian Pokutta,
and Berkant Turan



Computing How Life Works

Most life forms, including plants, animals, and humans, are composed of cells. The cell itself is a kind of tiny factory where millions of molecules interact continuously to perform the tasks needed to keep life going.

Despite the cell's diminutive size, which is typically on the order of a hundredth of a millimeter, the molecules within it are about 1,000 times smaller. These molecules exhibit rapid, constant motion, with each one executing billions (!) of twists and turns per second. Remarkably, within this complex dance of millions of molecules, a meaningful and functional cell emerges.

Researchers worldwide are dedicated to unraveling the mystery of how cellular function arises from this seemingly chaotic whirlwind of motion. To gain insights, they employ the most powerful supercomputers for "molecular dynamics," a scientific discipline focused on simulating the movements and interactions of molecules. The underlying concept of molecular dynamics simulations is akin to creating a computational laboratory, offering a glimpse into the molecular world in motion within each living organism.

One of the main challenges in molecular dynamics is overcoming the "timescale barrier." This term stands for the fact that the important events are hidden within many insignificant details like a needle in a haystack: they are "rare," in the sense that the probability of seeing such an event even in the longest possible simulation is very low. This is true, for example, for so-called ligand–target docking processes, that is, for understanding whether and how a drug deactivates disease-related processes in the cells of a patient.

These important rare events occur on timescales that are not accessible to direct simulation, even on the largest or specifically dedicated supercomputers. They lack the speed required for the task, and unfortunately, the anticipated advancements in computing power over the next few decades will still fall short of making them sufficiently fast.

Motivated by this challenge, ZIB researchers have worked hard for many years to overcome the timescale barrier by devising innovative approaches for performing rare event simulations more efficiently. The basic idea is straightforward: glean insights from simulations to identify molecular motions of lesser importance, channeling computational efforts exclusively toward the crucial ones. Although easily articulated, this necessitated the formulation of a novel mathematical theory that enables the development of alternative methods for molecular dynamics, coupled with the training of artificial intelligence to differentiate between insignificant and significant molecular motions. Berlin's mathematical community, including ZIB's researchers, spearheaded this groundbreaking development.

In fact, we are now able to simulate important processes like ligand–target docking or protein–protein association with unprecedented accuracy and at much lower computational cost, allowing for important breakthroughs like the design of novel pain relief drugs. Such simulations now require weeks of computing time, a vast improvement compared to the potential decades (!) it would have taken using conventional approaches.

While this progress is commendable, a full in-depth understanding of the molecular world in motion within a living organism necessitates another substantial acceleration of our computational methods. The next formidable challenge is waiting!

Stefanie Winkelmann,
Marcus Weber, and Christof Schuette

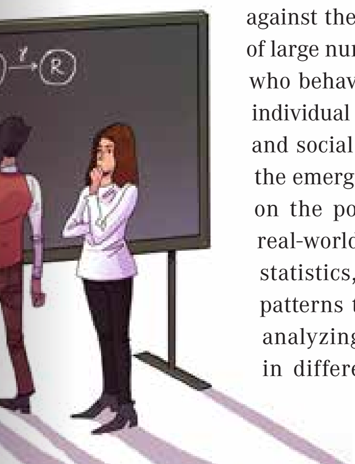
Modeling Tomorrow:

COMPUTATIONAL LENS ON SOCIAL DYNAMICS

Modern societies face numerous significant challenges, including climate change, health pandemics, forced migration, political instability, and social injustice. Understanding and addressing the underlying causes of these issues are essential steps toward fostering a more resilient and fair society.

At ZIB we actively advance this objective by developing large-scale computational models that can simulate human actions and their interactions with other people as well as with their environment. These models are simplified representations of reality that serve as valuable tools for learning about complex social dynamics, testing hypotheses, evaluating the impact of different policies, and predicting potential future scenarios. Our goal is to provide mathematical formulations that describe the underlying principles of social systems and develop methods for their thorough computational analysis, and efficient simulation and optimization to support decision-making processes in diverse societal domains.

In 2020, while facing the COVID-19 pandemic, our team collaborated with researchers from TU Berlin and the MATH+ Cluster of Excellence to develop a so-called agent-based model (ABM) for simulating the spread of infection that enabled an accurate assessment of different non-pharmaceutical measures against the virus. This ABM consists of large numbers of individual agents who behave like humans that make individual choices regarding mobility and social interactions, resulting in the emergence of collective patterns on the population scale. We used real-world mobility data, infection statistics, and realistic behavioral patterns to calibrate the model for analyzing the infection dynamics in different regions in Germany.



Within the project MODUS-COVID, we implemented this ABM on ZIB's supercomputer for millions of agents and tested different scenarios, which we published as periodic reports to the German federal government.

The abstract formulation of this model not only makes it generalizable to other forms of epidemic spreading, providing a framework that can be applied in future contexts, but also extends its application to different settings. We apply these models to study spreading processes in ancient times, offering a long-term historical perspective on the fundamental aspects of human societies. Through interdisciplinary collaborations with archaeologists, anthropologists, and geographers we formulated several mathematical models to investigate the complex relationship between human mobility and the cultural evolution of past societies. In particular, with our colleagues from the German Archaeological Institute (DAI), we studied the interplay between the process of Romanization in northern Tunisia and the temporal changes in the region's road network. Our results provide valuable insights for understanding the evolution of Roman culture, whose achievements continue to shape and inspire modern society.

Our current research is on expanding these computational approaches for diverse problems of social relevance, including the formation and evolution of opinions influenced by social media, political currents, and socioeconomic impacts. Our goal is to build models that provide underpinning on how people shape their opinions and facilitate the development of strategies to address challenges such as polarization, the creation of echo chambers, and potential manipulation by influencers or automated bots. Ultimately, we envision contributing to the establishment of a more resilient society.

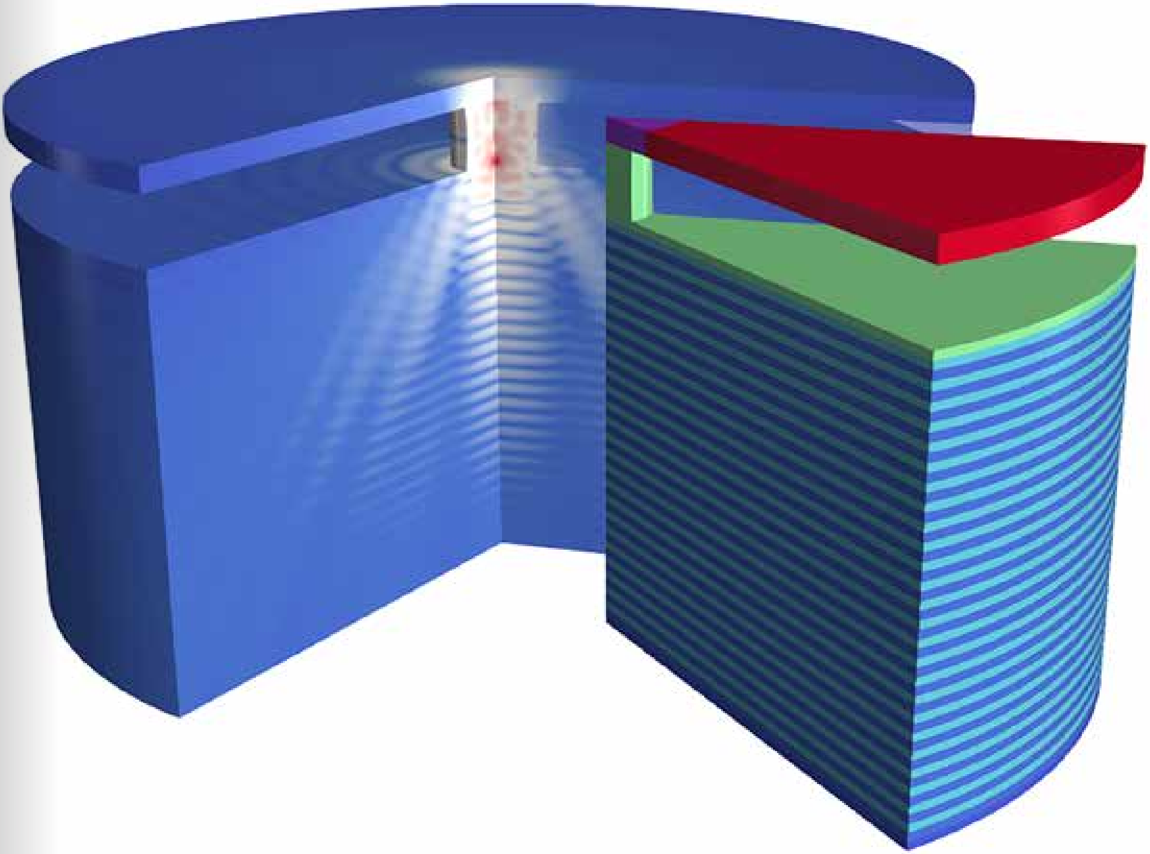
Natasa Djurdjevac Conrad

MATHEMATICS FOR QUANTUM TECHNOLOGY

For centuries, classical physics has been the foundation for our understanding of the world around us. This still is true for large-scale phenomena, including our everyday perception of the world, and most engineering problems. However, for about 100 years now there exists another theory for describing nature on the atomic and subatomic scales. This theory is called quantum mechanics and it introduces rules vastly differing from our classical intuitions. Phenomena predicted by quantum mechanics can seem paradoxical and have surprised scientists ever since. One famous example of this is entanglement: the properties of two microscopic particles cannot be described independently of each other, even when they are very far apart and cannot exchange information. The setting of this example can be paraphrased as a game in which two players are being simultaneously asked questions in separate rooms. By leveraging quantum entanglement, they can establish a link between their answers that cannot be explained by classical physics. The experimental demonstration of this groundbreaking concept, proposed by physicist John Bell in the 1960s, earned the Nobel Prize in Physics in 2022. In a recently published work, researchers at ZIB were able to provide better theoretical bounds, which characterize when this effect can occur.

Historically, quantum mechanics has been indispensable in advancing technology, facilitating the creation of groundbreaking devices like transistors, lasers, and atomic clocks. Accordingly, another area of focus is on engineering quantum sources that emit single photons, the basic units of light. These devices have potential applications in secure quantum communication, where interception is impossible. Together with external partners, researchers at ZIB were able to realize transportable quantum light sources with record-breaking photon generation rates, close to commercialization in quantum cryptography systems.

These devices can further be used as building blocks for the development of quantum computers, which are expected to be able to drastically outperform classical computers in certain computational tasks. Despite much effort, creating new quantum algorithms is still extremely challenging. At ZIB, researchers are exploring various methods to develop new quantum algorithms and to improve existing ones. One promising area of active research involves running dynamical systems on quantum computers. This is of great interest for studying various physical phenomena, such as many particle systems in different energy environments.



Schematic of a source of flying Q-bits for quantum key distribution.

Unfortunately, quantum computers are still in the developmental phase, struggling with hardware scalability limitations and other persistent obstacles. Interestingly however, classical computers can simulate quantum algorithms, offering a pathway to a deeper understanding of quantum processes. This often leads to the generation of vast amounts of data, which are too big to be processed. To tackle this challenge, researchers at ZIB are developing techniques to decompose large data structures into smaller components, helping classical computers to use their resources more efficiently for faster and improved simulations of quantum algorithms. By collaborating with international research institutes and combining expertise from diverse fields such as mathematics, computer science, and physics, we aim to push the boundaries of quantum algorithm development and pioneer revolutionary applications in computation, communication, and beyond.

Sven Burger, and Patrick Gelß

EXCELLENT SUPPORT FOR DIGITAL SCIENCE

Berlin's High-End Data and Computing Center

ZIB hosts Berlin's main data and computing center. It provides an expansive and sophisticated infrastructure to handle vast amounts of data and complex computational tasks. ZIB offers scalable and high-performance computing resources, including supercomputers, clusters, and cloud-based solutions, to support scientific research, including artificial intelligence, big data analytics, digitalization support, and more. With Berlin's largest storage capabilities in a special fireproof data facility, it can securely manage and process massive datasets, enabling researchers, businesses, and institutions to extract valuable insights and make data-driven decisions.

Additionally, ZIB provides advanced networking capabilities, ensuring seamless connectivity and collaboration. With its headquarters at ZIB, Berlin's scientific high-speed data network BRAIN is available to all scientific, cultural, and educational institutions based in Berlin. Recently, the core capacities have been significantly improved, including an extension of the superfast, high-throughput fiber-optic transmission network.

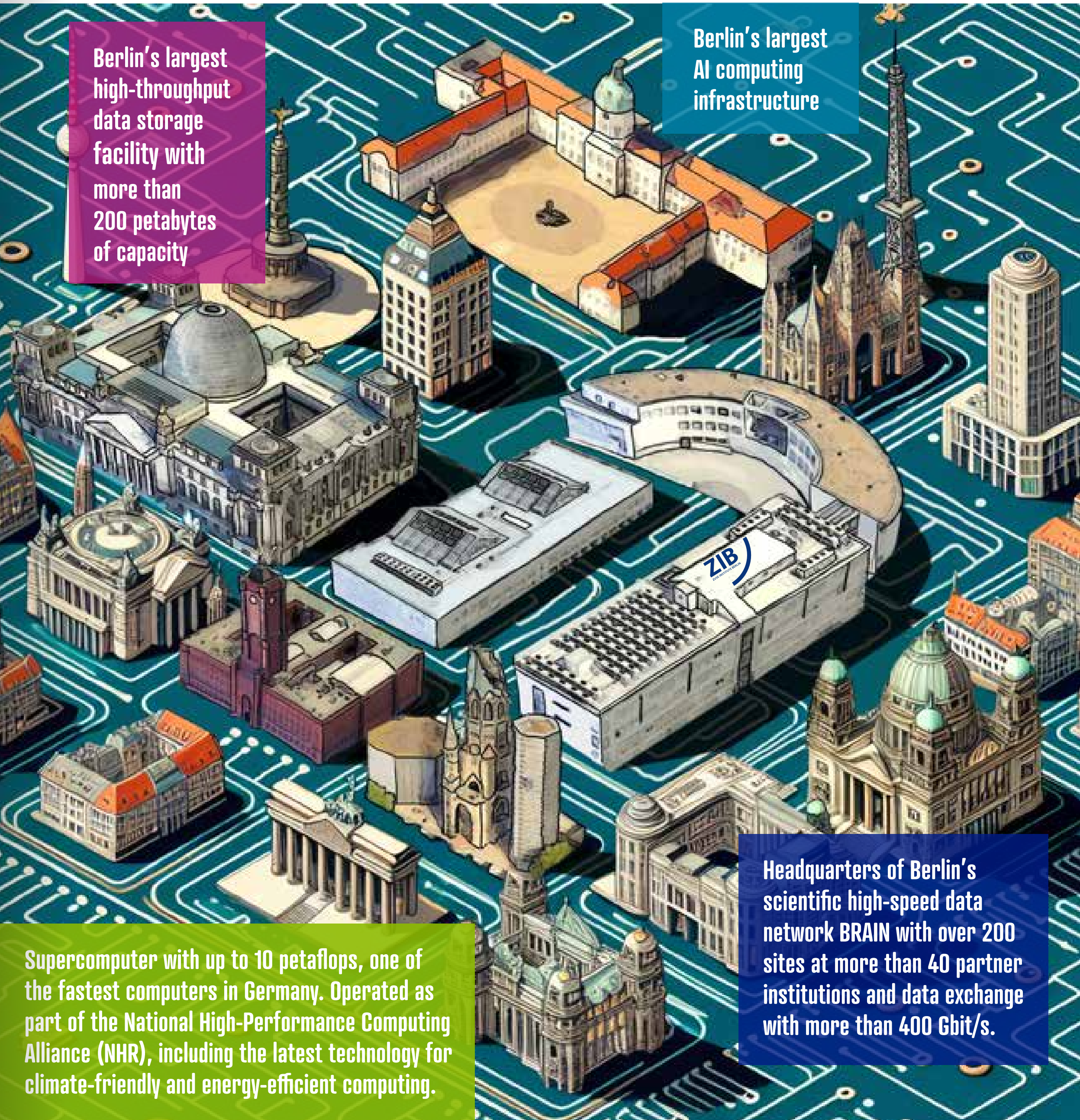
Overall, ZIB serves as a powerhouse for innovation and discovery across various fields by offering cutting-edge technologies and resources to meet the ever-growing demands of data-intensive tasks.

Digital Data and Information for Society, Science, and Culture

Universal access to knowledge has always been a dream of humankind. Today's democratic societies rightfully demand open access to data, code, methodologies, and results of scientific research. Open science is the key to transparent and trustworthy science. Our task is to support researchers in this endeavor. Together with galleries, libraries, archives, and museums, we make knowledge accessible, digitize and preserve our cultural heritage, and together with the universities, we make research data reusable.

One of the main drivers of knowledge accessibility, the Cooperative Library Network Berlin-Brandenburg (KOBV), is the association of all university and university of applied sciences libraries, all public libraries, and numerous special and public libraries in the Berlin-Brandenburg region with its headquarters at ZIB. Its aim is to improve the regional information infrastructure and to develop new services for users with a strong commitment to the open access movement and open science. The KOBV cooperates closely with the Research and Competence Center Digitalization Berlin (digiS), which is also located at ZIB.

KEY DATA ON ZIB'S DATA AND COMPUTING FACILITIES



Berlin's largest high-throughput data storage facility with more than 200 petabytes of capacity

Berlin's largest AI computing infrastructure

Headquarters of Berlin's scientific high-speed data network BRAIN with over 200 sites at more than 40 partner institutions and data exchange with more than 400 Gbit/s.

Supercomputer with up to 10 petaflops, one of the fastest computers in Germany. Operated as part of the National High-Performance Computing Alliance (NHR), including the latest technology for climate-friendly and energy-efficient computing.

"Shaping the Future in Berlin."

Prof. Dr. Christof Schütte and Prof. Dr. Sebastian Pokutta, President and Vice President of the Zuse Institute Berlin, on 40 years of research at ZIB

TO WHAT EXTENT IS THE EPONYM KONRAD ZUSE A ROLE MODEL FOR RESEARCH AT ZIB?

Prof. Schütte:

We are proud that our institute is named after the "father of computers." Konrad Zuse was an inventor in the truest sense of the word. He was even involved in the planning of ZIB in the early 1980s. Although his role during the Second World War has not yet been conclusively assessed historically, as a technological visionary Zuse is certainly a role model for ZIB.

Prof. Pokutta:

Konrad Zuse was a pioneer of our scientific field. You can draw a direct line from his calculating machines to the supercomputer that stands in our institute today. It is astonishing that even a simple computer today has millions of times the performance of the Z3, Zuse's first functional model, which he developed in Berlin in 1941, but the working principle is still the same in many respects: freely programmable, organized in binary form, and, thanks to input keyboards and the ability to read in programs, theoretically universally applicable. In this respect, we naturally see ourselves in the tradition of Zuse.

Not only did he build advanced calculating machines, but Zuse also started thinking about computational space itself. His first programming language was called "Plankalkül" – with a view to using it for planning and not only as an end in itself. This approach is also firmly anchored at ZIB. We have many projects that span the entire spectrum from mathematics to methodology and application. We are therefore happy to follow in the footsteps of this visionary thinking.

HOW WAS ZIB FOUNDED?

From the very beginning, ZIB was a place for research on and with high-performance computers. In the 1980s, it was recognized in Berlin that modern research is not possible without large-scale computers, which is how the idea for our institute was born. In 1984, it was founded precisely for this purpose – to operate Berlin's first high-performance computer. The founding president, Peter Deuflhard, was also very committed to the research component and was interested in how this powerful computer could be used particularly efficiently for science. From the very beginning, ZIB was not only a high-performance computing center, but above all a research institute for scientific computing. This approach has been imitated worldwide and has also significantly shaped the discipline "Scientific Computing."

To this day, high-performance computing and research are not taking place in parallel. Rather, the two are integrated: we do research on the computer, carry out algorithm research on the computer, conduct research with the computer in related areas such as simulation and artificial intelligence, and even use it to gain new insights into mathematics itself.

HOW DID ZIB GET ITS CURRENT LOCATION AND HIGH-PERFORMANCE COMPUTER?

Until 1996, ZIB was housed in a high-rise building in Charlottenburg. The first computer was huge by the standards of the time, but small by today's at around 3 cubic meters. The move was therefore an important step for ZIB. The current mainframe computer – we call it Lise – takes up around 500 square meters, including the network, transformers, and cooling system. The new building also made it possible to back up our enormous amounts of data. There is a special fire-protected high-security room with storage robots for this purpose.

Our building in Dahlem was literally built around the idea of a high-performance computer – first financed by the state of Berlin alone, then by the North German Supercomputing Alliance (Norddeutscher Verbund für Hoch- und Höchstleistungsrechnen). Since 2021, funding has been provided by the National High-Performance Computing Alliance (Verbund Nationales Hochleistungsrechnen). Within this framework, researchers from all German universities have access to the nine high-performance computing centers in Germany and receive technical support. The costs are shared between the federal and state governments, with 15 million euros invested in the ZIB mainframe alone every four years. This is also a computer of superlatives: it is one of the 100 fastest supercomputers in the world.

WHAT IS ZIB CURRENTLY RESEARCHING AND WHAT ROLE DOES ARTIFICIAL INTELLIGENCE PLAY?

There are currently 25 research groups in very diverse areas – from visualization and the mathematics of complex systems to optimization, high-performance computing, and big data. For example, we are driving forward drug development with machine learning and have successfully researched new pain-relieving drugs. In the context of the supercomputer, a lot of software development naturally also takes place, which we make available to science and the public.

ZIB is also very active in the fields of energy and transport. Major German mobility providers use our algorithms. Not only do they optimize their processes, but they also save a significant amount of $C0_2$. Then, of course, we are working in artificial intelligence. Possibly we will even modify the supercomputer to meet the new requirements and provide even more data capacity and AI computing power.

ZIB is primarily concerned with the noncommercial use of AI. We are interested in how artificial intelligence can be used for science. How can questions that require a high degree of creativity be answered? To give an example: how tightly can one pack spheres in high-dimensional space? If you program an AI system for this problem, you can have it constantly search for new solutions.

Large simulations – climate simulations or simulations of materials, of molecules, of processes in cells – produce so much data that humans can no longer understand and evaluate it in detail. AI can now be trained to find a structure in data. This means that we can not only run the simulations digitally, but also evaluate them digitally. This opens up completely new fields of application. One example is the optimization of Berlin's transport system. So far, we have used the high-performance computer to optimize the transport system in terms of departure times, utilization of certain routes, and so on. But there is one aspect that we have not yet been able to take into account: the people in this system with their millions of decisions. The combination of simulation and AI enables completely new possibilities for incorporating many more psychosocial aspects.

HOW DOES ZIB BRING SCIENCE TO THE PUBLIC?

Prof. Pokutta:

ZIB cooperates with around 150 partners from science and industry. We see ourselves as starting with method development, followed by application tests with supercomputing, and then developing a specific application together with our partners. The Research Campus MODAL, for example, is one of our private–public partnerships and the largest of its kind in applied mathematics in Germany. Together with Freie Universität Berlin, we are cooperating with more than 30 industrial partners, funded by the Federal Ministry of Education and Research. The aim is to bring our research to companies and society. The focus is on optimization in energy, mobility, health, and communication.

Prof. Schütte:

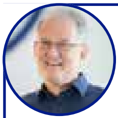
We are also heavily involved in the MATH+ Cluster of Excellence. Here, all of Berlin's mathematics institutes cooperate with major application institutions, such as Charité, the Helmholtz Institute, and the transport companies. Together with the Helmholtz Institute, for example, we are developing more efficient solar cells. This type of collaboration between research and application must be the future of supercomputing, because it offers a great deal of potential and societal impact.

WHAT DOES THE DAY-TO-DAY WORK AT ZIB LOOK LIKE?

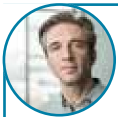
Our work here is more interdisciplinary than that of many universities. Our employees have a very diverse range of knowledge and many different application interests. So, there is a lot of discussion at ZIB and we sometimes build completely new bridges between the sciences. There are also quite a lot of us: around 300 people are currently conducting research at ZIB or carrying out research-supporting activities.

It's obvious that mathematicians and computer scientists are employed here. But physicists, chemists, physicians, biologists, psychologists, social scientists, materials scientists, and engineers also carry out research here. Our day-to-day work at the institute is characterized by synergistic cooperation. This is the only way, for instance, for mathematicians and physicians to develop new pain relievers together with the help of AI. Research into sustainable batteries or the translation of historical documents written in forgotten languages are further examples where a broad scientific spectrum and collaboration between multiple disciplines is very useful.

HOW ABOUT THE NEXT GENERATION OF SCIENTISTS?



Junior researchers are highly interested in ZIB. There are usually around 50 PhD students here whom we integrate into the research groups. Some of them are employed at our institute, but many are also part of graduate schools, and all are also enrolled at a university. However, their research mainly takes place here on-site.



There are no traditional university structures here. We give young scientists the opportunity to think outside the proverbial box right at the start of their career and thus help to develop completely new fields of work. Interdisciplinary thinking is very important to us because doctoral students will encounter it more and more in the future. We are no longer just looking for specialists with a narrow, clearly delineated area of expertise, but for people with a wide range of education and a great ability for transfer thinking.

HOW DOES ZIB INFORM THE INTERESTED PUBLIC?

We are of course happy to take part in events such as the "Lange Nacht der Wissenschaften," and the guided tours of our supercomputer are always very popular. As part of MATH+, we also give talks at the Urania, where we provide insights into our work. MATHINSIDE is a format for school classes in which we explain where mathematics can be found everywhere today. The Decision Theatre event, a collaboration between MATH+, the Global Climate Forum, and Arizona State University, is particularly interesting – also for us as scientists. The participants use simulations to examine how their ideas would affect society, with sustainable mobility being one of the topics. Who will succeed in achieving climate neutrality in Berlin by 2035 with their concepts and decisions? So far, no one really has.

Science transfer goes both ways, of course. For example, the results of Decision Theatre events can provide important hands-on value for decision-makers in the energy transition. This may then lead to exciting new research questions and collaborations.

WHAT DOES THE FUTURE OF RESEARCH AT ZIB LOOK LIKE?

Prof. Pokutta:

The mission of science is currently changing. If you look at the United States, for instance, you can see that expert commissions on urgent topics are being formed much more frequently there, which then prepare scientifically sound proposals for action. ZIB can make a major contribution, particularly in the areas of visions of the future, simulations, or multi-agent systems – because we can recreate systems in great detail and thus derive recommendations.

Prof. Schütte:

During Covid, we advised the government with a simulation model. There was a lively exchange between politics and science on how certain measures would affect the spread of the pandemic. There is a lot of potential in the dialogue between research and politics and this is one of the central tasks that now lie ahead for ZIB. We also want to further promote the participation of citizens in science. If we stay with the example of Covid: people have not always behaved rationally – and neither have politicians. This is an aspect that must be included in the models and is strengthened by public participation. In particular, we want ZIB to think even more about how we want to shape our future and how different options will affect us in the medium and long term within the framework of computational thinking. AI offers great opportunities for science here but is also precisely one of the challenges facing us as a society.

Interview by Jennifer Gaschler

Sudoku

EASY

4	7	2			8	3	9	
		8	1			2		4
6				4			8	5
2	8	7			8	3	9	
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3	5	9				8	1	2
8	2			7				6
7		5			1	9		
	1	3	5			4	7	8

DIFFICULT

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9	2			3				
					9			3
		3		5	7	8		2
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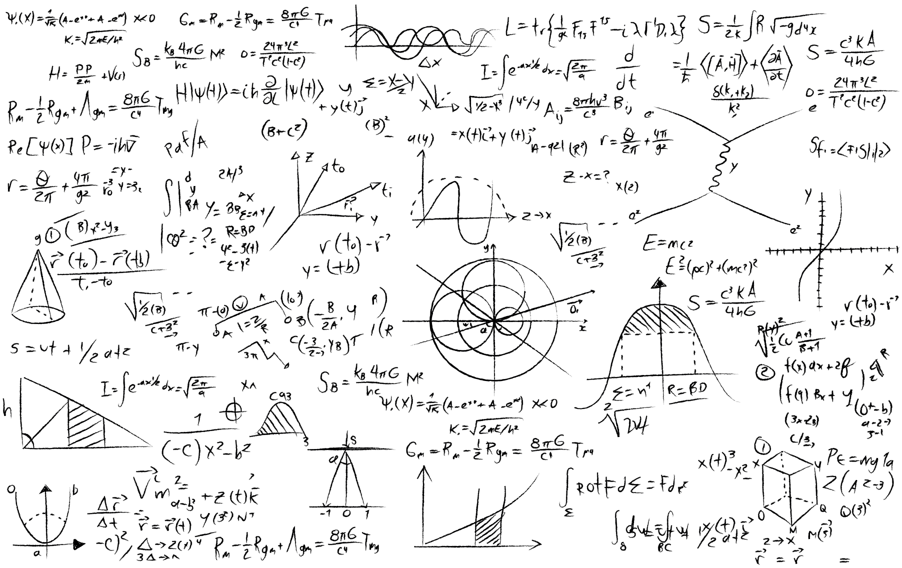
6			1					
				7			6	1
8	7			2	6	3		

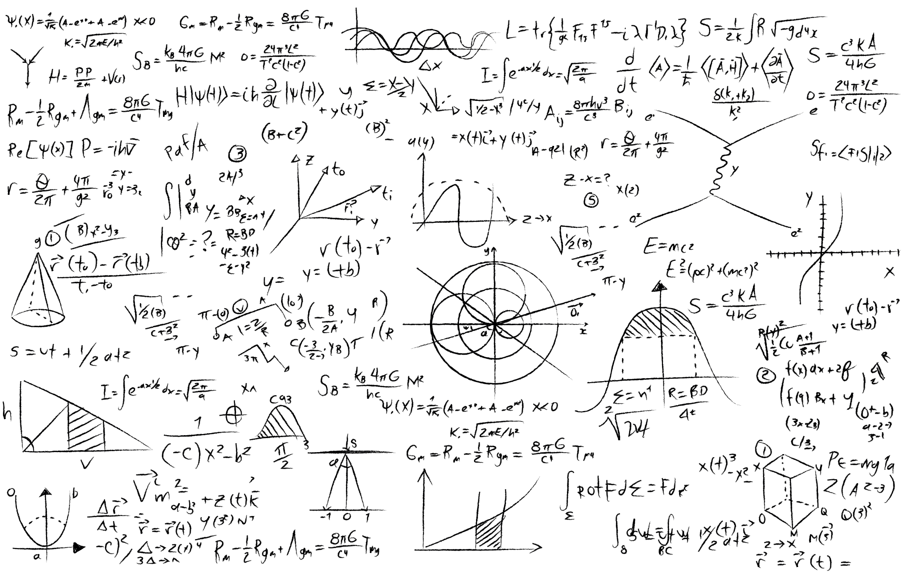
Picture Puzzle

Find 10 differences

IMITATION



ORIGINAL

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Solutions

EASY

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6	3	1	2	4	9	7	8	5
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DIFFICULT

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