





I am honored to present to you the first report of the Munich Data Science Institute (MDSI), underscoring our shared dedication to advancing the knowledge in Data Science, Machine Learning (ML), and Artificial Intelligence (AI).

In our inaugural years, we have worked towards creating an environment that fosters collaboration and knowledge exchange. The diverse programs and activities offered have created a vibrant hub for experts, bridging theoretical foundations with practical applications. As the executive director, I am proud to witness the commitment and enthusiasm of our team and all members

On behalf of the board of directors, I express my gratitude for the privilege of building this institute, made possible by the generous support of the Technical University of Munich (TUM) and the German Excellence Initiative. This report showcases our achievements and sets the stage for future endeavors. With continued support, we are confident that our institute will make lasting contributions to the field. We are grateful for the trust placed in us on this opportunity.

Prof. Stephan Günnemann Executive Director





raditional research is characterized by two components: experiment and theory. Computers and modern algorithmics have revolutionized this picture by introducing a third path to gaining insight via data. On the one hand, simulations can create data from theoretical models. On the other hand, data gathered from any kind of process can lead to hypotheses and models via computations. Both substantially help to understand, optimize, or predict reality. Although the term data science is not precisely defined, the paradigm of "from data to knowledge," the data-centered and data-driven path to insight marks the essence of data science. This is what characterizes the scope of the MDSI.

Data takes many forms, including text data, images, natural language, sensor data, measurements, or simulation data. To glean knowledge from collected data, data science relies on a technical and an analytical foundation. The former revolves around data generation, storage, compression, curation, processing, and transmission. The latter contains, among others, ML and AI techniques. All of these depend on methods and tools from mathematics and informatics. By applying these, scientists strive to automatically infer correlations or causal relations, to identify patterns, to make reliable predictions, or to optimize processes.

Data science is a core driver of future developments in many research fields, including e.g. computational sciences, digital medicine, and materials science. Furthermore, it will facilitate a significantly increased accuracy of the predictions and extrapolations that can be inferred from many kinds of data, such as in earth observation, particle physics, or social media. Additionally, data science will help tremendously to extend analyses to multiple scales, whether in time or spatially. These ground-breaking advances in data science made possible by ML and AI together with the increasing computational power already are and will continue to impact research, technology development, and our daily lives. MDSI is at the forefront of this epistemological paradigm shift where the paths of acquiring knowledge increasingly converge.

Today's data science landscape is centered around three pillars. For the first, emphasis is put on the foundations of data science, e.g. fundamental data science-specific algorithmic research in mathematics and computer science. A second component constitutes research in data-intensive domains such as natural, engineering, life, or social sciences. Thirdly, data science services and consulting can be identified, establishing an interface to various communities.





Over the last ca. 70 years, scientists have invented a variety of very successful algorithms for extracting information from data, e.g. support vector machines and kenel methods, neural networks, probabilistic graphic models, auto-encoders, or clustering techniques. Deep learning is one of the most sensational developments in this field. Despite the spectacular and broad success of deep learning and the respective deep neural networks, understanding how these networks function is still in its infancy. This black-box property entails that success cannot be guaranteed and that acceptance is still limited. Indeed, the mathematical proof of the results of AI methods must be considered at the same basic level as in general relativity or quantum mechanics for predictions in physics. Without such theoretical guarantees, purely empirical successes are challenged by the doubt about their reliability. In the context of scientific and technical applications,

Data Science Services & Consulting

With the increasing amounts and complexities of research data, scientists face tremendous challenges in exploiting it for cutting-edge research. Accessing, sharing, and fusing relevant data, selecting and using tools, and interpreting and analyzing results have never been so important. To cope with this situation, MDSI offers timely support structures and a central service hub, the recently founded TUM Research Data Hub, to bundle and link the various efforts on data-related research at

Foundations of Data Science

however, many of today's methods are limited and do not fully cover basic requirements. The reliable consideration of uncertainties in the decision-making process, learning based on complex structured data (non-Euclidean geometries, graphs), the integration of (physical) prior knowledge into the learning process, as well as the robustness, transparency, and efficiency of learning methods only represent a small part of the foundational questions in data science that still need to be answered. The MDSI considers an essential part of its agenda to foster talents that tackle the grand challenges of Al e.g. in the Konrad Zuse School of Excellence in Reliable AI (Konrad Zuse School relAI or relAI) funded by the **7** German Academic Exchange Service (DAAD) along with the development of novel, reliable, and intelligent algorithms that can bridge the gap to future applications (e.g. via MDSI's various focus topics or seed funds projects).

TUM. For MDSI, the term "service" encompasses several aspects. Amongst them are data-related services that complement hardware infrastructure and close-to-hardware services as offered, e.g. by the *¬ Leibniz Super*computing Center (LRZ), statistics services, advice on research data management, or links to and integration of data sources.

Domain-Specific Data Science

In recent years, modern data analytics and AI have been increasingly shaping essentially all areas of research in the natural and engineering sciences, humanities and social sciences, business management, as well as in medicine and the life sciences. Although often only in their initial stages, ML and related approaches are already among the most potent innovation drivers. This innovative power goes far beyond the domainspecific research outcome of merely applying the existing methodology. Instead, it extends equally to a co-design of applications and algorithms, to algorithmic tailoring or advancement, to its combination with first principle-based field-specific simulation models, to an efficient presentation and visualization of widely varying data, or the development of data ontologies specific to different application areas and research communities. Therefore, the few links between early adopters driving such pioneering research in their domain and foundational Al experts driving general algorithmic work must be extended, and today's separation of the respective scientific communities with topically quite disparate conferences and journals being the rule rather than the exception must be overcome. MDSI focuses on tailored, domain-specific AI research to address our society's fundamental challenges. Examples of such initiatives bundled under the MDSI are the Center for Digital Medicine and Health (ZDMG), the Georg Nemetschek Institute of AI for the Built World (GNI), or the International AI Future Lab: Artificial Intelligence for Earth Observation (AI4EO).



In a changing society dominated by digital transformation with the immense potential offered by vast amounts of data and intelligent machines, MDSI tries to establish a **central interface and innovation hub** for all stakeholders in academia, the industry, and the public.





Structure and Strategy





In formulating its mission, MDSI has set ambitious goals. It bridges the gap between scientific disciplines, particularly between their foundations and their application areas. Thus, scientists will experience the ideal environment for cutting-edge research. Beyond the interdisciplinary collaboration among scientists, MDSI promotes innovation and transfer from the academic to the industrial world. Moreover, MDSI has taken a great leap forward by creating a novel platform to train future scientists and professionals.

MDSI offers easy access to data-related services and consulting, and it engages in discourse between scientists, industry, and society on various data-related topics.







Welcome

neural network-related topics in particular, and in domain-specific data science and ML across TUM's portfolio of disciplines, covering **applications** such as material, catalysis, quantum, astrophysics and climate research, as well as research on the dynamics of social, political, and economic systems.

Consequently, MDSI promotes inter- and transdisciplinarity, aligning many of its actions to meet this mission. In particular, MDSI fosters joint research activities with many of them specifically designed to incentivize collaboration across the various research fields at TUM, such as the MDSI Seed Funds, the MDSI Focus Topics, and the MDSI Workshops & Retreats program. Several programs have also been established to implement interdisciplinarity early in academic careers, such as the MDSI Doctoral Training Program and the Konrad Zuse School relAI.

Furthermore, MDSI is continually expanding its internal research network while seeking collaboration with various partners at the university and beyond. In the same way, the networks and contacts with partners at the local (Munich eco-system), national (NFDI), and international levels (7 European Laboratory for Learning and Intelligent Systems, ELLIS; **7** University of Oxford; **7** Massachusetts Institute of Technology, MIT; 7 Institut Mines Télécom, IMT) are constantly growing via MDSI Core Members as well.

MDSI is dedicated to connecting expertise and providing an inspiring environment for cutting-edge research. It brings data science applications and foundational research into diverse domains.







MDSI creates a sustainable platform to train future scientists and educate professionals.

s the importance of data analytics and machine learning continuously increases across fields and disciplines, many researchers today need to be adequately prepared. To support future generations of scientists and help today's professionals in their careers, one of MDSI's mandates includes offering specialized training and education specific to data science, machine learning, and artificial intelligence.

A vital aspect of the educational formats at MDSI is enabling the transfer of knowledge across scientific boundaries and helping establish interdisciplinary connections. Additionally, these activities are tailored to



audiences ranging from students and doctoral researchers to professionals outside academia. MDSI's educational platform enables long-term collaboration and lays the foundation for future exchange.

MDSI fulfills its educational mandate in many ways. Via the *Linde/MDSI Programs*, MDSI offers scholarships and fellowships for students and doctoral researchers, supporting in particular the programs "Data Engineering and Analytics" and "Mathematics in Data Science."

MDSI also hosts the Konrad Zuse School *relAI*, one of three schools funded nationwide via the \neg Zuse Schools program.

he digital revolution is transforming societies, economies, and even science and its paths to knowledge. The MDSI is anticipating, accompanying, and shaping this change. Specifically, innovation in data science requires a deep understanding of state-of-the-art methods, techniques, and the vision to generate the necessary synergies, motivation, and strong networks for researchers, industry experts, and students to expand the frontier of knowledge in data science techniques.

With the appointment of the MDSI Advisory *Board*, consisting of renowned researchers and industry experts in data science from ↗ Alibaba, ↗ BMW, ↗ Google, ↗ Helmholtz

Munich, *A Leibniz Supercomputing Centre* (LRZ), the **7** University of Oxford, TUM, and many more, an important foundation for this mission has been set. Drawing on this expertise, MDSI actively establishes new collaborations and extends existing relationships with industry partners. Formats like the renowned TUM-DI-LAB further expand the successful cooperation and innovation between industry partners, researchers, and master's students. Moreover, with the new format "Research with Industry Groups" (RIG), MDSI plans to establish a setting to transfer cutting-edge applied research innovations to industry.



Additionally, the *TUM-DI-LAB* at MDSI coordinates industry projects for groups of master's students, and MDSI furthermore developed a training program for data scientists that offers tailored workshops and focuses on interdisciplinary exchange.

Aiming at professional education, MDSI has partnered with the **7** TUM Institute for LifeLong Learning (TUM IL³) to design and subsequently provide learning opportunities on data-related topics in continuing education. Finally, it is developing training programs based on the expertise of its core members, thus complementing their mutual expertise.



Service

he increasingly extensive data expertise necessary to perform cutting-edge research in data science underscores, together with data literacy, the need for dedicated training of researchers on the one hand and professionalized data services to alleviate the challenge for researchers of extracting knowledge from data on the other. MDSI provides both, specialized educational formats and complementary data-related services for TUM researchers. This requires identifying and continuously monitoring scientists' needs as well as providing datarelated services that complement existing offers, e.g. by the **7** TUM University Library or the **7** Leibniz Supercomputing Centre (LRZ).

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MDSI offers easy access to resources, services, and knowledge to enable top-notch research.

As part of a concrete measure to fulfil this mission, MDSI has partnered with the TUM University Library to establish the TUM Research Data Hub (RDH) to bundle all research data-related services at TUM and set up a single contact point for each stakeholder group at the university. In this context, MDSI's offer encompasses consulting, networking, and training formats as well as infrastructure support, and assistance from data stewards.

To facilitate all data-related tasks in health research and tackling major challenges related to security and privacy of health data, MDSI is also contributing to the concept and planning of the Bavarian Cloud for Health Research (BCHR).

Moreover, MDSI is supporting its core members by offering facilities such as office space and rooms for research and workshops. It also currently prepares GPU compute resources as an offer to its members.

MDSI drives the interaction and discussion between the scientific community, industry, public administration, and society on data-related topics.



ata science, machine learning (ML), and artificial intelligence (AI) are vital aspects of current developments – in science, industry, and society. Accordingly, the topics generate much interest and discussion, and MDSI acts as a driver of and platform for discussions centered on these topics. At MDSI, the ongoing discourse may be broadly mapped into "scientific exchange" and "public debate." The former looks to engage and connect scientists at TUM and beyond, while the latter invites the general public to learn about and engage with the latest developments in data science, ML, and AI.

Several MDSI programs and activities engage with the public and society in various ways. Aside from communicating research findings and events on MDSI's website and social media, the *Munich AI Lectures* offer an opportunity to listen to and engage with top

Networks

international researchers. In June 2023, MDSI co-organized the *Women in Data Science* (WiDS) conference in Munich and brought together participants from academia and industry. MDSI also co-organizes Hackathons as well as *data competitions* such as the IceCube Kaggle Challenge, and it channels the expertise of its core members to consult on policy questions and support public endeavors such as \nearrow "Jugend forscht".

Furthermore, the *TUM-DI-LAB* projects regularly bring together students with experts from industry and research, the Linde/MDSI *Programs* aims to support talented young female researchers, and *relAI* seeks to promote diversity and internationality. Training on how to reach out to society and the practical application of this training content is implemented in the MDSI Doctoral Training Program.

Munich Data Science Institute Technical University of Munich

2021-2023



Structure and Strategy

The > TUM Agenda 2030 future concept has for the 2nd time ensured the university's status as a University of Excellence. At its core are the new TUM Schools and 7 TUM's Integrative Research Institutes (IRIs) like MDSI.

A central feature of the TUM Agenda 2030 is expanding the technically-oriented humanities and social sciences and reorganizing the discipline-based internal structure to become even more innovation-focused. It envisions a matrix layout consisting of seven schools linked by IRIs.

These IRIs form an interdisciplinary basis on specific research focus areas with pronounced future potential. They consolidate intellectual and financial resources to fulfill their mission. The MDSI is an IRI within the broad scope of data science. This is reflected in its structural organization and offers very specific opportunities and challenges.







Organization As a 7 TUM Integrative Research Institute, MDSI directly reports to the TUM Board of Management. MDSI consists of and lives through its **members.** This is manifested in the MDSI statute by defining the following bodies: the MDSI Board of Directors headed by the MDSI Executive Director, the MDSI General Assembly, and the MDSI Advisory Board.

POSITIONING WITHIN TUM

Acting as an umbrella organization for different projects, initiatives, centers, and institutes, it has been pivotal in pooling TUM's activities in these critical research areas. Multiple stakeholders now proactively approach MDSI to dock future initiatives and programs to MDSI (e.g., endeavors in AI in finance or material science), clearly showcasing the mutual benefit and synergies such a collaboration brings.

ORGANIZATIONAL MILESTONES

Filling of core MDSI Management

- Office positions (Managing Director, Scientific Assistant, Science Manager, Project Manager, Program Manager, and Research Assistant) Integration of the *TUM-DI-LAB* into MDSI Implementation of *formats and activities* in line with the MDSI mandates • 1st MDSI General Assembly
- (11 November 2021)



MDSI is also actively integrated into strategically important university-wide initiatives such as *¬* DFG Clusters of Excellence and *¬* DFG Collaborative Research Centers, streamlining the activities in data science. Typically, these initiatives are supported by data stewards, which MDSI co-hosts and trains. This support of data stewards has also become a central element of the TUM Research Data Hub's (RDH) services, established by MDSI and the ■ TUM University Library.

MDSI is an active and vibrant entity that proactively takes initiative to promote exchange and engagement. It thrives on collaboration across units and institutes, operates beyond structural boundaries, and has established a broad research network. Joint initiatives and programs with the TUM University Library (the above mentioned RDH), the **7** TUM Institute for LifeLong Learning (TUM IL³) (professional education program), and the **7** TUM Global & Alumni Office (Visiting Researchers Program) highlight this engagement. MDSI has also initiated national and Bavarian activities with high visibility and significance, such as the Konrad Zuse School relAI. Furthermore, MDSI's members are fundamental to various activities, including **7** TUM Innovation Networks and DFG Clusters of Excellence.

- Expanding the portfolio of formats and activities along the mandates of the MDSI
- Appointment of the MDSI Advisory Board
- Successful start of the Konrad Zuse School relAl
- 2nd General Assembly (4 and 5 October 2022)

MDSI is located in the Galileo Building on TUM Campus Garching



The interest from multiple academic partners, nationally and internationally, who have requested best-practice models to set up similar structures, initiate and handle cross-department activities, underlines the positive outside perception of the MDSI. Likewise, MDSI has established itself as a contact point for the broader public, e.g. by supporting **7** "Jugend" forscht" and public media.



FUNDING

The **↗** *"Excellence Strategy"* of the German federal and state governments provides strategic financial support for German cutting-edge research. Via this initiative, TUM has received the "University of Excellence" distinction and is the only technical university to have continuously retained this status since 2006. As part of the future concept *TUM Agenda 2030* this support provides
 [→]
 MDSI's basic funding. Further funding comes from successfully acquired third-party funds such as the Konrad Zuse School relAI, the TUM-DI-LAB, and Linde as a Doctoral Fellowship and Master's Scholarship Programs sponsor. Moreover, MDSI will receive further funding for setting up additional research projects and long-term support within the scope of the **7** TUM Campus Heilbronn initiative.



MDSI BOARD OF DIREC-TORS AND EXECUTIVE DIRECTOR

Five directors oversee the institute. These professors are elected from the *MDSI Core Members* such that their professional background covers MDSI's main pillars: "Foundations of Data Analytics," "Domain-specific Data Analytics," and "Data Science Services & Consulting."

The tasks of the MDSI Board of Directors range from defining the research and innovation strategy to deciding on specific funding measures. The Board is headed by the MDSI Executive Director, who is responsible for convening and chairing board and general assembly meetings, representing MDSI within and outside TUM, communicating MDSI's activities, and executing <u>MDSI programs</u> with the help of the MDSI Management Office.

MDSI ADVISORY BOARD

The MDSI Advisory Board consists of representatives of TUM and TUM's institutional cooperation partners as well as external experts from science and industry. They discuss the direction of future research and innovation activities at MDSI, develop strategic and organizational development recommendations, and define measures for an internationally successful innovation and technology transfer strategy for MDSI. In addition, the MDSI Advisory Board contributes recommendations on quality assurance in research, e.g. by participating in institutional evaluations. Since its establishment in 2022, the MDSI Advisory Board has met annually at the general assembly.

MDSI MEMBERS

At the heart of MDSI are its core members and project members. *MDSI Core Members* are TUM professors, TUM Junior Fellows, or similar senior researchers. The President of TUM appoints the core members for a sixyear term. Through them, junior researchers working on relevant topics are affiliated. MDSI Project Members actively participate in MDSI individual projects and programs, or conduct an MDSI-relevant individual or collaborative research project e.g. *> DFG Collaborative Research Centers*, *> DFG Research Training Groups*.

Currently, MDSI has 70 core members originating from all seven TUM Schools, and the number is continuously growing. All members contribute to the development of MDSI and are highly encouraged to actively set up interdisciplinary MDSI Focus Topics. MDSI has established numerous formats to facilitate and foster exchange among its members. The most important platform for exchange is the annual MDSI General Assembly. It serves not only for networking, but also for discussion and further development of the MDSI Program and Activities, above all, represents an important quality assurance instrument for MDSI. Involving all members, the MDSI General Assembly evaluates the MDSI Program. The resulting discussions are instrumental in improving the upcoming year's program or developing new formats.



Anna Brückner Team Assistant

MDSI MANAGEMENT OFFICE

The MDSI Management Office, headed by the MDSI Managing Director, is responsible for designing and implementing the <u>MDSI</u> <u>Program and Activities</u> and providing organizational support at the institute. It also acts as a communication channel between MDSI's members, transmitting information from and to the target groups of the <u>MDSI Program</u> <u>and Activities</u>. Furthermore, it is a source of ideas for the MDSI Executive Director.



Dr. Ricardo Acevedo Cabra Project Manager



Dr. Mónica Campillos González Science Manager (relAl and MDSI)



Dr. Marco Barden Science Manager



Dr. Jody-Ann Jones *Coordinator Research Data Management*



Anna Mayevska Scientific Assistant

> Dr. Leo Schwinn Science Manager Machine Learning



Dr. Emmelie Korell

Program Manager



Dr. Drew Behrens Project Manager



Dr. Arielle Helmick *TUM General Manager of Munich Center for Machine Learning (MCML)*





Sylvia Kortüm Managing Director

Dr. Andrea Schafferhans *Coordinator of Konrad Zuse School of Excellence in Reliable Artificial Intelligence (relAl)*

Vasiliki Sdralia Project Manager







Carefully tailored to different target groups and stakeholders, MDSI Program and Activities are continuously developed and adjusted to promote interdisciplinarity in machine learning (ML) and artificial intelligence (Al) along its *mandates* of research, innovation, education, service, and outreach.





management services are examples of the current MDSI repertoire. In consultation with its members, MDSI regularly adapts its program and activities to the needs of different target groups and stakeholders, as well as to new challenges in the data science field. Following its <u>mandates</u>, the varied program and activities cover research, innovation, education, service, and outreach aspects.



Program and Activities

Overview of MDSI Program and Activities, their target groups, stakeholders and relation to MDSI Mandates:

ddressed or involved groups are depicted on the right and denote either the collective the program is designed for (target groups) or a participating group (stakeholders).

The mandates related to the program and activity are represented on the left.



Mandates

Mandate O Partially addressed Mandate



		Junior	Resea
MDSI Doctoral Training Program			
Doctoral Seminar & Workshop	•		
Linde/MDSI Programs			
Industry Engagement	•	•	
TUM-DI-LAB			
Konrad Zuse School relAl			
Hackathons			
Data Competition		\blacklozenge	
MDSI Best Paper of the Year Award			•
MDSI Visiting Researchers Program	•		•
MDSI Workshops & Retreats		\blacklozenge	•
Munich AI Lectures			
Focus Topics		\blacklozenge	
Seed Funds		\blacklozenge	
MDSI Interdisciplinary Exchange			
TUM RDH	•		•
Consultancy & Services for NFDI			•
Professional Education		•	•
Events			•

Program & Activities





Partially involved Stakeholders





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The MDSI Doctoral Training Program endows participants with subject-related and interdisciplinary skills and exhibits a central focus on networking and fostering interdisciplinary connections.

Events

MDSI Doctoral Seminar & Workshop, MDSI Module

Entrepreneurial Mindset for Data Scientists, Module Entrepreneurship

Public Science Communication for Data Scientists, Module Outreach

Scientific Writing in the Era of AI (for Data Scientists), Module Research

GreenHack IT Hackathon: a great first edition of TUM, IMT, and ArianeGroup, Module Research

Machine Learning approaches in Lattice QCD – An Interdisciplinary Exchange, Module Research

Multidisciplinary Workshop on **Stochastic Modelling and Monte** Carlo Tree Search, Module Research

TUM Distinguished Lecture Series on AI & Healthcare, Module Research

MDSI Workshop Computational Material Design powered by Machine Learning (CMD-ML), Module Research

French-German Machine Learning Symposium, Module Research

esearchers need expertise and a toolkit of subject-related and interdisciplinary skills for success. Often, research questions cross disciplinary boundaries, audience-oriented communication decides the success or failure of a proposal, and entrepreneurial thinking is required to tackle common obstacles. The MDSI Doctoral Training Program gives its participants the skills to meet these challenges successfully and prepares them for their next career stage in academia or the industry.

The MDSI Research Seminar & Workshop on Data Science, machine learning, and artifi*cial intelligence* is at the heart of the program. While the one-day workshop provides attendees with in-depth know-how on interdisciplinary communication in these fields, the subsequent seminar sessions allow young researchers to meet, share ideas, and collaborate to overcome common problems. In addition to teaching the necessary skills, the MDSI Doctoral Seminar & Workshop enables young researchers to form interdisciplinary networks.

MANDATES: RESEARCH, EDUCATION Training Program

Additional mandatory training program elements include attending the MDSI General Assembly, participating in an MDSI Science Blog Series, and a workshop on responsible research. The MDSI General Assembly offers an opportunity to forge interdisciplinary connections with and present research to senior researchers at TUM and beyond. Additionally, the MDSI Science Blog Series addresses an even wider audience. Short, informative blog articles published online introduce the doctoral researchers' thesis work not just to scientists but to interested audiences across the globe. Responsible research and research ethics are intrinsic to data science, ML, and AI. Recognizing their importance, MDSI is currently planning to offer tailored courses on this subject geared explicitly toward data scientists soon. Meanwhile, courses offered by other institutions, e.g. **7** TUM Graduate School (TUM-GS) are recognized in the program.

Apart from the "MDSI Module" comprising the elements above, the program's participants complete two additional focus modules. They can choose from research, entrepreneurship, or outreach. In 2023, MDSI already hosted the mandatory workshops for two focus modules: science communication



and entrepreneurship for data scientists. The latter was so successful that a repeat was scheduled for the same year. Regarding the research module, MDSI and the **7** TUM University Library joined forces to form the TUM Research Data Hub (RDH), which centralizes educational offers on research data management. Through this module, workshops and long-term certificate programs in research data management will be conducted and acknowledged as part of the MDSI Doctoral Training Program.

Complementing the mandatory elements of the training program are several optional offers and opportunities. Participation in the Munich AI Lectures constitutes a voluntary element along with research stays, internships, and outreach projects. An extraordinary opportunity comes with workshop organization since MDSI, through its Workshops & Retreats program, also offers funding for doctoral researchers to organize their workshops. As an example, one interdisciplinary workshop was successfully held in the fall of 2022. All doctoral researchers completing the four mandatory activities from the MDSI Module plus at least two mandatory activities from the focus modules receive the MDSI Doctoral Training Program Completion Certificate.

TRAINING PROGRAM STRUCTURE

mandatory

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MDSI Doctoral Seminar & Workshop Munich Al Lectures MDSI General Assembly **MDSI Science Blog Series Responsible Research**

RESEARCH

Research Data Management

ENTREPRENEURSHIP

Entrepreneurship Training

OUTREACH

Science Communication

optional

Research Stay Workshop Organization

Industry Internship Industry/Entrepreneurship Project

Outreach Project



Doctoral Seminar & Vorkshop

As a result of a high degree of specialization, communication across disciplines can be challenging. The "Research Seminar & Workshop on Data Science, machine learning (ML), and artificial intelligence (AI) topics Topics" aims to **connect young researchers,** facilitate interdisciplinary communication, and enable new collaboration.

> A s the primary element in bringing together the doctoral researchers in data science at TUM, the MDSI Doctoral Seminar & Workshop provides a forum for young researchers to establish connections to peers in other fields and find help for challenging aspects of their thesis. The seminar sessions are held in MDSI's comfortable lounge area. The informal atmosphere helps stimulate an open discussion, and often groups of participants stay longer to continue collaborating. Every semester, the seminar is preceded by a workshop preparing the participants for their presentations.

> From its launch until today, the workshop & seminar series has been a great success. On average, 30 doctoral researchers and a small fraction of master's students participated in the event in the three semesters from summer 2022 to summer 2023. The format continued in the winter semester of 2023/2024. All early career researchers (including advanced master's students) are invited to come and stay – for future sessions or to use MDSI's facilities and collaborate.

WORKSHOP

The workshop presents a means to introduce the participants to each other and provides suitable preparation for the subsequent seminar sessions. The primary goal is to inform the participants that presenting their research to listeners from other fields requires a significantly different approach than talks within their community. Traditionally, scientists from foundation and application fields face the biggest challenge when talking to the other group. In this, the workshop has fully achieved its goal as participants observed a distinct difference in the seminar presentations of those who participated in the workshop and those who did not. This distinction stresses the importance of regularly offering formats to train interdisciplinary communication and related themes like science communication. The workshop is a full-day event that precedes the first presentation of the seminar series.

SEMINAR

The seminar sessions take place regularly during lecture times. Usually, two doctoral researchers present their research to an interdisciplinary audience, and popular topics, methods, and challenges allow everyone to join the discussion. A vital element of the presentations is the integration of connecting points with other participants. On the one hand, the presenters are asked to portray the expertise that they would be willing to offer their peers. On the other hand, they introduce issues where they seek input and help from others. This tremendously serves to stimulate intense exchange that is occasion-





ally carried on until after the session and into a joint lunch. The approach aims to connect researchers from application and foundation areas. Ideally, the application researchers receive help from the foundation scientists when they are presented with problems that challenge them to design new codes.

On two outstanding occasions, the seminar featured special guest appearances by representatives from *¬ Intel* and *¬ Amazon,* who offered insights on research at their respective companies. Moreover, they provided a glimpse into what it is like to work there, and they introduced different career path options for scientists.

JOURNAL CLUB

During the term break in spring 2023, a group of doctoral researchers met at the regular seminar time slot to continue collaborating in a self-organized journal club mode. They took turns and presented hot topics from the ML community (e.g. diffusion models or transformer models) and other exciting content (e.g. structuring papers). Interdisciplinary communication – workshop held in spring 2022

Journal Club

Sparsity in Deep Learning: Increasing Expressiveness, Decreasing Costs

Denoising Diffusion Probabilistic Models

Towards ChatGPT – the Development of Transformer Models

Neural Search and Information Retrieval: More Knowledge without More Parameters

Ten Simple Rules for Structuring Papers

Neural Radiance Fields (NeRFs)

Data-Centric AI: How to Make AI Perform Well in Real-World Scenarios

How I Almost Failed to Search a 37 GB Text File in Under 1 Millisecond (in Python): Efficient Data Handling for Big Files

Seminar Talks

Non-Invasive Transcriptomics by Vesicular Export

Modeling of Time-Resolved Calcium Imaging Data of Mouse Brains

Deep Learning for Cold Regions

Geometric Deep Learning

Neural Networks from the Perspective of Multiscale Dynamical Systems

Natural Language Processing

Incentivizing Truthfulness in Production Capacity Exchanges with Budget Constraints

Thermal 3D Mapping and CNN Analysis for Enrichment of Building Models

Vision for Autonomy

Applications of Data Science in the Logistics Domain

Lattice QCD Correlators in Effective Field Theories

Visual Understanding of 3D Urban Street Environment Using MLS Point Clouds

Optical Coherence Tomography – OCT

Neural Networks as Dynamical Systems

Short-Term Solar Forecasts/ Segmenting Solar Panels/Data Engineering (fortiss)

Causality and Graphical Models

Network Adaptation in Si Electrodissolution

AI for design?



Linde/MDSI Programs for Doctoral Researchers

To battle the lack of specialists in data science, ➤ Linde and MDSI are partnering to sponsor future generations of researchers, paying special attention to female scientists.

n late 2020, Linde and TUM intensified their relationship to promote future data scientists and interdisciplinary experts in developing, adapting, and applying data analytics methods in a broad array of research domains with the goal of preparing a new generation of data analysts for the needs of increasingly digitized workflows and value chains beyond academia. This idea was combined with a strong focus on sponsoring female students, which ties nicely into MDSI's efforts to promote diversity in data science. These efforts culminated in Linde committing to make a total gift of €1,500,000 targeted at doctoral researchers and students at TUM. The natural partner at TUM for initiating a program and coordinating these funds was MDSI.

"Like many other international students, I felt socially and financially lost during the pandemic. I was fortunate to receive Lthe Linde/MDSI Master's Scholarship, which provided support and expanded my scientific contacts in the field. Thanks to MDSI, I could focus on my studies, successfully finish the degree, and continue my research career as a Ph.D. candidate."

– Iryna Burak (scholarship holder)

and Master's Students

LINDE/MDSI **DOCTORAL FELLOWSHIP PROGRAM**

The Linde/MDSI Doctoral Fellowship Program aims to promote excellent doctoral researchers from data science, machine learning (ML), and artificial intelligence (AI), their mathematical foundations, and their application in the various scientific fields represented at TUM to strengthen interdisciplinary research. These Linde/MDSI Doctoral Fellows are essential to MDSI's thriving and dynamic research atmosphere. They participate in the specially tailored MDSI Doctoral Training Program and share the location at the institute's facilities as needed. MDSI strongly supports their collaboration and interaction with fellows and faculty from other research areas.

To participate in the program, candidates must stand out at the beginning of their doctorate in one of MDSI's annual calls and convince a jury of their plans for a doctoral thesis. The reward is a three-year co-funded fellowship and integration into the MDSI research environment, including all activities and programs tailored to doctoral researchers, such as the MDSI Doctoral Seminar & Workshop, the entrepreneurship workshop, the science communication training, or the Al writing course. Furthermore, they meet their Linde sponsor and receive an introduction to a global company's career opportunities. Additionally, MDSI provides funds to doctoral researchers to participate in conferences or workshops or invite guests they would like to collaborate with.

Currently, the program numbers 15 doctoral fellows: six, five, and four each from the 2020, 2021, and 2022 calls. Initial results can already be seen, with the first doctoral researchers currently close to completing their doctoral thesis.



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LINDE/MDSI **MASTER'S SCHOLARSHIP PROGRAM**

The second component of the Linde/MDSI Programs is a one-year scholarship for talented master's students. Matching the topical focus of MDSI, students from the TUM master's programs **>** "Data Engineering and Analytics" and **7** "Mathematics in Data Science" are entitled to apply in the bi-annual calls for applications. A panel consisting of MDSI Core Members from mathematics and computer science reviews applications to identify the most promising candidates for the €1,000 per month scholarship. The decisive factor for being selected is demonstration of outstanding academic achievements and commitment.

Currently, MDSI is initiating further activities to strengthen the integration of scholarship holders into the MDSI ecosystem. The pandemic hampered many ideas for interaction with the students at the beginning of the program. Nevertheless, the first students were welcomed by the MDSI Executive Director Prof. Stephan Günnemann and they have been invited to participate in MDSI Doctoral Seminar & Workshop to help them establish first contacts with doctoral researchers already pursuing a career in a field of interest. To further solidify the connection between the two groups – doctoral researchers and master's students – MDSI also includes them in a research assistant program. Moreover, the Linde/MDSI scholars may participate in the TUM Research Data Hub's (RDH) various activities.

OUTLOOK

MDSI is planning to introduce further accompanying support elements to the Linde/MDSI Programs, e.g. establishing a welcome event with a meeting at MDSI and an introduction to the Garching campus, a program featuring former Linde/ MDSI scholars and fellows, and a joint dinner. Further activities include an annual excursion to Linde, an academic retreat including TUM and Linde senior researchers, fireside chats with MDSI Core Members or site visits at their chairs.



"My fellowship has enabled me to pursue my research on deployable ML-based models and tools to assist analysts, policymakers, and market participants in understanding and analyzing the power market economics in the context of the muchneeded energy transition."

– Shiva Madadkhani (doctoral fellow)



Linde/MDSI Programs

"During these first years of my Ph.D., the MDSI has played a pivotal role in connecting me with researchers across diverse fields. It has provided a platform where I can freely exchange ideas and experiences with other Ph.D. students with whom I might not have crossed paths otherwise. At the MDSI, researchers from all fields come together to tackle shared problems." – Johanna Sommer (doctoral fellow)

Johanna Sommer:

Generative Modelling of Molecules for Drug Discovery

eep molecule generation promises a more efficient exploration of the vast chemical space compared to traditional methods, and it may help design molecules with unique properties that would otherwise go undiscovered.

Current deep molecule generation methods have shown initial successes on popular benchmarks that measure a model's ability to learn the space of drug-like molecules. Many rely on so-called motifs — building blocks or commonly occurring subgraphs that aid the generation procedure. Johanna investigates what constitutes suitable motifs: Should they reflect chemical rules and properties, or is a data-driven approach favorable? This goes together with a better understanding of where motifs can help models learn to build molecules and where it limits them. She disentangles such motifs' structure and features for the first time with the novel molecule generation model MAGNet, enabling models to benefit from such building blocks without limitations when navigating the space of drug-like molecules. The flexibility and expressiveness of her approach helps pave the way for new drug discoveries.

Achievements

→ Hetzel, L.*, Sommer, J.*, Rieck, B., Theis, F., & Günnemann, S. (2023). MAGNet: Motif-Agnostic Generation of Molecules from Shapes.

S. (2023). The power of motifs as inductive bias for learning molecular distributions.

*equal contribution

Team

Johanna Sommer¹, Leon Hetzel^{2,3}, Stephan Günnemann¹, Bastian Rieck^{2,3}, David Lüdke¹, Fabian Theis^{2,3}

¹ ¬ Data Analytics and Machine Learning ² ¬ Mathematical Modelling of Biological Systems ³ ¬ Helmholtz Munich

> Comparative model of new molecule generation with MAGnet



Level of detail



Shiva Madadkhani: **Analysis & Projection of the Power Market: An ML Approach**

s witnessed in the recent period, increased power price fluctuations raise the financial risks for electricity market participants. A machine learning-based approach helps identify key variables and improves price predictions.

Electrification of carbon-intensive sectors and decarbonization of power supply are widely acknowledged as essential in transitioning to a carbon-neutral future. In light of this, understanding the dynamics of electricity prices and how the prices may change is critical for navigating the energy transition. The relationship between power prices and the underlying factors is complex and changes non-trivially over time.

Shiva has applied a machine learning (ML) model to identify the most important factors from a list of 80 which are driving electricity prices in Germany. The results of the feature selection analysis align well with econometrics-based and structural modeling approaches. Furthermore, Shiva used the code to predict the power prices in 2016 – 2021. The models exhibit good prediction accuracy, as measured by the relevant error metrics, and the tests help narrow down the limitations of the prediction.

Achievements

↗ Madadkhani, S., & Ikonnikova, S. (2022). Analyzing the Power Market and Projecting the Future with High Energy and Carbon Prices: A Machine-Learning Approach.

Madadkhani, S., & Ikonnikova, S. (2022). What Machine Learning Can Tell Us about the Drivers of Electricity Prices: The Case of Germany. 43rd IAEE International Conference. International Association for Energy Economics.

Team

Shiva Madadkhani, Svetlana Ikonnikova Center for Energy Markets, TUM School of Management



Example of the detection and tracking of moving objects with Dynamic Simultaneous Localization and Mapping



Mariia Gladkova: **Dynamic Simultaneous Localization and Mapping**

oday, Simultaneous Localization and Mapping (SLAM) and multiobject tracking are critical components in autonomous systems. However, real-world scenarios with numerous moving objects push current algorithms to their limits.

In SLAM, a location, e.g. of a robot, car, or drone, is jointly estimated with the 3D mapping of the environment. When analyzing the recorded visual data by a moving sensor like a camera, the surrounding is often assumed to be static. Moving objects in the scene adversely affect this process. To mitigate this disruption, Mariia combines the detection and tracking of moving objects with classical visual odometry/SLAM methods. Such a hybrid system has a high accuracy of the camera and objects' pose estimation and allows consistent reconstruction of the 3D environment. Moreover, the new system can adequately model the motion of each observed object in the scene. Additionally, Mariia integrates map-based relocalization into direct visual odometry to further improve global localization in case of an unreliable GPS signal. In combination, these methods contribute immensely to a richer and more reliable scene understanding.

Achievements

¬ Gladkova, M., Wang, R., Zeller, N., & Cremers, D. (2021). Tight Integration of Feature-based Relocalization in Monocular Direct Visual Odometry.

 ¬ Gladkova, M., Korobov, N., Demmel,
 N., Ošep, A., Leal-Taixé, L., & Cremers, D. (2022). DirectTracker: 3D Multi-Object Tracking Using Direct Image Alignment and Photometric Bundle Adjustment.

Presentations at 7 IEEE ICRA 2021, Xi'an, China, and \neg IEEE IROS 2022, Kyoto, Japan.

Team

Mariia Gladkova, Rui Wang, Niclas Zeller, Daniel Cremers

Intelligence

Munich Data Science Institute Technical University of Munich

2021-2023



ndustry

Since its operational start in 2021, MDSI has been active in establishing and expanding industry contacts to foster various collaborations. In this context, the collaborations aim for knowledge exchange, promoting R&D projects, or funding young scientists.

Industry Students Exchange

Motivation: Companies are interested in recruiting students with a data analysis background.

Concept: MDSI facilitates the communication of jobs and positions through its webpage and career fairs for all TUM students.

Collaboration contracts between €5,000-€10,000 annually per company.

n the past years, several intensive discussions have commenced with representatives of MDSI and companies across various industries, e.g. **↗** Amazon, **↗** Audi, **↗** BayWa, → BMW, → Mercedes-Benz, → Muon Space, and \neg SAP, exploring various potential models for collaboration.

Following the advice of the MDSI Advisory *Board* to identify topics and formats that may be of interest to potential industry partners, MDSI developed the **"Research with Indus**try Groups" (RIG) program. With the newly established RIGs, MDSI seeks to intensify the exchange of its members with industry partners. RIGs are built around an interdisciplinary team of doctoral researchers participating in MDSI Doctoral Training Program.

Furthermore, RIGs also integrate master's students seeking to gain hands-on experience in applied research. The doctoral researchers and master's students will

Engagement

interact intensely with the industry partner to achieve the proposed research goals.

Zeiss

gen

Specifically, RIGs comprise one or two principal investigators affiliated with TUM and an industry collaboration partner. Each project hosts a team of several doctoral researchers collaborating on a common scientific theme, each pursuing their own doctoral thesis topic. Industry partners and TUM chairs co-fund and co-supervise the doctoral researchers. MDSI supplies funds for travel, student assistants, and an additional doctoral researcher.

Industry Research Support

Motivation: *TUM-DI-LAB* internal projects with TUM chairs might include industry sponsors. These sponsors do not participate actively in the research project. However, their financial contribution is duly acknowledged on the MDSI webpage and in the final reports of the respective projects.

Concept: collaboration/sponsoring contracts between €5,000–€10,000 per supported project.





At the end of 2022, MDSI started gathering potential companies interested in such a format. Preliminary discussions have been held with various industry partners.

Beyond the RIG program, several further ideas were discussed extensively with the industry partners: "Industry students exchange," "Industry research support," and "Lunch talk/fire-side chat."

As a long-standing partner of TUM, 7 Linde recently announced extending their MDSIcommitment and aims to intensify collaboration. To this end, a constant, close exchange with MDSI is planned to share information about events and to develop joint actions, lectures, and programs such as plant visits, excursions, etc.

Lunch talk/fire-side chat

Motivation: To bring together the scientific community and representatives from various industries to discuss potential future collaboration.

Concept: Talks on topics of interest for industry partners and the scientific community (e.g. latest developments or recent challenges in the industry).

Onsite meeting at MDSI, depending on the audience size, the format, and time/space for networking with snacks sponsored by industry partners.



MANDATES: RESEARCH, INNOVATION, EDUCATION IJM-DI-AB**TUM Data Innovation Lab**

7 TUM-DI-LAB embodies an educational and early research initiative, fostering the exchange of cutting-edge knowledge in data science among researchers, industry experts, and master's **students** with a keen interest in the practical application of data analysis and artificial intelligence (AI).

TUM-DI-LAB in a nutshell

Started in 2017 and joined MDSI in 2021

103 projects until 2022, 50% industry and 50% research

83 partners from industry, TUM, and other research institutions

Since 2017, participation of 435 master's students. 25 master's degree programs, and 9 TUM departments

Project supervision by 83 industry mentors, 35 TUM doctoral students, 16 TUM postdocs, and 8 TUM professors

IDEA

UM-DI-LAB aims to connect researchers from industry and academia via innovative projects incorporating dynamic teams of master's students from diverse fields of expertise. This constellation exhibits a multitude of benefits for all involved: Researchers at TUM and in the industry can establish new contacts with each other, they profit from the results generated in the interdisciplinary teams, and they can attract valuable members for their research groups. Likewise, the master's students can tremendously broaden their experience, open up new avenues for their upcoming careers and receive additional credit for their ongoing studies.

CONCEPT

Each semester, partners from industry and academia offer data science-related topics and data, and data science experts to supervise the teams. Selected TUM master's students from different TUM departments then get the opportunity to work on these interdisciplinary projects. The selection of projects and the composition of the teams involves a meticulous evaluation coordinated by the TUM-DI-LAB. In this context, relevant aspects such as educational potential, subject, innovation, applicability, ethical implications, and potential societal impact are considered.

Similarly, all members comprising each project team, potentially including industry experts, TUM researchers, and master's students, are thoughtfully selected based on their expertise, academic transcripts, motivation, interdisciplinary skills, and diversity considerations like gender and nationality. This approach for matching projects and teams while optimizing their composition maximizes educational benefits and ideally promotes cross-fertilization through engaged joint learning.

The teams of the lab operate under the guidance of TUM researchers throughout the lecture period and produce a comprehensive final report at the end of the semester. Moreover, they prepare a presentation of the project's outcomes, doubling as a final exam for the master's students.

TUM-DI-LAB IN 2022

In the summer and winter of 2022, the lab hosted 20 projects with the participation of 96 students and 24 supervisors.

INDUSTRY PROJECTS	RES
 Alyne GmbH, "Enterprise Risk Autopilot" 	• 7 1
 Amazon, "Uncertainty Quantification and Probabilistic Forecasting of Big Data Time Series at Amazon Supply Chain" 	"Di Do Red
 ABMW, "Prediction and Clustering Critical Suppliers" 	• 7 7 Bu: "NI
 A Horváth & Partners GmbH, "NLP for Intelligent Data Mining and Augmentation of Probabilistic Graphical Networks" 	Clu • 7 7 Bio
 <i>KPMG</i>, "Deep xVA: Speeding-Up Derivative Pricing" 	"Cr • 7 7
 Intel and Leibniz Supercomputing Centre (LRZ), "How to Train the Best Deep Learning Models for the Edge?" 	Sys Brc • 7 7
 PreciTaste, "Detecting Novel Objects With Only Few Examples" 	and "To
 Inovex GmbH, "Graph Learning Based Fashion Recommendations" 	in E • 7 7
 ¬PwC, "Innovative Machine Learning Algorithm Meets Carrera for Auto-Piloting" 	Sys "Ge Ima
 A Lidl and A TUM Associate Professorship of Business Analytics, "Practical Machine Learning Solutions for Uncertainty Quantifi- cation in Regression Problems" 	• 7 1 Pro "Pa
 AMW, "Anomaly Detection and Prediction of Charging Station Failure" 	• 7 7 <i>Me</i> Tra
	• 77
	"So Lea

SEARCH PROJECTS

MIT and 7 TUM Chair of Bioinformatics, iffusion Models for Rigid Protein-Protein ocking and Binding Pocket Conditioned ceptor Flexibility"

TUM Chair of Software Engineering for siness Information Systems,

LP and Knowledge Graphs for Research uster Prediction and Analysis"

TUM Chair of Mathematical Modeling of ological Systems and 7 Helmholtz AI, reating a Single-Cell Atlas of Human Blood"

TUM Chair of Robotics, AI and Real-time stems, "Meta-Reinforcement Learning for oad Non-Parametric Tasks"

TUM Data Science in Earth Observation d 7 German Aerospace Center (DLR),

owards a NAS Benchmark for Classification Earth Observation"

TUM Chair of Decentralized Information stems and Data Management,

eneration of Synthetic Segmented Medical ages for Tumor Detection"

TUM Chair for Computer Aided Medical ocedures and Augmented Reality, artial 3D Thyroid Registration"

TUM Chair of Aerodynamics and Fluid echanics, "Acceleration of Neural Network aining with Microsoft DeepSpeed"

TUM Chair of Digital Agriculture, oybean Yield Estimation with Machine arning and Remote Sensing in Brazil"



Selected TUM-DI-LAB projects



About the project

Sponsor

7 TUM Chair of Bioinformatics

Supervisors

- Doctoral researcher Hannes Stärk (MIT)
- Doctoral researcher Céline Marquet (TUM Chair of Bioinformatics)

Student master's programs

- Mathematics in Science and Engineering
- Robotics, Cognition, and Intelligence
- Informatics
- Electrical Engineering and Information Technology

Results

7 Paper published at the MLDD workshop, ICLR 2023: Ketata, M. A., Laue, C., Mammadov, R., Stärk, H., Wu, M., Corso, G., Marquet, C., Barzilay, R., & Jaakkola, T. S. (2023) DiffDock-PP: Rigid Protein-Protein Docking with Diffusion Models.

nderstanding how proteins interact with other molecules or other proteins is crucial to modern biology, with applications ranging from drug discovery to protein design. The recent machine learning method DiffDock has formulated protein-size molecule docking as a generative problem, with significant performance boosts over traditional and current deep learning baselines.

In this project, students investigated ways to extend DiffDock and improve its results. In the first part, students modeled the proteins as semi-flexible to account for structural changes upon docking and to predict the amino acid sidechains' conformations near the ligand's proposed binding site. The experiments presented in the paper show promising results. This additional task can aid in predicting better ligand poses alongside structural changes during binding, especially when relying on unbound protein structures. Most prominently, students were able to show that the underlying model mainly relies on information from atoms near the binding site, allowing thus to gain a significant speedup when discarding atoms too far away without losing accuracy. State-of-the-art performance was achieved, outperforming all considered baselines.

Binding Pocket Conditioned Receptor Flexibility



Uncertainty Quantification and Probabilistic Forecasting of Big Data Time Series at Amazon Supply Chain



ime series forecasting in supply chains has several applications, such as predicting future inbound flows of goods or the future demand for products. Since business decisions (e.g. inventory replenishment strategy) may be based on those forecasts, ensuring accurate, robust, and interpretable predictions is critical. Additionally, supply chain disruptions such as the COVID-19 pandemic, the Suez Canal blockage, the Shanghai lockdown, or the current geopolitical/economic context have increased the uncertainty on inbound and outbound flows.

In this project, students focused on researching probabilistic forecasting methods. By combining the state-of-the-art fixed quantile forecaster MQTransformer with an existing generative copula-based approach, they created a new model, the MQCopulaTransformer, which achieves competitive results compared to the MQTransformer. In addition, the model prevents issues like quantile crossing and adds the capability of learning cross-series and cross-time correlations.

Finally, the students worked on increasing the interpretability of how these models estimate uncertainty by researching explainable artificial intelligence techniques and embedding them on top of the created deep learning models pipeline. These techniques allow a researcher to understand the inputs (previous timestamp or exogenous variable) driving the models' predictions and assess how the models learn from data and whether their predictions are reliable.

This research and package implementation work is a basis for further Amazon internal research on uncertainty quantification within the supply chain.

About the project

Sponsor

Amazon

Supervisors

- Filippo Lentoni and Aurélien Amiyao Ouattara (Amazon
- Doctoral researcher Cristina Cipriani (**7** TUM Chair of Applied and Numerical Analy-

Students' master's programs

- Mathematics in Data Science
- Mathematics in Operations Research
- Mathematics
- Electrical Engineering and Information Technology
- Information Systems

Results

This research and package implementation work is a basis for further Amazon-internal research on uncertainty quantification within the global supply chain.

In addition to modeling the uncertainty, the students researched physics-informed machine learning to leverage prior knowledge about the system and predictable variables. In this way, the students enhanced a data-driven approach given laws of physics or economic properties specific to the supply chain environment.



Konrad Zuse School of Excelence in Reliable AI -

The **7** Konrad Zuse School relAl **trains M.Sc. and** Ph.D. students on technical aspects of artificial intelligence (AI) as well as issues related to the importance of **reliable AI** for society. relAI is a joint TUM and Ludwig Maximilian University of Munich (Ludwig-Maximilians-Universität München, LMU) educational and research program.

> n 2022, MDSI was instrumental in securing funding for relAl, a joint educational and research initiative of TUM and LMU. The overall project management is hosted by MDSI, tightly cooperating with local project management at LMU and integrating relAl into the MDSI activities. The funded budget of €13.8 Mio will secure the project for its first six years.

relAI is one of only three **>** Konrad Zuse Schools for AI the 7 German Academic Exchange Service (DAAD) initiated to attract excellent young AI specialists worldwide. The Konrad Zuse School relAl is the first graduate training program in Germany dedicated to the reliability of AI technology.

MANDATES: RESEARCH, INNOVATION, EDUCATION

Reliable AI is an emerging field focusing on Al aspects such as safety, security, privacy, and responsibility. These factors are essential prerequisites for adopting AI by industry and society across AI application areas in the public domain, including autonomous driving and human-robot interaction, healthcare, or decision-making for business optimization. Training talents skilled in transferring research results to corresponding applications in the industry is crucial to guarantee successful adoption. The relAI project takes the lead in this endeavor by developing a research and educational program to train future generations of AI experts who, for the first time, combine technical brilliance with awareness of AI's implications on society.

EDUCATION

The Konrad Zuse School relAl educates top international master's students and doctoral researchers in the end-to-end development of reliable AI systems. The relAI school's concept is based on three pillars:

- coherent, personalized training,
- (early) exposure to real-life challenges and awareness of the (business) impact of AI research, and
- fully embracing the international scope of reliable AI.

With these aims in mind, the school is set up to offer an innovative program that covers the full spectrum of scientific knowledge, business expertise, and industrial exposure, preparing students and doctoral researchers for diverse career paths in industry and academia. The relAI training program highlights collaboration with and work experience in top international AI centers combined with a strong interaction with industry partners to foster high-impact interdisciplinary research.





Munich Data Science Institute Technical University of Munich

2021-2023

RESEARCH

The relAl research program encompasses four research areas: mathematical and algorithmic foundations of reliable artificial intelligence (Al) and domain knowledge in three core application domains: medicine & healthcare, robotics & interacting systems, and algorithmic decision-making. Each of the research areas covers central themes of reliable Al:

- Safety, i.e., ensuring that AI systems (e.g., robots) do not cause harm or danger.
- Security, i.e., making AI systems resilient against threats, external attacks, and information leakage, such as avoiding manipulation of decision-making systems against adversaries.
- Privacy, i.e., ensuring protection and confidentiality of (individual) data and information, such as medical AI systems incorporating sensitive patient data.
- Responsibility, i.e., developing AI systems while taking societal norms, ethical principles, and human needs into consideration, such as by making decisions understandable and protecting individuals against discrimination.







relAI FAMILY

In setting up the project, relAl has brought together three member groups to support the research and academic training of the relAI master's & doctoral candidates: the school's fellows, international academic partners, and industry partners. The school's fellows, wellknown academics in areas of central importance for relAI, provide the supervision of the doctoral researchers and jointly conduct research together. The academic partners are the anchor point to the world-class AI centers and support the school's international network. Industry partners provide practical Al expertise as well as insights on application-focused challenges. They participate in supervision activities, provide internship opportunities, and engage in activities such as career fairs or other public events.

relAI OPENING CEREMONY

On 26 July 2023, relAl celebrated the opening ceremony at the Residenz in Munich. Markus Blume, the Bavarian Minister of Science, TUM's Vice President, Prof. Gerhard Kramer, LMU's Vice President, Prof. Francesca Biagini, and the *¬ DAAD* General Secretary Dr. Kai Sicks introduced the event with welcome speeches. The agenda was enriched by discussions among relAl members on relAl and its different focus areas.



"I am a master's student at TUM and a member of relAI's first cohort since September 2022. When I first heard about relAI as one of the few Al schools in Germany, I wanted to join to gain research experience in Al and ML already during my master's thesis. After I joined and during our first get-together, I was amazed by the amount of gifted and highly motivated individuals coming together to discuss AI. From master's students to Ph.D. students to fellows and professors, everyone is very excited to collaborate and help advance the foundations of reliable AI. Since I joined relAI, I have improved my research, communication, and presentation skills, and I am very excited about the months and years to come. I hope to continue as a relAI member when I start my Ph.D."

– Mohamed Amine Ketata





"I have been part of relAl for less than a year, and it has definitely been a fun and enriching experience. I'm particularly excited about relAl's focus on the societal impact of Al, which I find very relevant. The program's extensive network of universities and industry partners brings together a wide range of perspectives from diverse research and application areas, offering interesting insights into the topic. Moreover, connecting with fellow students who share similar interests but come from different backgrounds has been both fun and inspiring. I'm genuinely excited to see what exciting things the future holds for relAl!"

- Cecilia Casolo

Munich Data Science Institute

Thematic Setting

MDSI offers hackathons as an exciting means to support young researchers. Together with ↗ Institut Mines Télécom (IMT), MDSI hosted the hackathon GreenHack~IT, built around a challenge provided by 7 Ariane Group.

> Getting together to crack problems: moments from GreenHack~IT

o foster innovative learning platforms for applied coding and to engage in interdisciplinary exchange with peers from different research fields, the MDSI organizes hackathons: multi-day collaborative software and hardware development events where participants from different (research) areas, including many applied fields beyond computer science, produce software products in cross-functional teams to solve problems.

GREENHACK~IT – **A COLLABORATION BETWEEN MDSI & IMT**

GreenHack~IT aims to let final-year French and German graduate students well versed in machine learning (ML) and data analytics unleash their creativity and skills. During the hackathon they tackle a significant industrial problem considering sustainable development goals in the context of Industry 4.0. This hands-on experience in real-life problems within a time-constrained setting resembles challenges they would face in their future jobs. The main goal of this hackathon was to promote the spirit of bilateral collaboration between Germany and France and teach the engineers of tomorrow how to collaborate across borders, following the principles of the European Union.

Hackathons

Ariane Group, IMT's industrial partner for the first edition, provided the topic of the Hackathon.

Target group: The hackathon (four days and three nights, from Thursday to Sunday) brought together 30 French students from all IMT schools and 15 German students from TUM, who formed mixed teams, each mentored by a coach (organizer or graduate student). The hackathon was hosted at the premises of MDSI.

Implementation methods and measures:

The main technical aim was to predict and/ or explain a phenomenon through varied factors or attributes using ML and data science tools, mainly on data provided by the industry partner. However, each group was also free to collect supplementary relevant data on the web. One of the critical factors considered beyond technical merit was the ecological footprint of the proposed methods, as it is one of the fundamental tenants of Industry 4.0. The topic for the first edition revolved around image classification to detect defective parts in an industrial process automatically to lessen the ecological impact of the process. Today, defects are detected by pre-emptively destroying a sample of produced parts, as noninvasive probing is currently too costly. The students'

MANDATES: RESEARCH, INNOVATION, EDUCATION, OUTREACH

task was to propose a solution to remove the need for destructive probing and significantly improve the process's ecological footprint.

German-French cooperation: The organization committee comprises equal parts of German and French members. Ariane Group, the industrial partner, is a French-German company. The hackathon involved mixed teams of French and German students working in tandem. On all counts, GreenHack~IT is the very embodiment of French-German collaboration.

Perspectives: Beyond fostering French-German collaboration, the initiative laid the foundation for a more durable R&D collaboration. The industrial partner has expressed interest in engaging in contractual work with researchers from IMT and TUM to continue working on the project. Additionally, the event is meant to be recurrent and held (bi)annually, depending on the availability of suitable topics. IMT has successfully applied for another GreenHack~IT envisioned for January 2024.

Researchers at MDSI and linked projects generate vast amounts of data. Exploring ways to work with that data sometimes takes the shape of a data competition.

mong the events MDSI co-organized, the Kaggle competition **IceCube** – **Neutrinos in Deep Ice** was undoubtedly outstanding. Based on data collected in Antarctica, the challenge called on participants to develop a machine learning (ML) solution to predict the direction of neutrinos passing the detector array. Endowed with a generous prize and organized by MDSI member Dr. Philipp Eller and a well-known group of international research units, this exciting challenge attracted widespread interest. When it ended on 19 April 2023, 901 participants had written over eleven thousand entries. Altogether, 6460 teams registered from 74 countries.

The top three placements applied so-called "transformers," the same architecture that powers the latest generation of large language models such as ChatGPT. This new technique applied to IceCube surpassed the quality of previous ML-based reconstructions significantly, opening up new possibilities to apply these algorithms to vast numbers of events, if not the entire IceCube data stream at once. Up to now, such high precision was reserved for select neutrino event candidates that needed to be processed with computationally intensive methods, taking minutes to hours per event. In contrast, the methods developed during the Kaggle competition perform at lightning speed and can be applied to millions of events within a few hours.

MANDATE: RESEARCH

MDSI Best Paper of the Year AWard

The MDSI Best Paper of the Year Award, initiated in 2022, showcases the excellent work of MDSI researchers.

very year, *MDSI Core Members*, MDSI Project Members, and affiliated researchers publish volumes of excellent research. Among all these remarkable publications, the MDSI Best Paper of the Year Award highlights outstanding results in data science, machine learning (ML), and artificial intelligence (AI), and shares these with the MDSI community. An anonymous reviewing board consisting of MDSI Core Members select three papers for first, second, and third place. The primary criteria for receiving the award are the publication's advancements to the field of data science/ML, its interdisciplinarity and potential impact, as well as the paper's relevance to society.

Awards ceremony 2023 during the MDSI Opening Ceremony & 3rd General Assembly. From left to right: Prof. Thomas F. Hofmann (TUM President), Christine Eilers (honorable mention), Marten Lienen (runner-up), Leon Hetzel (winner of the MDSI Best Paper of the Year Award), Viviana Sutedjo (honorable mention), Markus Blume (Bavarian State Minister for Science and the Arts) and Prof. Stephan Günnemann (MDSI Executive Director).

AWARDS 2021:

Winner: > Stephan Thaler and Julija Zavadlav: Learning Neural Network Potentials from Experimental Data via Differentiable Trajectory Reweighting. Nature Communications (2021).

Runner-up: *¬ Mohammad Lotfollahi, Mohsen* Naghipourfar, Malte D. Luecken, Matin Khajavi, Maren Büttner, Marco Wagenstetter, Žiga Avsec, Adam Gayoso, Nir Yosef, Marta Interlandi, Sergei Rybakov, Alexander V. Misharin and Fabian J. Theis. Mapping Single-Cell Data to Reference Atlases by Transfer Learning. Nature Biotechnology (2021).

Honorable mention: 7 *Georgios Kaissis,* Alexander Ziller, Jonathan Passerat-Palmbach, Théo Ryffel, Dmitrii Usynin, Andrew Trask, Ionésio Lima Jr, Jason Mancuso, Friederike Jungmann, Marc-Matthias Steinborn, Andreas Saleh, Marcus Makowski, Daniel Rueckert, Rickmer Braren. End-to-End Privacy Preserving Deep Learning on Multi-Institutional Medical Imaging. Nature Machine Intelligence volume 3, pages 473–484 (2021).

AWARDS 2022:

Winner: 7 Leon Hetzel, Simon Boehm, Niki Kilbertus, Stephan Günnemann, Mohammad Lotfollahi, Fabian Theis. Predicting Cellular Responses to Novel Drug Perturbations at a Single-Cell Resolution, 36th Conference on Neural Information Processing Systems (NeurIPS), 2022.

Runner-up: 7 Marten Lienen, Stephan Günnemann. Learning the Dynamics of Physical Systems from Sparse Observations with Finite Element Networks, International Conference on Learning Representations (ICLR), 2022.

Honorable mention: *¬Viviana Sutedjo,* Maria Tirindelli, Christine Eilers, Walter Simson, Benjamin Busam, and Nassir Navab. Acoustic Shadowing Aware Robotic Ultrasound: Lighting up the Dark, in IEEE Robotics and Automation Letters, 2022.

Awards ceremony 2022 during the 2nd MDSI General Assembly. From left to right: Prof. Gerhard Kramer (TUM Senior Vice President for Research and Innovation), Stephan Thaler (winner of the MDSI Best Paper of the Year Award), Georgios Kaissis & Alexander Ziller (honorable mention), Mohammad Lotfollahi (runner-up) and Prof. Stephan Günnemann (MDSI Executive Director).

MANDATE: RESEARCH

MDSI Visiting Researchers Program

The MDSI Visiting Researchers Program aims to support scientists at TUM in inviting guests from abroad. With this program, MDSI connects experts, supports joint research projects and publications, and facilitates scientific exchange.

Visiting Researcher Prof. Shanahan in discussion with scientists at TUM.

ince late 2022, MDSI Core Members can invite researchers from other institutions to TUM for data science-related stays via the MDSI Visiting Researchers Program. In 2023, MDSI joined forces with **7** TUM Global & Alumni Office to further develop the program. While the TUM Global & Alumni Office provides different funding programs for incoming and outgoing visitors for extended periods, MDSI's Visiting Researchers Program is complementary in that it primarily looks to fund short-term visits with interdisciplinary research interests.

Applications to the program are assessed for their relationship to MDSI's core mission. Additionally, MDSI looks to support primarily interdisciplinary undertakings and seeks to bring foundation and application researchers together.

The first researcher to receive MDSI support was 🛪 Prof. Phiala Shanahan (🛪 Massachusetts Institute of Technology, MIT). At TUM,

she organized a joint interdisciplinary workshop on "Machine Learning approaches in Lattice QCD" with Prof. Nora Brambilla (TUM). In the second call, three visitors were invited. **>** Prof. Matthias Auf der Maur (
 University of Rome) and Prof. Alessio Gagliardi (TUM) are working on a project integrating ML methods to continuum-atomistic multiscale simulations for photovoltaic and optoelectronic nanostructured devices. ↗ Prof. Zheng Liu (↗ University of British) Columbia) explores a research collaboration with *Prof. Xiaoxiang Zhu* and the *AI4EO*. ↗ Prof. Gregory Macfarlane (↗ Brigham Young) University) and Prof. Rolf Moeckel investigate a coherent and regionally transferable transport modelling platform with exchangeable elements.

> Participants of the Machine Learning approaches for Lattice QCD workshop

MANDATES: RESEARCH, INNOVATION, Λ / I EDUCATION, OUTREACH **Vorkshops** & Retreats

The MDSI Workshops and Retreats program co-funds different formats that bring together researchers from within TUM and/or from other institutions. This program further stimulates interdisciplinary networking and international collaboration.

> ithin the program, a mixed group of TUM researchers and selected exter experts aim to explore topics related to da science and its applications from a multidisciplinary perspective during a single or multi-day event. The program also promot transdisciplinary approaches and collaborations, especially those of an exploratory, creative nature.

> Particularly, MDSI looks to support young researchers in exploring academic and ent preneurial topics off the beaten track of the primary research agenda. Accordingly, teal of doctoral and postdoctoral researchers can also apply for funding to organize a workshop that brings together young scho ars and experts for in-depth discussions. This format complements the interdisciplin ary networking engendered by the MDSI

Thematic Setting

Illustration used for the Machine Learning approaches for Lattice QCD workshop

rnal ata	Doctoral Seminar & Workshop. It allows doctoral researchers to deepen their under- standing of interdisciplinary approaches and strengthen their networks.
tes ,	In 2022 and 2023, MDSI supported three workshops, two led by doctoral research- ers. The first, "Tobitate," has been organized by <i>Linde/MDSI Doctoral Fellow</i> Yukiteru Murakami. "Tobitate" brought together Japanese scholars working at or affiliated
tre- ieir ams	with TUM to exchange their research and contextualize more general topics. The broad reach of the event mirrored the relevance of <i>MDSI's mandate</i> in wider society.
ว เ - า-	In the fall of 2022, doctoral researchers Larkin Liu and Jun Tao Luo organized a work- shop on "¬ Stochastic Modelling and Monte Carlo Tree Search." Focusing on Monte Carlo methods, they brought together a diverse

group of researchers and featured a student tutoring session. Moreover, the workshop attracted select international researchers. The MDSI funding gave the young organizers the unique opportunity to promote and discuss these topics.

MDSI also sponsored a large international conference on "
Machine Learning approaches in Lattice QCD," led by Prof. Nora Brambilla in March 2023 at 7 TUM Institute for Advanced Study (TUM IAS). Its support included, together with other partners, co-funding of the multi-day workshop and help with the organization and advertising. This major event was a great success that attracted numerous international attendees. With its focus on the intersection of physics and machine learning, the workshop impressively highlighted the possibilities and challenges of bringing these two fields together.

MANDATES: RESEARCH, EDUCATION, OUTREACH

and an extended discussion session.

he Munich AI Lectures were initiated jointly by the Munich-based AI research institutions 7 Center for Advanced Studies (CAS), European Laboratory for Learning and Intelligent Systems (ELLIS) Munich, Munich Center for Machine Learning (MCML), and MDSI. It offers presentations by top-level artificial intelligence and machine learning researchers on topics of their ongoing work and the future of AI.

The lectures consist of a short presentation and a Q&A session to foster a lively discussion with our speakers. Each lecture lasts about one hour; most are streamed live and recorded on the 7 Munich AI Lectures YouTube *channel*. During the stream, all audience members can pose questions or comment. The Munich AI Lectures YouTube channel has approx. 300 followers and the lectures have been viewed around 3500 times.

PAST SPEAKERS

→ Yann LeCun
↗ Meta Al Research – ↗ New Ye
Jürgen Schmidhuber
Al Initiative KAUST – A Swiss
Ludwig Schmidt
University of Washington
University of Pennsylvania
Peter A. Flach
Iniversity of Bristol
Michael Bronstein
Iniversity of Oxford
↗ Max Welling
University of Amsterdam
↗ Collège de France
↗ Harvard University

The *Munich AI Lectures* brings together scientists and the public via short presentations by international experts

	29 September 2023	From Machine Learning to Autonomous Intelligence
ork University		
	14 July 2023	Thoughts on Artificial Intelligence
AI Lab IDSIA		
	11 July 2023	A Data-centric View on Reliable Generalization:
		From ImageNet to LAION-5B & DataComp
	8 March 2023	Explainable AI via Semantic Information Pursuit
	8 February 2023	The Highs and Lows of Performance Evaluation:
		Towards a Measurement Theory for Machine Learning
	2 November 2022	Physics-Inspired Learning on Graphs
	5 October 2022	The PDE Prior
	7 September 2022	Mathematical Mysteries of Deep Neural Networks
	-	
	4 May 2022	Fairness, Randomness, and the Crystal Ball
	•	

MANDATES: RESEARCH, INNOVATION, EDUCATION

MDSI Focus Topics help identify scientific highlights with enormous strategic importance for MDSI and the university. They aim to support measures related to such topics that have a long-lasting impact beyond MDSI's seed funding contribution.

he MDSI Focus Topics aim to establish a project or program employing innovative formats with high visibility and a pronounced long-term character. MDSI Core Members initiate the focus topics, and together with its members ranging from professors to doctoral researchers or even motivated master's students – they define the focus topic's mode of operation. However, focus topics might also integrate other researchers even beyond TUM.

Activities initiated by MDSI Focus Topics include the application for large collaborative programs funded by third parties, the organization of regular workshops or conferences, the publication of papers, or setting up a science blog series that introduces the group's research to the scientific community or the broad (non-academic) public. New ideas for innovative activities with high visibility are very welcome.

MDSI supports its focus topics by offering collaboration space at its premises, help, and financial support for organizing workshops or conferences, and funds for visiting researchers via the MDSI Visiting Researchers Program.

In 2023, MDSI started supplying the focus topics with additional funds via the MDSI Seed Funding scheme. This new means of support aims to establish long-lasting, sustainable activities. Many of these activities represent ideal complements to other MDSI formats, including the MDSI Doctoral Training Program and the MDSI Interdisciplinary Exchange

Selected Focus Topics:

Artificial Intelligence in Finance (AIF)

Artificial intelligence (AI) and machine learning (ML) tools and techniques have the potential to significantly impact the financial sector. The focus topic AIF will support tool development, consumer education, and professionals training in this domain.

he focus topic AIF, founded by MDSI Core Member Gjergji Kasneci and Ibrahim Karasu, Managing Director **7** Bundesverband deutscher Banken, bridges the gap between research and application in financial services and develops AI innovations for the financial sector. Furthermore, it promotes an undestanding of digital finance systems and fosters continuous professional education. These efforts will establish a long-term, symbiotic relationship between academia and industry, driving forward the financial sector's evolution with AI at the core.

The development of new AI solutions and technologies for the financial industry will include automated topics like trading systems, risk management, fraud detection, identity protection, and sustainability management. Addressing the finance sector's needs will create long-term partnerships and support startup incubation.

To adopt these technologies, consumers and society will need a deep understanding of Al and digital financial systems. With MDSI, **TUM Center for Educational Technologies** (EdTech Center), and **7** TUM Institute for Life-Long Learning (TUM IL³), TUM covers all formal education and knowledge transfer aspects in modern AI technologies.

Furthermore, AIF will provide professionals in the financial sector with up-to-date, flexible learning content adapted to individual needs and previous knowledge in AI and data science, including online courses, workshops, or other continuing learning resources.

Privacy-Preserving and Trustworthy Machine Learning – PPTML

PPTML aims to enable research in fields such as medicine, where the world's most critical problems are constrained by a lack of available scientific data resulting from legal or ethical restrictions.

n combination with owners being discouraged from sharing data that could provide them a competitive advantage, the lack of privacy-preserving and trustworthy analysis techniques significantly hamper progress despite the growing availability of high-performance algorithmic tools. Privacy-enhancing technologies like differential privacy, encrypted computation, or distributed learning represent potential solutions and are investigated in the focus topic. The researchers of PPTML further develop and apply these techniques to enable the exploitation of vast amounts of existing data. A major outcome of the focus topic is the successful application for funding for the Konrad *Zuse School relAI*, which targets privacy and security as major research pillars. Moreover, focus topic members Georg Kaissis, Daniel *Rückert*, and Alexander Ziller were awarded the 2021 **7** Eugen-Münch-Preis and the 2023 German **7** Society for Digital Medicine Publication Prize; Daniel Rückert and Georg Kaissis were awarded the **7** Federal Ministry of Education and Research (Bundesministerium für Bildung und Forschung, BMBF) *PrivateAIM* research project grant.

Illustration depicting the concept of privacy-preserving data analysis using ML algorithms.

Outcome

Konrad Zuse School relAI, awards from the **7** Münch Foundation and the German ↗ Society for Digital Medicine, → PrivateAIM research grant.

Team

Georg Kaissis; Daniel Rückert ↗ Artificial Intelligence in Healthcare and Medicine

Stephan Günnemann Data Analytics and Machine Learning

Twelve additional members from the three TUM Schools 'Computation, Information and Technology', 'Medicine and Health', and 'Life Sciences':

Pramod Bhatotia (7 Engineering Software for Decentralized Systems)

Alena Buyx (MDSI Advisory Board Member **7** Ethics in Medicine and Health Technologies)

Georg Carle (7 Network Architectures and Services/Information and Technology)

Javier Esparza (
Theoretical Computer Science)

Debarghya Ghoshdastidar (7 Theoretical Foundations of Artificial Intelligence)

Jens Großklags (7 Cyber Trust)

Jan Křetínský (*7 Formal Methods for* Software Reliability)

Markus List (*¬ Data Science in Systems* Biology)

Josch Konstantin Pauling (7 LipiTUM) - Computational Systems Medicine on Lipids and Metabolism)

Georg Sigl (
 Security in Information Technology)

Antonia Wachter-Zeh (7 Coding and Cryptography)

> Munich Data Science Institute Technical University of Munich

> > 2021-2023

Mathias Wilhelm (7 Computational Mass Spectrometry)

Focus Topics

Illustration of the Focus Topic CMD-ML

CMD-ML researchers are collaborating to fuse computational and machine learning (ML) techniques ir material design to further propel the field forward.

While computational science has been paramount in provide ing physical understanding and technological advancemer for material and device development for some time, the introduction of ML techniques has been relatively recent. Several approaches were proposed, including directly moc ing atomistic structure-property relations, using ML as a surrogate model, or incorporating ML models directly within simulations. Although different spatial scales in materials face different obstacles, many challenges are common to all scales. Thus, knowledge transfer between computationa science subfields can boost method development tremendously. To that end, the researchers of the focus topic have established a workshop series bringing together TUM researchers and international experts. They are also collaborating in the **7** TUM innovation network ARTEMIS.

Thematic Setting

Interdisciplinary Research on Graphs, Networks, and Connectivity Structures (InterConnect)

Graphs and networks represent complex rela-Graphs and networks exchange tionships in various fields, including social sci-Bimonthly, principal investigators (PIs) will ences, biology, transportation and computer give blackboard talks on graphs and networks topics. Similarly, doctoral researchers networks, recommendation systems, and computer graphics. Inter-Connect will foster will meet with a coach every second month interaction between these communities. to enhance exchange.

Graph neural networks and topological data analy-Visiting early-stage researchers sis provide strong potential for gaining deeper InterConnect will invite international junior insights into global patterns in graph-structured researchers for short stays at TUM to collabdata, utilizing a combination of machine learning orate with TUM scientists. (ML), combinatorics, geometry, algebra, and statis-Workshops and conferences tics techniques. Studying these networks' connec-InterConnect PIs co-organize the 7 ICCV tivity provides insights into information flow, social 2023 workshop on Scene Graphs and Graph dynamics, disease spread, traffic optimization, Representation Learning and are hosting the network resilience, and much more. InterConnect Munich meetup of the *¬ Learning on Graphs* will stimulate novel research ideas in these fields Conference 2023. They will initiate a workby promoting and enhancing networks between shop at the **7** TUM Science & Study Center TUM researchers and scientists worldwide. in Raitenhaslach for internal and external PIs and junior researchers.

n	Outcome	
d-	International Workshop CMD-ML, 24 February 2022, featuring three mini-symposia, each with a keynote by an external speaker and three	Five additional members from the three TUM Schools 'Engineering and Design', 'Natural Sciences', and 'Com- putation, Information and Technology':
nt	short presentations.	Nikolaus Adams (<a>Aerodynamics and Fluid Mechanics)
	Team Alessio Gagliardi	David Egger (<a>Theory of Functional En- ergy Materials)
del-	Simulation of Nanosystems for Energy Conversion	Phaedon-Stelios Koutsourelakis (⁊ Data-driven materials Modeling)
in	Julija Zavadlav A Multiscale Modeling of Fluid Materials	Wolfgang Polifke (<i>¬ Thermo-Fluid</i> Dynamics)
	Stephan Günnemann Data Analytics and Machine Learning	Nils Thuerey (<a a="" physics-based="" simulation)<="">
al		
е		
)-		

Teaching

New joint lectures by multiple PIs and block seminars for master's students represent innovative formats, especially because they target students from different schools. In the future, InterConnect plans to host a summer school in Munich on graphs and networks.

Data repository

As benchmark data are essential for many ML applications, InterConnect will develop a repository of graph data sets, including a curated list of external websites as a central hub for such data.

Causal Inference (CAUSE)

Research in causal inference has gained tremendous momentum in the current era of massively growing data complexity with its increased need for evidence-based decision-making. CAUSE will further this field through various innovative formats, promoting collaboration between researchers.

Causal inference aims to equip domain scientists with tools to move beyond mere correlations and conduct data analyses that discern and quantify the effects of the true drivers of observed outcomes. These will help in many areas, including biomedical and social sciences and public policy. CAUSE focuses on three key areas: climate science, computational biology, and economics. To connect researchers engaged in advancing the methodological and theoretical foundations of causal inference and domain scientists at TUM, CAUSE will offer several activities.

Two external speakers representing combined foundational and applied aspects will talk about, e.g. climate science and the analysis of temporal/spatial data, economics and heterogeneous causal effects, as well as computational biology and interventional data. In addition, TUM junior scientists will hold a day of research talks.

Summer course on causality

Thomas Richardson from the University of Washington in Seattle will teach doctoral researchers from TUM and CAUSE's external partners for one week on causality.

Workshops

Two workshops will initiate and deepen cooperation with causal inference researchers from other German institutions, including dedicated workshops for junior researchers.

Competitions

CAUSE will organize a data-driven competition on its primary topics. A competition about causal experimental design for biomedical applications is already in preparation.

Double-header seminar

MANDATES: RESEARCH

In light of growing national and international competition, TUM has tasked itself with increasing the number of **large, collaborative research proposals.** MDSI tries to further this goal by promoting joint proposals in data science via the MDSI Seed Funds.

M DSI has taken up the idea of the TUM Seed Fund and transferred it to research fields related to data science. The goal is to promote collaboration between data scientists who are in the process of initiating joint projects. The MDSI Seed Funds aim at boosting such projects by stimulating the identification of common research topics and the production of initial methods for subsequent research or other preparatory work. Ideally, MDSI Seed Funds projects result in the composition of first publications or the acquisition of external funding. Annually, MDSI opens calls for proposals to identify the most promising projects in the field. In the peer review process, critical factors for selecting the best-ranking proposals are interdisciplinarity, originality, feasibility, impact, and subsidiarity.

Achievements

Schaefer, S., Henning, D. F., & Leutenegger, S. (2023, September 19). GloPro: Globally-Consistent Uncertainty-Aware 3D Human Pose Estimation & Tracking in the Wild.

Mitterberger, D., Atanasova, L., Dörfler,
 K., Gramazio, F., & Kohler, M. (2022). Tie a
 knot: human-robot cooperative workflow
 for assembling wooden structures using
 rope joints. Construction Robotics, 6(3-4),
 277–292.

Simon Schaefer @ *¬ IROS'23 conference*.
Collection of real-world human-robot
collaborative construction data with a
human expert (construction operative)
and integrated robot assistant.

 Collaboration "Cooperative Mobile Brickwork", TUM Digital Fabrication and Bauinnung München-Ebersberg
 GNI: SPAICR: Spatial AI for Cooperative Construction Robotics

Atanasova, L., Dörfler, K.: Contribution to Exhibition: "The Great Repair," Academy of the Arts, Berlin

Team

Stefan Leutenegger; Simon Schaefer Machine Learning for Robotics

Kathrin Dörfler, Lidia Atanasova Digital Fabrication

d Funds

In the most recent edition of these seed funds, MDSI promotes MDSI Kickstarter projects initiated by two TUM principal investigators and introduces support for *MDSI Focus Topics* connecting at least five TUM researchers. The latter aims to promote additional high-profile themes as MDSI's key research areas, going beyond project character and aiming to initiate innovative formats with high visibility and a distinct long-term character. The goal of these projects is to establish activities and structures that will continue beyond the end of the MDSI funding, thus creating a lasting impact. So far, MDSI has supported *15 Kickstarter projects*, each spanning a funding period of typically six months. Moreover, two new MDSI Focus Topics have been established via the seed funds.

Selected Kickstarter Projects:

3D Human Motion Capture for Cooperative Construction Robotics – HuMoCap

n many mobile robotics applications, robots must understand and forecast human movement to avoid collisions and work collaboratively. HuMoCap develops 3D human pose and posture estimation algorithms for robots that move themselves, too.

Human-Robot collaboration, e.g. for building construction, is highly challenging as the robots need a precise spatial understanding of their complex environment, must interpret and forecast human poses, deal with heavy occlusions in their field of view, and handle ego-motion. Additionally, the development of algorithms for such robots is impacted by a lack of readily available, contextualized ground truth data required to learn data-driven models.

HuMoCap is developing an in-the-wild human motion capturing system which can cope with these challenges and has a better performance, a significantly reduced reconstruction

intensifying drough

2071 - 2100

In darkest areas drought and frost frequencies rise in unison

Joint probability of a mildly extreme event occurring within three periods for Bavaria. The darker the color, the lower the likelihood of an extreme event.

Drought and late frost risk in a changing climate – ClimVine

ClimVine has developed a tailored vine copula-based regression model to predict forest tree drought and late frost risk. The integrated model enables accurate forecasting of the temporal evolution of future risks based on transient climatic drivers.

Climate change increases the frequency and intensity of droughts and, at the same time, leads to an increased risk of late spring frost. Both climate extremes can influence forest health detrimentally, especially when they occur in close temporal sequence. Unfortunately, the statistical coupling between the two extreme events is not yet understood. Based on a dataset for Bavarian forests covering the last ~70 years, ClimVine has developed a Y-vine copula regression model that efficiently captures heavy tails and asymmetric dependence structures in the data. It incorporates a prediction model that enables the identification of spatial and temporal "at-risk" regions for forest ecosystems across multiple projected climate change trajectories. This work paves the way for expanding the model's spatial scope to larger geometric domains.

error, and is faster and more memory efficient than other state-of-the-art methods. This was successfully implemented in a semi-automated human-robot collaborative workflow for brickwork constructions in a test environment. This test case validated the system's capabilities and provided an opportunity to collect valuable real-world datasets. Leveraging human-pose estimation demonstrates the technology's immense potential in collaborative construction settings.

Achievements

Tepegjozova, M., & Czado, C.
 (2022). Bivariate vine copula based
 regression, bivariate level and quantile
 curves.

 Tepegjozova, M., Meyer, B. F.,
 Rammig, A., Zang, C. S., & Czado,
 C. (2023). Assessing univariate and bivariate risks of late-frost and drought
 using vine copulas: A historical study
 for Bavaria.

Conference participations: Tepegjozova: *¬ ICRA9, 2022, Perugia,* Italy; *¬ CMStatistics, 2022, London, UK.*, Meyer: *¬ EGU General Assembly, 2023, Vienna, Austria.*

 Doctoral thesis M. Tepegjozova:
 "Statistical learning with vine copulas in regression settings," defended July 27, 2023.

Team

Claudia Czado; Marija Tepegjozova Applied Mathematical Statistics

Anja Rammig; Benjamin Meyer *Interactions*

Christian Zang
Forests and Climate Change,
HSWT

Munich Data Science Institute Technical University of Munich

2021-2023

Seed Funds

Achievements

(2022). Fast and precise model calculation for KATRIN using a neural network. The European Physical Journal C, 82(5).

↗ Thesis of C. Karl defended with summa-cum laude distinction (July 8, 2022)

Team

Susanne Mertens: Christian Karl

Debarghya Ghoshdastidar; Pascal Mattia Esser Theoretical Foundations of Artificial Intelligence

Philipp Eller Experimental Physics with Cosmic Particles

Precise and fast model prediction with machine learning – Netrium

Netrium has developed a machine learning-based method to tremendously improve the prediction of tritium model spectra for the *AKATRIN* experiment, which is designed to measure the neutrino mass with unprecedented precision.

limiting factor in this endeavor is the Computation speed of the model spectrum of individual decay events required to simultaneously process multiple data sets with various correlated and uncorrelated systematic uncertainties. The numerical calculations used for the first two KATRIN data releases do not meet this requirement. In the Netrium project, we have developed a novel method based on machine learning that applies a neural network to predict the tritium spectrum as a function of all relevant input parameters. The resulting predictions are highly accurate and reduce the computa-

Comparison between reference Monte Carlo simulation and neural net model fit.

tion time by at least three orders of magnitude compared to the previously published methods. This result can be considered a significant breakthrough in the KATRIN data analysis. The code has already reproduced the first two measurement campaigns; more analyses are underway. It will be applied to all forthcoming neutrino mass analyses and searches for physics beyond the Standard Model with KATRIN data.

"The MDSI always has an open door and has been incredibly supportive, ranging from the realization of large projects to the sharing of their space for seminars and workshops. In addition, their various funding programs offer fast turnaround opportunities for TUM students and scientists." – Philipp Eller

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Members

Enhancing Seismic Safety in Munich's Geothermal Energy Sector: Data-Driven Model **Updating for Building Vibrations under Induced** Seismicity (SeismicSafety)

Gerhard Müller (
 Structural Mechanics) Wolfgang Wall (> Computational Mechanics) 2023

Focus Topics

Causal Inference (CAUSE)

Donna Ankerst (
Biostatistics) Stefan Bauer (Algorithmic Machine Learning & Explainable AI) Niklas Boers (*> Earth System Modelling*) Mathias Drton (
Mathematical Statistics) Jalal Etesami (*¬ Decision Analytics*) Helmut Farbmacher (7 Applied Econometrics) Hanna Hottenrott (
 Economics of Innovation) Niki Kilbertus (7 Ethics in Systems Design and Machine Learning) Fabian Theis (
Mathematical Modelling of **Biological Systems**) 2023

Interdisciplinary Research on Graphs, **Networks, and Connectivity Structures**

(InterConnect) Karen Alim (7 Biological Physics and Morphogenesis Ulrich Bauer (¬ Applied Topology and Geometry) Ulrich Gerland (*¬ Physics of Complex Biosystems*) Stephan Günnemann (7 Data Analytics and Machine Learning) Debarghya Ghoshdastidar (
7 Theoretical Foundations of Artificial Intelligence) Christian Kühn (> Multiscale and Stochastic Dynamics) Nassir Navab (Computer Aided Medical Procedures & Augmented Reality) Bastian Rieck (> AIDOS Lab Helmholtz & Mathematical Modelling of Biological Systems) Daniel Rückert (
Artificial Intelligence in Healthcare and Medicine)

> Munich Data Science Institute Technical University of Munich

2023

MDS Interdisciplinary Exchange

20 JUNE 2023

Graph Neural Networks for Material Science Julija Zavadlav,

Multiscale Modeling of Fluid Materials Stephan Günnemann, Machine Learning

12 JULY 2023

Mass spectrometry, AI, and the dark proteome

lulien Gagneur, Computational Molecular Medicine Mathias Wilhelm, Computational Mass Spectrometry

20 SEPTEMBER 2023

Materials in precision engineering

Alessio Gagliardi, tems for Energy Conversion Nikolaus Adams, Aerodynamics and Fluid Mechanics

The MDSI Interdisciplinary Exchange allows MDSI Core Members to informally build connections across domains, which may later become the foundation for interdisciplinary research projects.

ith MDSI's main mission to bring together researchers across domains and disciplines, the MDSI Interdisciplinary Exchange format realizes just that. Roughly once every six weeks, starting in the summer of 2023, two core members give short presentations on a shared research topic and everyone else is invited to join the informal discussion. The format creates a platform to learn from each other, discuss methodologies that could be of interest across disciplines, and gain a better holistic understanding of common challenges.

TUM RDH TUM Research Data Hub

The 7 TUM RDH is the newly established central point for research data management (RDM) services at TUM. It is coordinated by MDSI and the **>** TUM University Library.

he TUM RDH supports researchers in implementing the TUM RDM regulations and serves as a point of contact and advice for all questions in this area. In addition, the RDH promotes the networking of all researchers in data-intensive fields, creates synergies between different research initiatives, and bundles expertise in data infrastructure and data research.

CONTACTS AND NETWORK

The RDH aims to share the expertise gained in National Research Data Infrastructure (Nationale Forschungsdateninfrastruktur, NFDI) projects and large coordinated programs with the TUM community. In this context, it coordinates the regular "round tables" for NFDI data officers, "tech meetings" for data stewards, and the "expert tables" for interested scientists. RDH aims to exchange ideas and challenges in RDM via these meetings and provide a discussion forum for technical issues in ongoing projects. The goal is to establish a knowledge base and connect researchers from the applied sciences with those from the foundation sciences.

MANDATES: EDUCATION, SERVICE

DATA STEWARDS

Over the next few years, the RDH will establish a pool of data stewards. These data stewards work in individual, large, coordinated programs or NFDI initiatives and will be anchored in the RDH. Data stewards coordinate the RDM activities of a project holistically. They maintain networks within TUM, exchange solutions and accept and convey support. Moreover, they participate in the RDH (training) program. This ensures the development, stemming from the RDH, of a competence network that secures long-term expertise in RDM for the entire TUM.

TRAINING AND CONSULTING

At the application stage, TUM members can contact the RDH to receive consultation for their third-party funding projects. Together with **7** TUM Office for Research and Innovation (TUM Forschungsförderung & Technologietransfer, TUM ForTe), the RDH team pro-

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vides targeted support in developing concepts for data management. Furthermore, the RDH offers all TUM members various courses and lectures on RDM to increase data literacy. The RDH training activities include hands-on training on multiple data analysis techniques, including machine learning methods. In addition, the RDH offers professional data-related services and advice on data publication and licenses, support with legal issues, and procurement of infrastructure.

INFRASTRUCTURE

Based on the **7** Leibniz Supercomputing Centre (LRZ) storage and backup system, the RDH offers the web-based software solutions *¬* mediaTUM for publishing and *¬* TUM
 Workbench as an electronic lab book. Furthermore, it supports users in finding software for research documentation and it cooperates with LRZ to provide adequate computing infrastructure.

> The SuperMUC supercomputer at LRZ

Consultancy and

TUM's partnership in half of all National Research Data Infrastructure (NFDI) consortia enhances the impact of exploiting synergies among participating TUM researchers and data stewards. MDSI connects these initiatives, combines their expertise, and broadcasts it to others.

he NFDI forms a network of consortia to systematically develop and secure data sets as well as make them accessible to scientists. The consortia gather data in a science-driven process according to the FAIR principles (Findable, Accessible, Interoperable, Re-Usable) and provide these to the research community. Over the past few years, 27 NFDI consortia have been initiated, with TUM partnering in 13 of them e.g. the here highlighted National Research Data Infrastructure for Engineering Sciences (**>** NFDI4Ing) and The German Human Genome-Phenome Archive (7 GHGA).

To harness the expertise of its researchers in these consortia and exploit the synergies that arise from the exchange between them, the NFDI data officers participate in the TUM Research Data Hub (RDH) program.

NFDI "ROUND TABLE"

The NFDI consortia's data officers come together in the NFDI Round Table meeting, a NFDI-dedicated format of TUM RDH. These meetings aim to enhance the researchers' knowledge and skills in research data management and broaden their network. The sessions cover various topics, including data management planning, data organization, data sharing, and ethical considerations. In this context, the MDSI premises offer a stimulating environment for exchanging ideas.

GHGAR THE GERMAN HUMAN GENOME-PHENOME ARCHIVE

NFDI4Ing

To make engineering research data FAIR, 7 NFDI4Ing's members have identified typical research profiles – the seven archetypes - which capture commonly recurring needs, methods, and workflows. Across all archetypes, they offer base services, including quality assurance, software development, metadata, storage, data security, training, and data discovery.

TUM coordinates the archetype **7** "Doris," which aims at enabling the exchange of enormous high-quality datasets, provisioning of high performance computing (HPC) data to foster widespread use, and driving new NFDI-wide methodological sharing approaches. "Doris" incorporates finding solutions to challenges related to accessibility and access rights, data security and sovereignty, metadata definitions and terminologies, support to data-generating groups, storage and archiving for very large data, reproducibility on largescale HPC systems, support for third-party users and community-based training, and provision of post-processing algorithms and modules.

GHGA has already reached the first operational phase of its metadata catalog, which contains a collection of existing national resources. It defines a standardized data set library with the GHGA Metadata Model. Soon, GHGA will be able to function as a data archive with streamlined data deposition. Further data products will include the GHGA Atlas offering data analysis and visualization tools as well as the GHGA Cloud representing community-specific data portals.

THE GERMAN HUMAN **GENOME-PHENOME ARCHIVE (GHGA)**

→ GHGA is building a national data infrastructure for human genome-phenome data, which is accessible to researchers but also secure. To achieve this, an ethico-legal framework is in place that guarantees General Data Protection Regulation (GDPR) compliance and development in exchange with and focused on patient needs. As data is extremely hard to find when stored de-centrally, GHGA connects the data and makes them FAIR. As part of this, GHGA is also embedded in the federated **>** European Genome-Phenome Archive.

DNA helices representing GHGA

n matters of professional education, MDSI takes on a coordinating role between its core members, providing the expertise on the training subject, and the TUM IL³, with the experience in developing and structuring these courses. Beyond coordination, MDSI disseminates information about these formats to its network and is also a point of contact for further projects and ideas related to professional education.

The offers are designed as continuing education courses, and participants receive a certificate upon completion. In 2022, two new programs were developed and implemented: "Data Science in political communication" and "Data Science".

The "Data Science in political communication" program introduced data science methods to analyze social media data in political communication to participants with a limited

technical, IT, or mathematical background. For this reason, the program first provided a solid understanding of how data is generated in social media and how it is used with data science methods to understand political communication in digital spheres. Furthermore, it equipped attendees with a basic understanding of how machine learning mechanisms work, utilizing the programming language R. It also delivered hands-on training in social media data network visualization using actual data and data analysis tools. To round it off, the program concluded with an in-depth discussion on the potential of social media to influence and shape current democratic developments. Additionally, the participants had the opportunity to exchange with experts from industry and academia about deploying data science methods to make social media a place for a healthier public conversation and the role of artificial intelligence now and in the future.

In cooperation with **7** TUM Institute for LifeLong Learning (TUM IL³), MDSI designs **learning opportunities** on data-related topics for professional users and other

interest groups

This program, developed under the leadership of MDSI Core Member Yannis Theo*charis*, was first offered at the end of 2022. Parts of the program were also open to *EuroTeQ Engineering University* students. The EuroTeQ initiative, with its members ↗ Technical University of Denmark, Findhoven University of Technology, École Polytechnique, Zech Technical University, **7** Tallinn University of Technology, and TUM, is committed to intra-European cooperation and a shared understanding of European values. As part of the EuroTeQ program, "Data Science in political communication" offered insight into the dynamics of political movements through the lens of social media data.

The "Data Science" certificate program introduced modern computational methods to process and visualize data and communicate data analysis results. This comprehensive program combined the latest research results with findings and challenges from the field. Participants learned about fundamental statistical principles, practical statistical methods, state-of-the-art prediction methods from machine learning, and optimization and randomization tools that help them tackle large-scale data-analytic problems.

Prof. Matthias Scherer and MDSI Core Member Prof. Mathias Drton led the development of this program. Other TUM professors and MDSI members also contributed, including Prof. Claudia Czado, 7 Prof. Blanka Horvath, and Prof. Felix Krahmer. After its successful first presentation in 2022, the program was offered again in the summer of 2023.

MANDATES: RESEARCH, INNOVATION, EDUCATION, OUTREACH

Workshops, competitions, talks, and gatherings:

MDSI hosts and (co-)organizes a wide variety of events to pursue its primary mission: **connecting people**,

ue to the COVID-19 pandemic in 2021 and 2022, events took place partly only online or in hybrid form. While this presented a challenge at the time, MDSI events are now held in-person again, thus facilitating the core mission of MDSI: connecting people, ideas, and knowledge.

Advisory Board Meeting

In its advisory role, the committee meets at least once a year, typically alongside the MDSI General Assembly to discuss research and innovation direction with the MDSI Board of Directors. Its constructive monitoring and recommendations aim at further developing MDSI's agenda of measures for an internationally successful innovation and technology transfer strategy.

General Assembly

The MDSI General Assembly convenes once a year and is an opportunity for MDSI's members to review, discuss, and shape the activities and formats of the institute. Alongside a report on progress and the state of MDSI's activities, the MDSI General Assembly features opportunities for scientific exchange and networking. MDSI Core Members, affiliated doctoral researchers, postdocs, principal investigators from research projects, and selected guests from industry and other research institutions participate.

ideas, and knowledge within academia and beyond.

1ST GENERAL ASSEMBLY

n accordance with the COVID-19 regulations which applied at the time, the event took place in hybrid form on 11 November 2021. Despite these restrictions, the event was a good opportunity for professional exchange, networking, discussion, and interaction, and for those who could be on site, the possibility to visit the premises of MDSI. Prof. Claudia Peus delivered her welcome address virtually, followed by a discussion on National Research Data Infrastructure (NFDI) activities led by Prof. Julien Gagneur and Prof. Christian Stemmer

Networks

Welcome address of Prof. Claudia Peus (above) and discussion workshop (left) at the 1st General Assembly

Highlights of the event included the research talks "Decoding the mysteries of modern machine learning" by Prof. Debarghya Ghoshdastidar, "Neural network potentials trained top-down" by *Prof. Julija Zavadlav*, and "The Robot Co-Builder – Human-in-the-Loop Computational Design and Fabrication" by *Prof. Kathrin Dörfler*. The talks excellently reflected the depth and breadth of expertise at MDSI. Particularly noteworthy was the discussion workshop, in which MDSI's members contributed new ideas for future activities and programs, which were discussed and defined together like the implementation of MDSI Focus Topics.

Events

2ND GENERAL ASSEMBLY

he 2nd MDSI General Assembly was also held at the **7** Science Congress Center at Galileo and the MDSI from 4–5 October 2022. Besides serving as a platform for networking and cross-disciplinary scientific discourse, it was combined with the 1st constituent meeting of the MDSI Advisory *Board*. On both days, the now extended circle of participants (representatives of the advisory board, MDSI Core Members and MDSI Project Members, and MDSI-funded doctoral researchers) was invited to reflect on the MDSI Program and actively shape it with new ideas and contributions. The results of the discussions formed the starting point for further priorities in 2023:

- Upgrading the MDSI Seed Funds program to offer flexible funding for MDSI Focus Topics,
- Creating further networking opportunities for Pls, e.g. in the form of an *Interdisciplin*ary exchange seminar,
- Establishing specific programs for women in data science.

Two research keynote addresses inspired in-depth discussions. Prof. Angela Dai talk's "Learning 3D Priors for Real-world Spatial Perception" and Prof. Lukas Heinrich's talk "Petabytes and Picobarns: Data Science in High Energy Physics" provided insights to stimulate conversation and emphasized the need for increased interdisciplinary exchange. The Guided Mingling – an activity designed to build connections based on shared research interests – offered a first start to this and laid the foundation for identifying the abovementioned priorities for 2023.

above: Group photo at the 2nd General Assembly

left: Guided Mingling at the 2nd General Assembly

ince the COVID-19 pandemic severely restricted in-person events, MDSI postponed its opening ceremony until September 2023. The ceremony could then take place in person and brought together MDSI Core Members and associated researchers and partners from science, industry, politics, and the public. Attended by the Bavarian State Minister for Science and the Arts,

Markus Blume, the President of TUM, and high-ranking representatives from science and industry, as well as international guests, the event highlighted ongoing research and connected both the scientific community and representatives from the industry and society as a starting point for in-depth discussions.

Outstanding contributions by MDSI Core Members included two keynote talks; the first by Prof. Elisa Resconi on "Artificial Intelligence and Fundamental Sciences," drawing onto her group's latest, prize-winning findings related to the use of artificial intelligence (AI) in physics. The second keynote, by Prof. Enkelejda Kasneci on "Generative AI: New Challenges for Education," debated the opportunities and challenges linked to the use of AI in education. After these talks, the panel discussion on "Finding the Right Balance in Data Science and AI: Regulation vs. Innovation" examined the benefits and risks of AI. The discussion profited from the expertise of the panelists: alongside TUM vice president Dr. Jeanne Rubner, who moderated the discussion, participants included TUM student representative Cristina Cipriani, Prof. Gjergji Kasneci (TUM),

MDSI OPENING CEREMONY AND 3RD GENERAL ASSEMBLY

MDSI Opening ceremony with the **Bavarian State Minister for Science** and the Arts, Markus Blume, and TUM president, Prof. Thomas Hofmann

Events

Dr. Gianluca Misuraca (7 Universidad Politécnica de Madrid), who acted as a consultant for the European Union (EU) on this topic, Dr. Iulia Pasov (*¬ Sixt*), and Prof. Julia Schnabel (*¬ Helmholtz Munich* & TUM).

Aside from the speeches by TUM president Prof. Thomas Hofmann and the Bavarian State Minister for Science and the Arts Markus Blume, highlights included presenting some of MDSI's research and collaboration projects. Two companies, **7** Amazon and Henkel, presented their TUM-DI-LAB projects, providing a glimpse into the project results and the role of different research fields within the company. Furthermore, Dr. Schafferhans-Fuhrmann introduced the Konrad Zuse School relAI and Prof. Daniel Cremers the Munich Center for Machine Learning (MCML). Finally, the MDSI Best Paper Award was presented on this day.

Panel discussion at the MDSI Opening Ceremony

Poster session at the MDSI Opening Ceremony

MISCELLANEOUS EVENTS: SELECTION

part from those mentioned above, MDSI (co-)organized various other in-person and virtual events including small meetings of research groups discussing shared problems or events offering opportunities to forge new connections across TUM and beyond. The meeting space at MDSI, including the lounge and meeting rooms, proved conducive to discussion and exchange.

Among the events organized and hosted by MDSI in 2022 was a **teacher training on "Artificial Intelligence and Autonomous Driving**" as part of the EU-funded project "Introducing Artificial Intelligence to Vocational Schools in Europe." It took place at MDSI and was led by doctoral researchers Leon Hetzel (TUM), Arne Nix (7 University of *Tübingen*) and Nicolas Berberich (TUM). After theoretical and practical introductions to the basics, history, and algorithms of artificial intelligence (AI) and autonomous driving, the highlight of the course was programming mobile robots.

Furthermore, the keynote lectures by the Buy-Side Quant of the Year Award winners Alex Lipton (7 Hebrew University & 7 Abu Dhabi Investment Authority) and Marcos Lopez de Prado (7 Cornell University & Abu Dhabi Investment Authority) were also co-organized by MDSI. They addressed "Blockchain and distributed ledgers" and "Escaping the Sisyphean Trap: How **Quants Can Achieve Their Full Potential,**" respectively. A simultaneous live stream of the two talks generated interest beyond the TUM community. In addition to the keynotes, various events took place at TUM, including discussions on future cooperation possibilities.

In 2023, the Bavarian **7** Jugend forscht section approached MDSI to prepare the winners of the Bavarian contest for the national competition. "Bahn-Vorhersage," the project which won in the mathematics & informatics category of the Bavarian contest, used existing data (over 400TB of datapoints) to evaluate and predict the reliability of trains through machine learning. MDSI Core Member Prof. Rolf Moeckel offered additional expertise to polish the project for the final contest.

and Autonomous

hile the personnel composition in MDSI-related TUM departments reflects the typical historic structural imbalances, several programs and activities aim to change this. TUM has especially considered gender aspects when filling positions over the past decade, and in the MDSI context, many of the recently appointed core members are women. Parity is also very carefully taken into account in awarding prizes (e.g. MDSI Best Paper Award) and funding (MDSI Seed Funds). The selection committees have equal representation or observe balanced funding quotas. Furthermore, MDSI promotes diversity in its programs for doctoral researchers.

The Linde/MDSI Master's Scholarship and the Linde/MDSI Doctoral Fellowship Programs are dedicated to female students. With the master's scholarship, *7 Linde* and MDSI are pursuing the advancement of women in two

study programs in which women are still strongly underrepresented. So far, 20 students have profited from the funding in the past five semesters. Out of these, 14 students were women. This corresponds to 2.5 times more female students in Linde & MDSI's scholarship program than in the

TUM fosters a university culture of appreciation, openness, and diversity by taking a holistic approach to implementing its gender and diversity strategy. MDSI adheres to this approach and adapts it to match the specific needs of its community.

corresponding study programs. In the Linde/MDSI Doctoral *Fellowship Program*, 60% of the 15 beneficiaries are female. This number can be compared with the fact that only 36% of all doctoral researchers at TUM are women. Thus, the candidate selection process in both programs efficiently ensures that predominately talented female applicants receive the Linde/MDSI support to help them flourish and thrive. With a substantial number of female students present, the programs strengthen not only the participation of women in these fields but also increase their visibility and impact.

Similarly aimed at master's students and doctoral researchers, the Konrad Zuse School relAI focuses on diversity alongside excellence to bring diverging perspectives into the discussion and development of reliable artificial intelligence. The program focuses on integrating culturally diverse perspectives to highlight current challenges resulting from the societal status quo. 55% and 65% of its doctoral researchers and master's students, respectively, do

not originate from Germany. Thus, it effectively works to stop transferring current social inadequacies into technology.

Moreover, MDSI's programs also pay attention to internationality. More than half (53%) of all *Linde/MDSI Doctoral Fellows* are internationals, while at TUM less than 40% of the doctoral researchers are not German. For the master's students in the *Linde/MDSI Programs* the fraction is even higher: 91% come from abroad, compared to a fraction of 78% in the two related TUM study programs.

Based on the feedback collected at 2nd MDSI General Assembly in 2022 and the WiDS Munich conference, further programs for women in data science, such as mentoring, training, and informal network meetings, are being discussed. As key underrepresented contributors in this field, participants in these discussions are interested in connecting with other women in similar positions and sharing their experiences. MDSI is looking to organize programs independently or jointly with other stakeholders.

MUNICH

Guests and participants at the WiDS Munich Conference

From discussions with MDSI Core Members and junior scientists during the 2nd MDSI General Assembly, an initiative to develop specific, career-supporting activities and programs for women in data science emerged. The starting point was the ↗ Women in Data Science (WiDS) Munich conference held on June 19, 2023, organized by **7** Business, Economic, and Related Data (BERD)@NFDI, 7 Ludwig-Maximilians-Universität München (LMU), **>** SIXT SE, **>** TUM Think Tank, and MDSI, which invited academics and members of the industry and public to network and consider female perspectives in data science. The WiDS brand links to the annual **7** Global WiDS Conference held at **>** Stanford University and an estimated 150+ locations worldwide. Open to all genders, WiDS regional events feature outstanding women doing outstanding work. The WiDS Munich conference was a major success: the event was booked almost two weeks before the date. The event also received notable industry and political interest.

MDSI maintains a strong network in data science, machine learning (ML), and artificial intelligence (AI). Utilizing this network, the institute interfaces with local, regional, national, and international projects, initiatives, and partners.

Stronger

Before the foundation of MDSI, many productive but unconnected activities related to data science were conducted at TUM. Now, MDSI, as TUM's central hub for data science, implements a reciprocal docking mechanism to facilitate exchange between such initiatives. Several institutes and initiatives, including the Center for Digital Medicine and Health (ZDMG), the Future Lab "Artificial Intelligence for Earth Observation" (AI4EO), the Munich Center for Machine Learning (MCML), the European Laboratory for Learning and Intelligent Systems (ELLIS)

Munich, the National Research Data Infrastructure (NFDI) and the Georg Nemetschek Institute (GNI), are and will be docked to MDSI in this way.

Others profit from MDSI's networking and further initiatives like NFDI consortia, and other large, coordinated programs with TUM participation. Various of MDSI's services are also offered via TUM Research Data Hub (RDH). Furthermore, MDSI collaborates with various partners project-based, e.g. via relAI with universities, research institutions, and companies.

Additionally, MDSI works closely with the ↗ Al agency baiosphere to strengthen Bavarian networks in Al-related fields and accelerate innovation in Bavaria.

Two of the most significant challenges of our time are the provision of medical care in an effective, efficient, and equitable way, and the prevention of diseases. Digitalization and the powerful use of data through innovative technologies from data science and artificial intelligence (AI) offer an outstanding opportunity to meet these challenges. The use of AI can lead to new and improved diagnostic, therapeutic, and preventive approaches that can be optimally adapted to individual patients. This not only brings significant benefits for patients but also enables improvements in healthcare as a whole.

Utilizing large amounts of data via artificial intelligence (AI) technologies offers enormous potential for revolutionizing the health sector. The ZDMG at TUM will integrate several fundamental and applied fields to tackle this challenge.

> The new > ZDMG, which will be established as part of the MDSI, pursues the ambitious goal of developing new and ground-breaking approaches in data science, AI, and machine learning and promoting their translation into medicine for the tangible benefit of patients. The integrative meshing of computer science, mathematics, and medicine in one research center visible at the highest global level has been lacking so far. It will now be established at the scientific location Munich.

Prof. Daniel Rückert, director of ZDMG.

AIEG Future Lab Artificial Intelligence for Earth Observation

AI4EO brings together 46 renowned international organizations in
20 countries and 70 scientists at all levels in Munich via guest professorships and visiting fellowships to research three fundamental yet rarely
addressed challenges in Earth observation-specific AI research:
reasoning, uncertainty, and ethics.

REASONING

Current AI4EO mostly focuses on perception and the direct recognition of materials, objects, and phenomena, or on measuring geo-physical parameters. Reasoning goes beyond recognition towards induction, deduction, spatial and temporal reasoning, and structural inference, which will lead to the evolution of a new generation of AI4EO.

UNCERTAINTY

Earth observation applications target retrieving physical or bio-chemical variables on a large scale. These predicted physical quantities are often used in data assimilation and in decision making, for example, to reach the *Inited Nations Sustainable Development Goals*. Therefore, besides high accuracy, traceability, and reproducibility of results, quantifying the uncertainty of these predictions from an artificial intelligence algorithm is indispensable towards a high-quality and reliable AI4EO research.

ETHICS

Ethical implications may arise at different stages of AI4EO research. Building a responsible AI4EO that embodies social norms and values while ensuring sustainable and inclusive development is of central relevance. AI4EO addresses issues of data protection/ privacy, data portability, and fairness/equality at the level not just of data collection, but also at the level of data use and dissemination within the sphere of ethics in AI4EO.

The future lab offers up to 12 guest professorships of 18 to 36 months to established researchers and up to 70 further fellowships to early career researchers for a paid research stay in Munich for a time period of three to six months.

The research carried out in the AI4EO aims at not only advancing Earth observation science but also making key contributions for the interpretability of artificial intelligence and its ethical implications, and towards AI4EO technology transfer. It consolidates the core position of Germany in AI4EO.

Munich Center for Machine Learning

↗ MCML advances the field of machine learning (ML) through cutting-edge research and innovation. It fosters interdisciplinary collaborations between researchers, industry experts, and policymakers, and strives to educate the next generation of ML experts.

> CML is one of the six **7** German Centres of Excellence for AI Research selected in a competitive process and permanently funded by the national and Bavarian government. As a joint initiative between TUM and *¬ Ludwig-Maximilians-*Universität München (LMU), MCML explores the potential of ML across diverse domains in collaboration with top experts. Known for its focus on theoretical and applied research, MCML develops innovative methodologies and collaborates with industry partners to address real-world challenges, bridging academia and industry for the advancement of artificial intelligence (AI).

Thematic Setting

Natural Language Processing **Multimodal Perception**

The institutional funding for MCML started on 1 July 2022; a kick-off event for the center was held on 27 July 2022 and included talks by all four directors and keynotes from MCML principal investigators and key players from the industry. Representatives from LMU, TUM, the Bavarian government, and the **7** Federal Ministry of Education and Research (BMBF) also gave short talks. Together with further initiatives, MCML organizes the Munich AI Lectures Series and worked with the A Leibniz Supercomputing Centre (LRZ) to set up a GPU cluster. Furthermore, in 2023, MCML launched the following programs for recruiting and training talent: Ph.D. Matchmaking, the Junior Research Groups in Machine Learning, the Junior Research Group in Ethics, and the Thomas Bayes Fellowship.

In the first six months of its institutional funding, twentyeight new PIs from LMU and TUM joined MCML together with ca. 100 new doctoral researchers. MCML members published 125 articles, 80 of which were on high-profile outlets. Additionally, over 100 MCML members presented at conferences during these months. Moreover, MCML built up its ML consulting, open-source and open-data programs as well as entrepreneurship training.

Meeting of MCML members at MDSI

¬ ELLIS Munich is a unit within the ¬ ELLIS network, the European Laboratory for Learning and Intelligent Systems, integrating expertise from TUM, the 7 Helmholtz Munich, and collaborating partners. ELLIS Munich scientists engage in artificial intelligence (AI) explicability and develop reliable, intelligent machine learning (ML) algorithms in a communal environment.

ELLIS Munich, along with six partners in Germany, was successful in receiving funding for the **7** Konrad Zuse School of Excellence in Learning and Intelligent Systems (ELIZA), a graduate training program in the field of AI funded by the research and training activities focus on four main areas: the basics of ML (including ML-driven fields like computer vision, natural language processing, or robot learning), ML systems, applications in autonomous systems, as well as transdisciplinary applications for ML in other scientific fields, from life sciences to physics.

Networks

Munich Unit

LLIS Munich contributes to the ELLIS Society programs on computer vision, health, earth & climate, natural language processing, and semantic, symbolic & interpretable ML. The unit also focuses on developing novel ML methods and deploying them in biomedicine, computer vision, and Earth observation.

Between 2022 and 2023, ELLIS Munich added new members and planned several networking events in Munich, including a lunch at the inaugural **AI.BAY** conference, sponsored by the Bavarian government in February 2023. ELLIS Munich members participated in the European-wide Ph.D. Matchmaking calls, which attracted over 1,000 interested students.

National Research Data Infrastructure

∧ NFDI represents a strategic initiative of the ∧ German Research Foundation (DFG) to establish a sustainable and interconnected infrastructure for managing and sharing research data across various disciplines.

The initiative promotes the adoption of interoperable data he primary mission of NFDI is to address challenges associated with the rapidly increasing volume, complexity, standards and protocols to enable seamless data exchange and diversity of research data. By providing the necessary and integration foremost within and across different discitools, services, and standards, the initiative supports not only plines and research communities. This facilitates data sharing, reusability, and collaboration while ensuring data interoperadata management but also curation and accessibility, consistently following the FAIR (Findable, Accessible, Interoperable, bility, metadata consistency, and the individual's privacy and Reusable) principles. (Interoperability and Standards).

NFDI is a collaborative effort involving 26 consortia repre-Another aspect is the development of training programs and educational resources to enhance researchers' skills and senting a wide range of scientific disciplines and over 250 research institutions across Germany. TUM is engaged knowledge in RDM. Training opportunities include workshops, and participates in 13 of these consortia. Each consortium courses, and resources on data management planning, focuses on a specific field of research and contributes to ethics, privacy, analysis techniques, and FAIR principles the overall development and implementation of the NFDI. (Training and Education).

By fostering interdisciplinary collaboration and driving inn-Finally, NFDI plays a role in the establishment of a govervation in various domains of scientific research, NFDI plays a nance structure involving various stakeholders, including crucial role in facilitating data-intensive research, supporting researchers, institutions, reproducibility and reusability, and maximizing the value of funding agencies, and data research data for the scientific community and society. infrastructure providers.

NFDI envisions long-term sustainability, funding, and **NFDI HAS FIVE MAIN OBJECTIVES:** coordination of the research It aims at developing and promoting best practices for data infrastructure and proresearch data management (RDM) throughout the data lifecymotes collaborative decicle. This includes data planning, documentation, organization, sion-making and strategic storage, and preservation to ensure long-term usability and planning (**Governance** reproducibility of research data (**Data Management**). and Sustainability).

In addition, it provides a comprehensive suite of services, tools, and workflows for data collection, analysis, visualization, and shares these with the scientific community via data repositories, portals, analysis platforms, and collaboration tools to facilitate interdisciplinary research and data integration (Data Services and Tools).

List of NFDIs with TUM involvement

	Consortium	TUM Participants
		Klaus Mayer
	GHGA	<i>Julien Gagneur</i> , Thomas Meitinger, Juliane Winkelmann
	→ NFDI4Cat	Johannes Lercher
	NFDI4Ing	Christian Stemmer
		Wiebke Lohstroh
	→ FAIRmat	Hans-Joachim Bungartz
		Mathias Drton
		Martin Werner
	↗ NFDI4Microbiota	llias Lagkouvardos, Michael Schloter
	↗ PUNCH4NFDi	Lukas Heinrich, Allen Caldwell
_	→ FAIRagro	Senthold Asseng
A	↗ NFDI4Immuno	Dietmar Zehn
	↗ NFDIxCS	Tobias Nipkow, Martin Schulz

TUM Georg Nemetschek Institute Artificial Intelligence for the Built World

7 TUM GNI is a flagship institute for research, teaching, and knowledge transfer related to artificial intelligence (AI) in the built world. It focuses on developing AI applications in areas including architecture, engineering, construction, and asset management (AECOM).

cological and economically sustainable solutions for the built environment are part of the grand societal challenges. Conceiving, designing, and sustaining the built environment will profit immensely from the latest modern computer technologies, AI, and machine learning (ML) techniques. TUM GNI develops and promotes a new generation of such technologies with strategic importance for general digital sciences, particularly AECOM industries. A byproduct of this will be additional contributions to challenges in research on environment, climate, information and communications, mobility, and non-AECOM infrastructure.

Research activities of the GNI revolve around the overarching concept of the trustworthiness of AI methods for engineering in the built world. Key research areas include intelligent interfaces, design explainability, probabilistic digital twins, and generative design for early stages. TUM GNI also awards and manages interdisciplinary projects among other TUM research groups in the built world and more fundamental domains such as mathematics and computer science. In addition to innovative research, TUM GNI contributes to the education of AI-literate built-world engineers who will lead the industry to meet future strategic challenges.

Members

Tobias Nipkow, Martin Schulz

TUM GNI POSTDOC PROGRAM

In 2021, TUM GNI initiated a support program for young postdoctoral researchers with significant experience in TUM GNIrelated research fields. The program aims to provide highly qualified scientists the opportunity to establish their research with a focus on scientific core questions on data science and ML within the interdisciplinary research field of TUM GNI. The postdocs receive funding for up to three years plus an annual research budget as part of the program. Thus, the program benefits the participants and helps to strengthen TUM GNI's scientific development, external impact, and visibility.

Welcome

This section is dedicated to the MDSI Core Members. It aims to present a selection of their research interests, research highlights and main achievements.

The MDSI Core Members play a key role for MDSI. They shape the institute with their engagement and by proposing initiatives to the MDSI Board of Directors for discussion and possible implementation, thus actively contributing to its profile.

The number of members has been growing steadily since 2021 – and with it the expertise, programs and activities of the MDSI.

MDSI's faces

Overview of all MDSI Core Members

Nora Brambilla **Theoretical Particle and Nuclear Physics**

Renormalization; confinement; non-perturbative calculations; computational QFT; lattice QCD

APS Fellow, 2012; Vice-President Marie Curie Assoc., 2002-5; Humboldt Fellow, 1997, 2002-3; Marie Curie Fellow, 1998-99

Angela Dai

3D scene acquisition & reconstruction; 3D-deep learning

ACM SIGGRAPH Diss. Award, 2019; ZDB Jun. Research Group, 2019+; M.J. Flynn Fellow, Stanford, 2013-18; Certificate Prize, Princeton, 2013; Google A. Borg Memo-rial Scholar, 2012-13

Allen Caldwell Zerimental Particles, MPP

Distinguished Alumnus, U Wisconsin, 2012; Hon. Prof. TUM, 2006; Fellow APS, 2000; Humboldt Fellow, 1995-97

Thematic Setting

Structure and Strategy

Fundamental building blocks of matter; particle accelerator technologies; fundamental properties of neutrinos

Ulrich Bauer Applied and Computational Topology

Connectivity of data; topological data analysis; persistent homology; discrete Morse theory

ATMCS Best New Software Award, 2016; Apple Design Award, 2003; O'Reilly Mac OS X Innovators Award, 2003

Kathrin Dörfler **7 Digital Fabrication**

Digital design & construction robotics; mobile robotics in architecture; augmented reality

ICRA Best Automation Paper Award, 2018; Concrete Innovation Award, 2017; Swiss Technology Award, 2016; archdipl.'13, TU Vienna, 2013

Nikolaus Adams Aerodynamics and Fluid Mechanics

Transitional & turbulent flows; unsteady flow-structure interaction; microfluidics; high-speed aerodynamics

Hon. Prof. Tsinghua U, 2019; ERC Adv. Grant, 2015 & 2023; Fellow Am. Phys. Soc., 2011

Angela Casini Medicinal and Bioinorganic Chemistry

Anticancer metallodrugs; supramolecular complexes for imaging and therapy; Theranostics design

Member European Academy of Science; ACS Inorganic Lectureship award, 2019; European Medal for Biol. Inorganic Chemistry, 2012

Donna Ankerst Biostatistics

Clinical risk prediction; deep learning; models for climate change impacts on forest & health

Editor, Biometrics Book Reviews; Ph.D. Supervisor Award, 2018; Prostate Cancer Dream Challenge winner 2015; NSF Math. Sciences Fellowship, 1997-2000

Daniel Cremers Computer Vision and AI

Pattern recognition; ML & deep networks; autonomous systems; PDEs; statistical inference; convex & combinatorial optimization

Leibniz-Prize, 2016; ERC Grants, 2014, 2009; UCLA Chancellor's Award Postdoc Research, 2005; Olympus Prize, 2004

Martin Boeker

Digitalization in health care; med. information models & semantic data integration; med. terminologies; machine processing

Game-based e-learning..., 2013, PloS one 8 (12), e82328; Google Scholar..., 2013, BMC med. res. method. 13 (1), 1-12

David Egger Theory of Functional Energy Materials

Materials science; Electronicstructure theory; Molecular dynamics; ML

Sofja-Kovalevskaja Award, Humboldt Foundation, 2017; Best Thesis Award, TU Graz, 2015; Koshland Prize, Weizmann Institute of Science, 2014

Pramod Bhatotia Decentralized Systems Engineering

Software systems; distributed systems; compilers; data analytics systems

ERC Starting Grant, 2022; AvH H. Herz-Scout Award, 2021; Turing Fellow, 2017-2021; Microsoft Azure Research Award, 2017

Mathias Drton Mathematical Statistics

Graphical models; analysis of complex multivariate data; algebraic statistics; causal inference

ERC Adv. Grant, 2020; Ethel Neubold Prize, Bernoulli Society, 2019; Member RDASL, 2018; Medallion Lecture, IMS, 2014; Sloan Research Fellow, 2009

Stefan Bauer

Data science & intelligent systems; causal representation learning; robust & transformative Al-based technologies

CIFAR Azrieli Fellowship, 2020; Best paper ICML, 2019; ETH medal for outstanding doctoral thesis, 2018

Multivariate statistical inference; vine copulas; copula-based state space and regression models

Fulbright Travel Grant, 2001; MSI Fellow, Cornell University, 1986-87; GSS Fellow, Cornell University, 1987/88; GE Fellow, U Göttingen / Cornell U, 1982-83

André Borrmann Computational Modeling and Simulation

3D/4D building information / infrastructure modeling; computer-aided life cycle management; simulation of construction processes & pedestrian flows

Best Paper Awards, 2009, 2013, 2014, 2016, 2018

Massimo Fornasier Applied Numerical Analysis

Image & signal processing; PDEs; optimization; nonlinear & numerical analysis; thin structures, sparsity & compression

ERC Grant, 2012; Biennial Prize SIMAI, 2012; FWF START, 2011; Best Paper, AAS, 2010; Prix de Boelpaepe, RAB, 2009

Munich Data Science Institute Technical University of Munich

2021-2023

David Franklin Neuromuscular Diagnostics

Neuromuscular control, sensorimotor adaptation, computational neuroscience, human-robot interaction

Best Paper, WeRob Conf., 2018; Wellcome Trust Fellow, 2010; Gold Medal, Governor General of Canada, 2005

Sandra Hirche Information-oriented Control

Control engineering & system theory; ML for dynamical systems and control; robotics; human-machine interaction

Fellow IEEE; ERC Cons. Grant, 2020 & Start. Grant, 2014; IEEE Biomed. Eng. Best Paper, 2022 & CDC Outstanding Paper, 2018

Stephan Günnemann Data Analytics and ML

ML reliability; temporal & dynamic data; robust & adversarial ML; uncertainty estimation; GNN

Heinz Maier-Leibnitz Medal, TUM, 2022; Google Faculty Research Award, 2020; Best Paper SIGKDD, 2018; Junior Fellow GI, 2017; DFG Emmy Noether, 2015

Stefanie Klug

Epidemiology; health services research; chronic diseases prevention; HPV infections

Exp. Committee Early Cancer Detection, 2017+; NaKo, 2014+; STIKO, 2011-20; Award Stiftung Präventive Pädiatrie, 2009; Bavarian Public Health Lion, 1999

Alessio Gagliardi for Energy Conversion

Organic semiconductors; electrochem. systems; deep learning in materials science; atomistic modeling & quantum transport

IEEE Member; Member Exc. Cluster NIM & e-conversion; NanoGe 18, Torremolinos, 2018

Hanna Hottenrott *¬* **Economics of Innovation**

Innovation & science policy; economic effects of technological change; industrial economics; applied econometrics

TUM Excellence in Teaching Award, 2022; TUM SoM Supervisory Award, 2018; FWO Fellowship Award, 2010

Reinhard Heckel ↗ Machine Learning

Inverse problems; deep learning; active learning; DNA data storage

Capital 40 under 40, 2022; Honor Werner-von-Siemens-Ring foundation, 2022; BBC "The genius behind: ...," 2015; ETHZ dissertation medal, 2015; IBM invention achievement award, 2015

Thomas H. Kolbe **7** Geoinformatics

Virtual 3D/4D city & landscape models; GIS; urban digital twins & smart cities; 3D geodatabases; indoor navigation

Chairman Runder Tisch GIS, 2013+; Founding member TUM LOC; (Vice) President DGPF, 2008-16; Award "Germany -Land of Ideas", 2016

Julien Gagneur Computational Molecular Medicine

Gene regulation; genetic disorders; statistical algorithms & ML; transcriptomics & proteomics

GHGA, Steering committee, 2020+; Model repository Kipoi founder 2019+; Journal reviewer Nature, PLoS, Science

Dimitrios Karampinos Zerimental Magnetic Resonance Imaging

MRI & biomarkers; image reconstruction; disease pathophysiology

TUM Supervisory Award, 2020; 22 ISMRM Merit Awards, 2014-20; ERC Grants, 2015, 2019; ISMRM Junior Fellow, 2011

Debarghya Ghoshdastidar Theoretical Foundations of AI

Statistical learning theory; network science; ML for graphs; Non-parametric methods for learning

Baden-Wuerttemberg Postdocs Elite Program, 2017; Google Ph.D. Fellowship, 2013

Lukas Heinrich ↗ Data Science in Physics

Simulation-based inference; differentiable & probabilistic programming; ML for science; large-scale statistical modeling

Coordinator ORIGINS Data Science Laboratory; CERN Fellow (ATLAS Experiment) 2018-21

Enkelejda Kasneci Human-Centered Technologies for Learning

Human-centered AI & technologies; AI for education; humancomputer interaction

Core Member Cyber Valley, 2020+; Junior Fellow GI, 2016+; Margarete-von-Wrangell Fellow 2014+, Fed. Südwestmetall Award, 2014

Felix Krahmer Optimization and Data Analysis

Signal & image processing; randomized meas. methods; dimension reduction; compressed sensing; analog-to-digital conversion

ISAM Award, 2018; Emmy-Noether, 2014+; C. Newman Fellow, 2008-09; C. Morawetz Fellow, 2004-09; H. Grad Prize, 2008

Members

Simon Hegelich Political Data Science

Political relevance of digitalization; ML, data mining, computer vision, simulations in pol. science

"Zukunft menschlich gestalten" (FoKoS), Siegen, 2011-16; GraSP, Münster, 2005-11; Facebook needs to share more with researchers. Nature, 2020

Phaedon-Stelios Koutsourelakis Data-driven Materials Modeling

Uncertainty quantification; stochastic aspects in mechanics systems; multiscale phenomena

ZiF Fellow, 2016; Teaching Trophy, MSE, 2014/15/16; Dean's Prize, Princeton, 1998; Performance Prize, NTU Athens 1994/97/98

Jana Giceva

Data management; computer systems; hardware/software co-design

SIGMOD Research Highlight, 2023; Paper Award VLDB, 2022; Paper Award SIGMOD, 2021; VMware Early Career Faculty, 2019; ETH Diss. Medal, 2018, Google Ph.D. Fellowship 2014

Andreas Herkersdorf ↗ Integrated Systems

Multi-core processors; FPGA platforms; MPSoC architectures; innovative hardware IP building blocks; SoC design; autonomic computing

IBM Technical & Innovation Achievement Awards, 5x 1996-2003; IBM Master Inventor, 1998

Gjergji Kasneci Responsible Data Science

Transparency, robustness & fairness in ML; responsible AI & data science; explainable, robust & scalable Al

Hon. Prof. U Tübingen, 2019; Seoul Test of Time Award, 2018; IoC Prof., U Tübingen, 2018-23; Core Member Cyber Valley

Contact

Christian Kühn Multiscale and Stochastic **Dynamics**

Differential equations; uncertainties; adaptive networks; patterns, bifurcations & scaling laws

R.-von-Mises Prize, 2017; Lichtenberg Prof., 2016; Best Paper Award, 2014; Leibniz Fellow, 2013; APART-Fellow, 2012

Bernhard Küster Proteomics and Bioanalytics

Precision medicine; molecular mechanisms in cancer; effects of therapeutic drugs

Distinguished Achievement in Proteomics Sciences Award, 2015/23; Member of Leopoldina, 2021; C. von Linde Fellow, 2018; H. Maier-Leibnitz Medal, 2014

Jürgen Pfeffer Computational Social Science and Big Data

Dynamic socio-technical systems; negative dynamics from social media; political & economic systems

Journal editor: Frontiers BD, JSS, EPJ Data Science, Connections; Committees: ASONAM, Complex Networks, IC2S2, ICWSM

Stefan Minner In Logistics & Supply Chain Mgmt

Logistics networks; inventory management; transportation & urban logistics; logistics planning

Editor in Chief, International Journal of Production Economics; Wirtschaftswoche: Top 1% BA, 2020; Winner M&SOM Comp., 2019; Fellow ISIR, 2016

Gerhard Rigoll → Human-Machine-**Communication**

Audiovisual information processing; handwriting, gesture, emotion, face recognition; object tracking; interact. graph. systems

IEEE Life Fellow 2023; Fellow Asia-Pacific Artificial Intelligence Assoc., 2021; DAGM-Award, 2000; Heisenberg-Stipend, DFG, 1993

Stefan Leutenegger

Mobile robotics; robot navigation; sensor data processing, ML & deep learning

ICL President's Award, 2018; Nominee SACA, 2018-20, Best Paper Hon. Mention CVPR, 2018; Best Paper ECCV, 2016; ETH Medal for doctoral thesis, 2015

Franz Pfeiffer *¬ Biomedical Physics*

Biomedical imaging; tomography; X-ray & neutron optics; microscopy; synchrotron instrumentation

Alfred-Breit-Prize, 2017; ERC Grant, 2009/16; Gottfried Wilhelm Leibniz Prize, 2011; Röntgen-Prize, U Giessen, 2010, National Latsis Prize, 2009

Rolf Moeckel 7 Travel Behavior

Agent-based transport modeling; survey methods; travel behavior analysis

Harter Rupert Paper Award, 2021; Teaching Award, 2019; Scholarship TRB Rising Star Workshop, 2016; Doct. Prize, 2007; Fulbright Scholarship, 2000

Daniel Rückert AI in Healthcare and Medicine

Innovative image acquisition / analysis / interpretation algorithms; computer-aided diagnosis

A. von Humboldt Prof., 2020; ERC Synergy Grant 2013, ERC Advanced Grant 2019, Member, Leopoldina, 2023; IEEE Fellow, 2015;

Daniel Link Performance Analysis and Sports Informatics

Performance & data analytics in sports; sports software engineering; training science

Head of Sports Informatics & Engineering dvs; General Secretary IACSS; former member Expert Group Football dvs

Daniel Pittich 7 Educational Sciences

Competencies & dev. in tech. domains, teaching & learning in digitally-enriched envir., learning analytics & adaptive learning.

Ed. JOTED – Journal of Tech. Education, Steering Committee Kompetenzzentren lernen:digital; DiF German Rectors' Conference

Quantitative molecular imaging & AI in radiology; ECM & immuno-imaging; quantitative biomarkers in radiology

Marie-Curie-Ring, 2018; Heisenberg Prof., Charité, 2016-20; Wilhelm-Conrad-Röntgen-Award, 2013

Matthias Niessner Visual Computing

3D vision & reconstruction; 3D environments; neural rendering & scene representations

ERC Grant, 2018; NVidia Prof. Award, 2018; Google Faculty Award, 2018; SIGGRAPH'16: Best Emerging Tech., 2016; MPC-VCC Fellowship, 2013

Chris-Carolin Schön

Breeding process optimization; molecular markers in crop breeding; native biodiversity

Member Acatech, Bavarian Academy of Sciences, Leopoldina; Bavarian Order of Mer-it, 2018; Max-Schönleutner Medal, 2016; Heinz-Maier-Leibnitz Medal, 2009

Robot-guided surgery; ML & computer vision in medical applications

Akademia Europaea, 2022; En-during Impact, MICCAI, 2021; IEEE Fellow, 2022; Lasting Impact, IEEE ISMAR, 2015; Guest Prof. Award, BRF, 2017-20

Maximilian Schiffer Intelligent Systems

Transport & logistics; autonomous systems control; production planning

INFORMS TSL Dissertation Prize, 2018; Friedrich-Wilhelm-Award, 2018; GOR Diss. Prize, 2018; Borcher's Badge, 2018

Oleksandra Poquet Zeria Educational Sciences

Educational technology; data analysis from educational environments; AI in education

Centre for Change and Complexity in Learning, U South Australia; Executive Committee SoLAR, 2017-21; "Networks in Learning Analytics", JLA, 9:1, 2022

Liqiu Meng

Cartography & Visual Analytics

Visual analytics & cartography; geodata integration; visual data mining; navigation services

Vice President ICA; Leopoldina, 2011+; BAW, 2013+; Carus Medal & Prize, 2011; Helmholtz Senator, 2009-12; SVP TUM, 2008-14; Heinz Maier-Leibnitz Medal, 2007

Neutrinos; oscillation experiments; astron. data combination

Heinz Maier-Leibnitz Medal, 2017; Max Planck Fellow, 2017; Heisenberg Prof., 2012; Emmy Noether Group, 2005; Marie Curie Fellowship, 2002

Frank Petzold Architectural Informatics

DDS in architecture & urban planning, public participation, building surveying

Spec. Iss. Ed. Buildings; VP DARL, 2015+; Scientific Spokesman "Innovative Building" at Bayern innovativ, 2020+; SOC eCAADe, ascaad, caadfutures, ICCCBE, 2004+

Peter Schüffler Computational Pathology

ML for cancer detection / segmentation / reporting; prognostic markers; ergonomic systems / digital systems for pathologists

Co-Founder Paige, 2018; Best Paper VIGOR++ Workshop, 2014; Outstanding Paper, ABD MICCAI, 2013

Ian Smith TUM GNI: AI for the Built World

Active & intelligent structures; Measurement system design; Computer-aided engineering; **Biomimetic structures**

Editor Frontiers, JAEI, JCCE; National Academy of Construction, USA, 2022; Computing in Civil Engineering Award, ASCE, 2005

Wolfgang Wall Computational Mechanics

Fluid & structural dynamics; coupled multi-field & multi-scale problems; HPC; uncertainty quantification; ML & inverse problems

ERC Advanced Grant, 2021; EUROMECH Fellow, 2018; Member BAS, 2017; Prandtl Medal, 2016; Member AAS, 2015

Yannis Theocharis ↗ Digital Governance

Political & online world behavior; influence of digital media on political communication & governance; political participation

Politic. Communication Top Paper Award, 2021; IT & Politics Conf. Paper Award, 2016; A. von Humboldt Postdoct. Fellowship, 2011

Helge Stein ↗ Digital Catalysis

Materials for catalysis & secondary batteries; material acceleration platform development; automated/autonomous workflows & ML in material design

KIT Idea Prize, 2023; Honorable Mention Masao Horiba Award, 2021; Eickhoff Prize RUB, 2018

Jingui Xie Business Analytics

Welcome

Thematic Setting

Structure and Strate

Healthcare data analytics; Prediction & optimization; ML in business analytics

POMS-HK Best Paper, 2018; ORSC-BOM Best Paper, 2017; Junior Teaching Award, USTC, 2016; Dissertation Award, Tsinghua U, 2010

Christoph Ungemach

Choice architecture in consumer choice; choice under risk & uncertainty; process models of decision making

Decision, Risk and Management Sciences Grant, NSF, 2012; Academy of Management, Making Connections Award, 2008

Christian Stemmer Aerodynamics and Fluid **Mechanics**

Transition in hypersonic boundary-layer flows; Direct Numerical Simulation on HPC; reactive flows; research data management

TUM Asia Faculty; Editor ,Adv. in Aerodynamics' & ,ing.grid'; NATO AVT Excellence Award, 2020

Julija Zavadlav ↗ Multiscale Modeling of Fluid Materials

Molecular dynamics; ML-based Molecular modeling; ML in material science; Multiscale simulations

ERC Starting Grant, 2022; 1st Prize Goldene Lehre, TUM, 2022; ETH Postdoctoral Fellowship, ETHZ, 2017

Fabian Theis Mathematical Modeling of **Biological Systems**

ML & statistical learning; dynamical systems; single-cell analysis; multi-omics; quantitative imaging

Leibniz Prize, 2023; Hamburger Science Prize, 2021; ERC Grant, 2010, 2022; Erwin Schrödinger Prize, 2017

Birgit Vogel-Heuser Automation and Information Systems

Systems & software engineering; embedded systems; distributed intelligent systems

Special Award Initiative D21, 2005; Borchers Badge RWTH, 1991; GfR promotional award, 1990; Adam Opel Award, 1989

Wolfgang Utschick Methods of Signal Processing

Multiantenna systems; signal processing & generative modeling for wireless communications; statistical inference & parameter estim. in engineering applications

IEEE Fellow, 2021; TUM Teaching Award, 2014; Best Paper Award, 2009/10/13; ITG Award 2007

Xiaoxiang Zhu Data Sci. in Earth Observation

Remote sensing; Earth observation; ML & data science; socially relevant apps. (global urbanization, UN's SDGs, climate change,...)

IEEE Fellow 2021; ERC Grants 2016/20/22; Heinz Maier-Leibnitz Medal 2018; Leopoldina Early Career Award, 2018

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