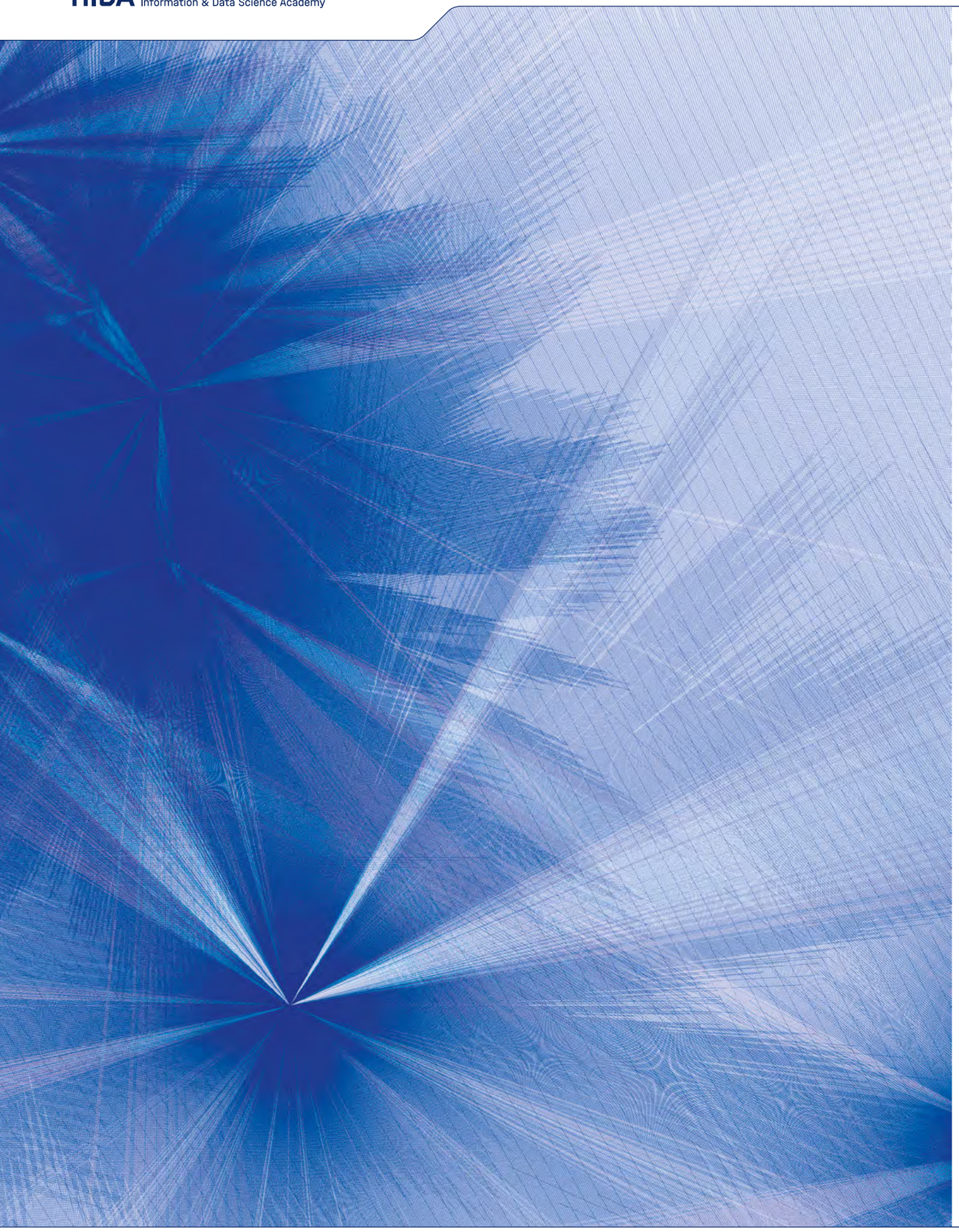
HiDA HELMHOLTZ
Information & Data Science Academy

HELMHOLTZ INFORMATION & DATA SCIENCE ACADEMY

REPORT 2022



I. HIDA IN GENERAL

In 2019, the Helmholtz Information & Data Science Academy (HIDA) was founded to attract and support excellent young scientists in the field of information and data science in the Helmholtz Association. In full extension, HIDA and the Helmholtz Information & Data Science Schools (HIDSS) will have trained over 330 doctoral researchers until 2025 (incl. associated doctoral researchers as reported by the schools). This makes the program the largest postgraduate training program in the field of information and data science in Germany.

HIDA offers networking activities, further education and training programs for information and data science talents from all Helmholtz Centers. The researchers combine knowledge in state-of-the-art information processing with scientific know-how in one of Helmholtz' research programs. HIDA strongly supports the worldwide recruitment of the most talented young scientists for all Helmholtz Centers and their university partners and contributes substantially to the associations' employer branding efforts.

In order to attract and qualify young talents, HIDA continued its diverse networking activities in 2022 together with the 18 Helmholtz Centers, a growing number of top universities and other partners from science and industry. In doing so, HIDA promotes and intensifies the collaboration between scientists and brings additional expertise in information and data science to the Helmholtz Centers.

HIDA also addresses the shortage of information and data science specialists, both in academia and in industry. Due to the scale of HIDA's education and training initiatives, they make a significant contribution to the training of information and data science experts in Germany.

Fall 2022 marked the beginning of a critical stage for HIDA. The first two schools - HEIBRIDS and HIDSS4Health - were successfully evaluated. In 2023, the remaining four schools will follow (See all the date on page 99).

For all these evaluations, HIDA is assembling panels of distinguished national and international experts to conduct an unbiased review of the schools' work. From 7 – 8 June 2023, HIDA itself will be evaluated, setting the course for the future of HIDA and the Schools.

II. HELMHOLTZ INFORMATION & DATA SCIENCE SCHOOLS

The HIDA network is the largest postgraduate training program in information and data science in Germany. The core of this program are the six Helmholtz Information & Data Science Schools, which form a network between 13 Helmholtz Centers and 17 top-tier universities. Together, they will have trained over 330 doctoral researchers (incl. associated doctoral researchers) until 2025. The schools are groundbreaking in the development of new collaborative approaches that help to evaluate complex, heterogeneous data in the natural sciences by using intelligent algorithms. HIDA thus is enabling modern cutting-edge research. Its doctoral researchers are always supervised by two PIs: one from the Helmholtz programs and one from the computer science, informatics or mathematics faculties of the schools' partner universities. As a result, HIDA is building bridges even beyond the scope of the individual doctoral projects.

In 2022, four doctoral researchers (HDS-LEE: 1, HEIBRiDS: 2, MarDATA: 1) successfully defended their dissertations and received their doctoral degrees. The schools have also achieved their ambitious goals in recruitment, training, and publication output in the field of information and data science and have further expanded their activities. Listed below are outstanding highlights of our schools (detailed information on the schools can be found in chapter IV):

- HEIBRiDS and HIDSS4Health underwent successful mid-term evaluations in 2022. The initial feedback from the review panels showed that both schools have been true to their mission of educating young researchers on the interface of data science and domain expertise. The continuation of the schools was strongly recommended.
- HIDSS4Health won two new industry partners: ZEISS and BioMedX.
- Three doctoral researchers from HIDSS4Health had an research exchange in the scope of i4Health in London.
- DASHH's first on-site retreat in August 2022 was a great success with numerous doctoral researchers and DASHH PIs joining this scientific get-together at the baltic sea.
- In September 2022, DASHH was proud to welcome the six members of its International Advisory Panel on-site in Hamburg to discuss and develop DASHH's future perspective with this board of excellent and renowned international scientists.
- HDS-LEE was able to record immense increase in 2022. The number of doctoral researchers grew from 26 to 46. The PhD positions are held by people from 16 nations, twenty-eight of them are Germans.
- HDS-LEE has extended the list of cooperation partners with the University Hospital Aachen thus expanding its expertise in the field of computational biomedicine. Contact person Prof. Andreas Schuppert is an important partner: In recent years, he gained particular recognition for his predictions on intensive care bed occupancy during the coronavirus pandemic.
- MarDATA doctoral researchers hosted their own session at AGU Fall Meeting 2022 in Chicago, USA, about "Interpretable Machine Learning for Marine Sciences".
- MUDS aligned four additional industry-funded collaborative projects.
- A total of nine MUDS doctoral researchers were awarded additional fellowships and prizes.
- MUDS doctoral researchers visited MILA Montreal for a research stay, as a result of the newly established research network between Canada and Helmholtz.

Currently, 331 doctoral researchers are trained at the schools in Hamburg, Bremerhaven/Kiel, Heidelberg/Karlsruhe, Berlin, Munich and Aachen/Cologne/Jülich.

Figure 1 shows the total number of recruited doctoral researchers from 2018 up to 2022. The number increased steadily from 13 doctoral researchers in 2018 to 331 doctoral researchers in 2022 (incl. 102 associated doctoral researchers, who are funded by third parties or other programs). The recruiting activities are according to plan and show the steady growth of the schools.

Recruitment at all schools shows a consistently high level of incoming applications.

Figure 2 summarizes the total number of received applications across all schools from 2018 to 2022. With more than 1.217 applications received in 2022, it is apparent that the demand for training at the interface between information and data science and research domain is high.

The doctoral researchers come from all over the world: Figure 3 shows the 44 countries of origin of the doctoral researchers across all six schools. Special efforts are made to attract more female candidates. These activities resulted in a gender ratio of 29% amongst the doctoral researchers over all schools, varying from 22 % (HDS-LEE and DASHH) up to 36% (MarDATA).

In 2022, 193 publications with contributions from HIDA doctoral researchers were published at all schools combined. Details of the publication output of each school are provided in chapter IV. In line with varying subject-specific publication practices, each school has structured and listed its publication data accordingly.

The schools' customized curricula offers a wide range of lectures, seminars, workshops, trainings and summer schools. 75 lectures were held at all schools. The lectures are specific to the subject matter of the schools.

In total, 45 courses took place across all schools in 2022. They aim to provide specific skills to the doctoral researchers, exemplified by courses like "Introduction to Machine Learning", (HIDSS4Health) or "Modern Fortran: Features for High-Performance Computing" (HDS-LEE/EU Regional School). 52 recruiting and networking events of various types were organized by the schools, including PhD seminars. This figure also contains events that are part of the schools' regular program, such as MarDATA's "Digital Science Mondays".

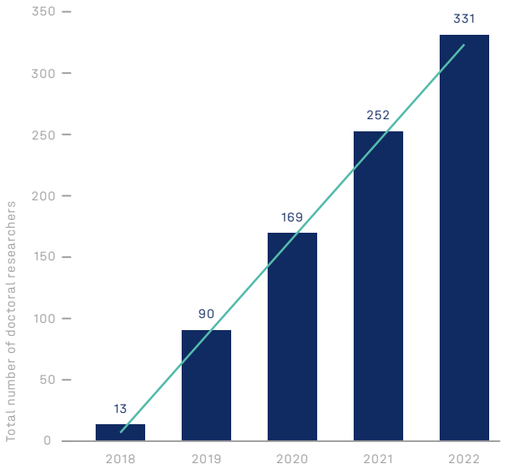


Fig. 1: Recruitment of doctoral researchers across the schools (incl. associated doctoral researchers)

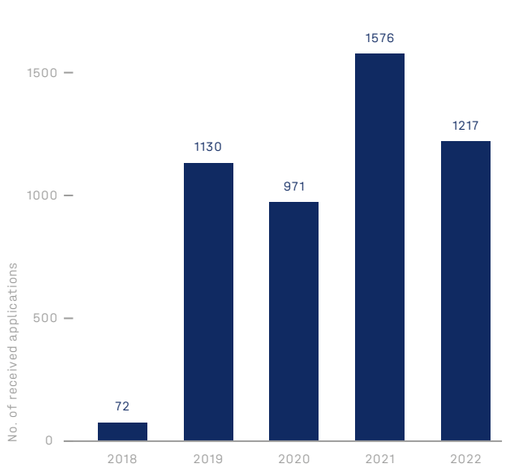


Fig. 2: Number of received applications across all schools (2018 - 2022)

Fig. 3: Countries of origin of the doctoral researchers of all six schools

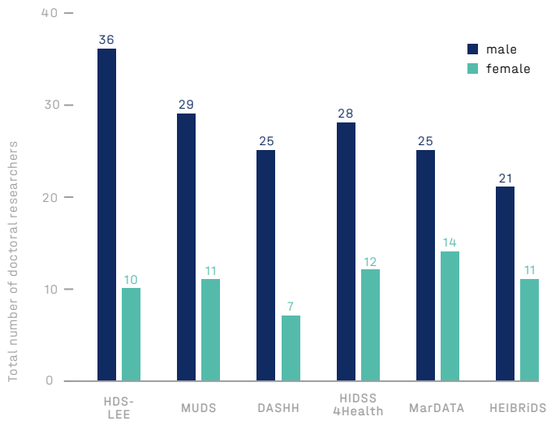


Fig. 4: Gender distribution of all doctoral researchers (excl. associated doctoral researchers)

III. HIDA ACTIVITIES

In 2022, HIDA continued to expand its recruiting, training and networking activities in the field of information and data science. Due to the high demand and basing on successful formats of 2020 and 2021, HIDA continued and intensified activities such as the Helmholtz Data Science Career Day and the Lecture Series in cooperation with the schools. HIDA also launched new activities such as the Incubator Summer Academy or the event series Helmholtz Entrepreneurs in cooperation with the other Helmholtz Incubator Platforms and further partners. HIDA's exchange programs grew significantly: In 2022, HIDA received 145 applications for the Helmholtz Visiting Researcher Grant, and a total of 38 doctoral researchers and postdocs applied for the Trainee Network. In addition, HIDA established a new exchange program with its partner NORA (Norwegian Artificial Intelligence Research Consortium). The British Council and the UK Science and Innovation Network became partners to HIDA's exchange project with the Israel Data Science Initiative.

HIDA AND THE HELMHOLTZ INCUBATOR PLATFORMS

HIDA is a central component of the Helmholtz Incubator and works in close collaboration with the other Information & Data Science Platforms in order to provide training and networking opportunities for Helmholtz researchers from all centers and programs. Outstanding joint activities were:

» TEACH - Talk about Education across Communities in Helmholtz

In cooperation with the Incubator platforms HIFIS and HMC, as well as the Helmholtz Open Science Office and the FZJ, HIDA organized the participant-driven event TEACH. The virtual event on November 09, 2022 provided an opportunity to exchange experiences and best practices in education, to develop innovative teaching ideas and to share teaching resources. (Learn more: page 32)

» Incubator Summer Academy 2022

The five Helmholtz Incubator platforms HIDA, Helmholtz AI, Helmholtz Imaging, HIFIS and HMC collaboratively organized the Incubator Summer Academy from September 12–23, 2022. It offered 19 courses and workshops, two lectures, a data challenge, a keynote as well as a career corner. (Learn more: page 33)

» Helmholtz Entrepreneurs Series (Helmholtz AI and HIDA)

In 2022, HIDA started the new event series Helmholtz Entrepreneurs in cooperation with Helmholtz Transfer and Helmholtz AI. On June 22, the first event took place, Helmholtz Entrepreneurs: From Idea to I Did. During the Helmholtz Incubator Summer Academy on September 20, the event was implemented a second time in a similar setting. (Learn more: page 38)

» HMC Fair Fridays (HMC supported by HIDA)

On March 18, 2022, the Helmholtz Metadata Collaboration (HMC) launched the HMC Fair Friday lecture series in cooperation with HIDA. The series is intended to stimulate interdisciplinary exchange on the responsible and sustainable use of research data. (Learn more: page 39)

» Helmholtz AI

- HIDSS4Health doctoral researchers attended the first AI HERO hackathon. It took place online from 01.-03.02.2022. Helmholtz AI, HIP, HMC, HIDSS4Health and HIDA organized the hackathon.
- Sugandha Doda, doctoral researcher at MUDS, co-organized the Helmholtz AI CountMeIn Challenge Hackathon, which took place from 11.04.–23.05.2022.
- Jannes Münchmeyer, doctoral researcher at HEIBRiDS, took part in the Helmholtz AI Conference 2022 on 02.–03.06.2022 in Dresden, Germany.
- Doctoral researchers at MarDATA participated at the Helmholtz AI Walk-in Consulting that took place on 15.12.2022.
- HDS-LEE doctoral researcher Danimir Doncevic published the teaching strategy of the HDS-LEE Hearts Gym Hackathon that took place in 2021 at the Teaching Workshop at the ECML Conference together with the Helmholtz AI team at FZJ: J. Ebert, D. T. Doncevic, R. Kloß, S. Kesselheim. Hearts Gym: Learning Reinforcement Learning as a Team Event.

III | 1. The Covid-19 Pandemic Impact

In 2022, the COVID-19 pandemic still had an impact on HIDA's and the schools' activities and reduced exchange programs and physical events until spring. Furthermore, it became apparent that the reduced exchange opportunities were limiting some doctoral researchers. As a result, the progress of some projects was delayed.

The Helmholtz Information & Data Science School's coordinators approached the head office in early 2022 to discuss possible immediate measures for doctoral researchers who have suffered severe restrictions of their work and personal lives due to the pandemic and whose PhD projects were threatened as a result.

The schools proposed a funding pool for extensions at HIDSS, which was established in June 2022. The funding is supposed to cover 50% of the personnel costs for up to three months, with corresponding co-financing from the participating centers' own funds. The total volume of the "Corona-Härtefallfonds" amounts up to 500,000 €.

The school coordinators handled the applications for their respective doctoral researchers. Application deadline was 31.12.2022. Applications consisted of three different assessments of the candidates' situation.

A panel, including the heads of HIDA and Strategy/IVF made the decisions based on the following criteria

- Risk of discontinuation of the PhD appears to be present
- Jeopardy to higher-level projects appears likely
- The duration of the extension (3 months) leads to the completion of the PhD

Nineteen applications from four schools were submitted. After a thorough review, all applications were approved.

With the establishment of the funding, the Helmholtz Association and HIDA acknowledge that the COVID-19 pandemic also affected computer-based doctoral theses and the need for a quick and unbureaucratic way to help. The contract extensions for the doctoral researchers concerned will take effect in 2023.

Moreover, the pandemic, its prevention and the corona virus itself also continued to be a scientific subject of lectures, seminars, events and publications:

- On April 27, Dirk Brockmann, expert in epidemiology and prominent figure in the management of the COVID-19 pandemic in Germany, gave a HIDA/HEIBRiDS lecture: The Data Donation Project – How Wearable Sensors Can Help in Dealing with the COVID-19 Crisis. Dirk Brockmann is professor at Humboldt Universität zu Berlin and group leader at Robert Koch Institute.
- Three articles by MUDS doctoral researchers on the COVID-19 pandemic have been accepted for publication.
- HIDSS4Health organized an online course on Mental Health First Aid for doctoral researchers. The training gave them an understanding of how to deal with stressful situations caused by the pandemic and its effects.
- HIDSS4Health has explored and is currently negotiating ways to reallocate unused HIDSS4Health funds, e.g. travel budgets and other expenses, to fund Corona enhancements for doctoral researchers.
- A HIDSS4Health doctoral researcher in collaboration with other researchers (see publication notes) published an article on Covid-19 prediction datasets.
- In November 2022, DASHH PI Dr. Alke Meents was awarded with the Bjørn Wiik Prize 2022 for his outstanding achievements in the COVID-19 drug research.
- Moein Einollahzadeh Samadi, associated doctoral researcher at HDS-LEE, presented two conference posters and gave a flash talk on his research about the COVID-19 pandemic.
- Three HDS-LEE PIs were involved in the successful project proposal "LOKI – Integrated Early Warning System for Local Recognition, Prevention, and Control for Epidemic Outbreaks".
- HIDA PI Sabine Attinger (UFZ), now leads the modeling and data science project "COCAP- COping CAPacity of nations facing systemic crisis - a global intercomparison exploring the SARS-CoV2 pandemic".

The COVID-19 pandemic also affected the way some of HIDA's and the schools' activities took place. Until spring 2022, many of the offered trainings and events were held online. However, with the end of contact restrictions the schools were able to organize many retreats in person in order to offer networking opportunities to the doctoral researchers. HIDA also began organizing on-site events in spring – such as the GPU Hackathon in March at AI Campus Berlin and the HIDA Office Opening in May.

Nevertheless, in the future, HIDA will also continue to expand its own and the schools' virtual activities in the areas of recruitment, joint events, and networking, utilizing the lessons learned during the COVID-19 pandemic.

III | 2. Exchange Programs

HIDA's exchange programs and especially the Helmholtz Visiting Researcher Grant have grown significantly in 2022. Their overall goal is to connect international and national data science talents (doctoral researchers and postdocs) with the scientists of the Helmholtz Association and getting them excited about Helmholtz as a potential future employer. In addition, they are intended to encourage research collaboration across borders and disciplines. Listed below are some highlights of HIDA's exchange programs in 2022:

- The launch of the exchange programs was heavily influenced by the pandemic in 2020 and 2021, which prohibited travel and physical exchange almost entirely. 2022 proved to be a year in which the programs' participants were able to carry out a considerable amount of their research stays on-site at the Helmholtz Centers.
- The number of Helmholtz PIs that requested to be listed as potential hosts surpassed 80 in 2022. Scientists from 17 Helmholtz Centers offer to host a visiting scientist for a short-term research stay in their group.
- As the number of applications for all exchange programs has increased in 2022, seven new reviewers were recruited in addition to the members of the HIDA Steering Committee.
- The Helmholtz Visiting Researcher Grant is now open to doctoral and postdoctoral researchers as well as researchers with a Master's degree and at least three years of research experience.
- The British Council and the UK Science and Innovation Network became partners to HIDA's exchange project with the Israel Data Science Initiative at the end of 2022. The now trilateral exchange program with top universities and research institutes from Israel, Germany, and the UK will take place for the first time in summer 2023.
- HIDA has established a new exchange program with its partner NORA (Norwegian Artificial Intelligence Research Consortium) in 2022. For the first time, HIDA had applicants sketch out their own project ideas for the three-month exchange program with Norway, instead of giving them projects.
- In view of the BMBF's directive to discontinue or critically review scientific cooperation with Russia against the backdrop of the Russian attack of Ukraine, no applications from Russian institutions were accepted in 2022.

HIDA has expanded its marketing efforts through holding information events and promoting the exchange programs through Research in Germany and the DAAD's social media channels. With virtual info sessions and according marketing measures, HIDA was able to inform interested participants (internal and external) and hosts about the Trainee Network and the Visiting Researcher Grant.

THE HIDA TRAINEE NETWORK

With the Trainee Network, HIDA has created new forms of collaboration and exchange between scientists of the different Helmholtz Centers and is still doing so. The program promotes research stays with a duration of one to three months at different Helmholtz Centers for doctoral and postdoctoral researchers (trainees) whose research has a strong connection to (applied) information or data sciences. The Trainee Network promotes the mutual transfer of expertise in the field of information and data science in the long term and ensures that methods and algorithms are shared between groups from different Helmholtz Centers and research domains, with the hosting labs gaining additional recruiting opportunities. Since its establishment in 2020, 81 doctoral and postdoctoral Helmholtz researchers have been awarded the grant.

Abhishek Cukkemane and Valentin Stefan successfully completed their research stay in 2022. (Photo: A. Cukkemane; German Center for Integrative Biodiversity Research (iDiv) Halle-Jena-Leipzig)

» Call for applications for the Trainee Network in 2022

In 2022, HIDA again organized two rounds of applications for the Trainee Network. With the easing of pandemic restrictions and the program becoming more well-known, the number of applications has increased for the two rounds in 2022. A total of 37 doctoral researchers and postdocs applied for the Trainee Network in 2022 (in 2021, a total of 21 researchers and postdocs applied to the program). The spring round of applications (application deadline March 2022) closed with 20 applications. After review, 19 of the applications were supported. 13 of the successful applicants were doctoral researchers while six of them were postdocs. In total, 15 of the 18 Helmholtz Centers were involved in this round of applications as the sending or receiving institution. As sending institutions (Home Center) took part: AWI, DESY, DLR, FZJ, Geomar, GSI, HZDR, HZI, UFZ, Hereon, GFZ, and MDC. As host institutions (Host Center) took part: DLR, FZJ, HZB, HZDR, UFZ, Hereon, Helmholtz Munich, KIT, and MDC.

For the autumn round of applications (application deadline October 2022), HIDA received 17 applications for the Trainee Network. All applications were granted. 15 of the successful applicants were doctoral researchers while two of them were postdocs. Twelve Helmholtz Centers were involved as potential sending or receiving institutions. The Home Centers were: AWI, DKFZ, DLR, FZJ, HZB, HZI, UFZ, Hereon, Helmholtz Munich, and MDC. The Host Centers were: AWI, CISPA, DKFZ, DLR, FZJ, HZI, UFZ, Hereon, Helmholtz Munich, and KIT.

FIG.5 - HIDA TRAINEE NETWORK APPLICATIONS

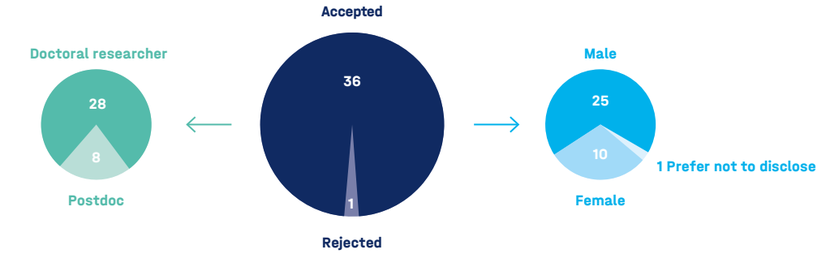
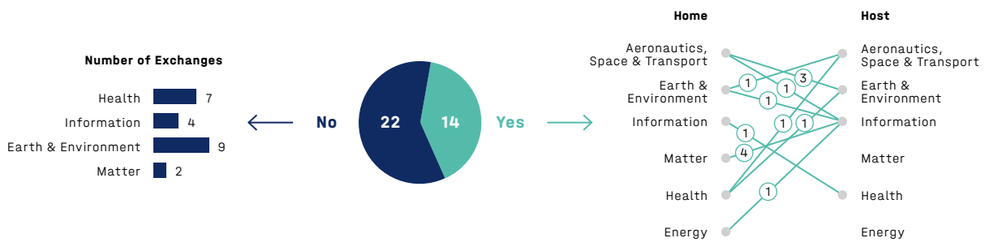


FIG.6 - PARTICIPATING HOME AND HOST CENTERS

FIG.7 - EXCHANGES ACROSS RESEARCH FIELDS

The number in the figure show the number of participants.



HIDA TRAINEE NETWORK PROJECTS ACCEPTED IN 2022 (MARCH ROUND)

Home	Host	Project Title
AWI	FZJ	In-depth investigation scaling/paralleling machine learning-based system for automated oceanographic data quality control in the JSC HPC system
DESY	HZB	Towards X-ray absorption spectra prediction using protein non-covalent interaction patterns as trained data for a supervised machine learning techniques
FZJ	DLR	Self-supervised learning for the semantic analysis of synthetic aperture radar images
GEOMAR	Hereon	A semi-supervised contrastive learning approach to predict sediment accumulation at the seafloor
DLR	Hereon	Semantic technologies for scientific laboratories to support polymer membrane research
GSI	HZDR	Artificial neural networks and deep learning methods for use in storage ring experiments with highly charged ions
UFZ	KIT	Exploring the relationships between drought hazard, vulnerability and socio-economic impacts
HZI	Helmholtz Munich	Mapping a novel COVID-19 lung atlas to the Human Lung Cell Atlas to reveal cellular trajectories that shape the resolution of ARDS
GFZ	KIT	Uncertainty quantification in a joint inversion of surface and body waves using multi-level Markov chain Monte Carlo
GFZ	UFZ	3D X-ray tomographic imaging of mineral-microbial aggregates in Greenland ice-cores
HZDR	KIT	Hybrid classical-quantum deep random neural networks
HZDR	MDC	3D reconstruction from focal series images of electron microscopy using machine learning
HZDR	FZJ	Establishing data-driven design thinking in the field of materials science
HZDR	FZJ	Application of deep learning for simultaneous standardized delineation of brain tumors and healthy reference regions in quantitative brain FET PET/MR
Hereon	Helmholtz Munich	Deep learning and computer vision to lens-free microscopic images for classification and regression tasks
Hereon	KIT	Cloud/fog pattern estimation using data-driven deep learning methods
Hereon	KIT	Machine learning based force field for layered double hydroxides
Hereon	HZB	Explainable AI for corrosion inhibition prediction
MDC	Helmholtz Munich	Link prediction in gene-gene network based on deep graph neural networks

HIDA TRAINEE NETWORK PROJECTS ACCEPTED IN 2022 (OCTOBER ROUND)

Home	Host	Project Title
HZB	KIT	Investigating the influence of unbalanced experimental data when applying quantum random forests on modeling superconducting critical temperature in the Supercon dataset
AWI	UFZ	Analysis of key features in LC-MS DOM samples from polar oceans
HZI	DKFZ	Protein domain annotation of divergent viral sequences
DKFZ	HZI	Establishing high-throughput screening pipelines at the DKFZ Cluster for the discovery of novel viruses in cancer sequencing data
AWI	Hereon	Coastline modifications and drivers: North Sea and Baltic Sea – past, present, and future perspective
DLR	UFZ	Machine learning for estimation of lateral and vertical distributions and dynamics of soil moisture from P-band SAR observations
DLR	CISPA	Investigate approaches to reconstruct the data flow graph from source code
Hereon	KIT	Quantifying uncertainties in phase contrast tomography
FZJ	KIT	Accelerating the experimental electrocatalyst optimization by machine learning
Hereon	FZJ	Virtual biopsies in brain tumor patients
DLR	KIT	Active learning of robot vision from humans
MDC	DLR	Fuzzy clustering for LIBS data of multi-phase geological targets measured in simulated martian conditions
Hereon	Helmholtz Munich	Machine learning (ML) based approaches to study the mechanosensation of cells
MDC	Helmholtz Munich	Investigating how cells interact in their 3D tissue niches through spatial transcriptomics
UFZ	AWI	Statistical heterospectroscopy, an approach to correlate FT-ICR MS and high-field NMR spectra of natural organic matter datasets
UFZ	FZJ	Computational methods for biotechnology and environmental toxicology. Use cases of Bayesian optimization in two different research fields
Helmholtz Munich	AWI	Statistical and data science methods integration for metagenomics data analysis

HELMHOLTZ VISITING RESEARCHER GRANT

The Helmholtz Visiting Researcher Grant was established in 2021, with the first research stays taking place in 2022. This program complements the HIDA Trainee Network funding line and enables short-term research stays with a duration of one to three months for researchers from outside the Helmholtz Association whose work has a strong link to (applied) information and data science. In 2022, the program was opened for applications by researchers with a Master's degree and at least three years of research experience. Doctoral researchers and postdocs from universities, research organizations, and industry worldwide are eligible to apply for this grant. Since its first round in June 2021, interest in the Helmholtz Visiting Researcher Grant has grown exponentially, showing the strong appeal of not only this funding line but also the Helmholtz Association nationally and especially internationally. Feedback from the first reports by participants that already finished their research stays has been overwhelmingly positive with many emphasizing the outstanding scientific reputation and prowess of the Helmholtz Association. Several of the researchers that HIDA supported plan to continue collaborating on their research with their respective hosts and/or centers.

» Call for applications for the Helmholtz Visiting Researcher Grant in 2022

While there were ten applications in the first application round (June 2021), HIDA received 47 applications for the second round (application deadline March 2022), of which 36 were approved by the HIDA reviewers in the end. The successful candidates came from 21 different countries. 24 of the accepted applicants were doctoral researchers while 12 of them were postdocs. The accepted candidates are going to one of 13 Helmholtz Centers: AWI, CISPA, DKFZ, DLR, Geomar, HZDR, HZI, UFZ, Hereon, Helmholtz Munich, GFZ, KIT, and MDC.

For the third round (application deadline October 2022), HIDA received 98 applications of which 73 were approved. The successful candidates came from 29 different countries. 48 of the successful applicants were doctoral researchers while 25 of them were postdocs. The accepted candidates are going to one of 16 Helmholtz Centers: AWI, CISPA, DESY, DKFZ, DLR, DZNE, FZJ, Geomar, HZDR, HZI, UFZ, Hereon, Helmholtz Munich, GFZ, KIT, and MDC.

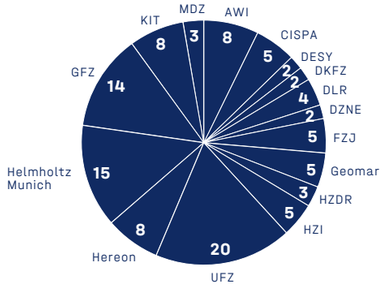
NATIONALITIES OF THE PARTICIPANTS

Country	No.
Germany	14
China (PRC)	10
India	9
USA	8
Brazil	6
Iran	5
Pakistan	5
United Kingdom	4
Italy	4
Nigeria	4
Spain	3
Australia	3
Mexico	3
Indonesia	2
Colombia	2
Ghana	2
Ethiopia	2
Chile	2
Poland	2
Cameroon	1
Romania	1
Ukraine	1
Thailand	1
Botswana	1
Israel	1
France	1
Philippines	1
Egypt	1
Netherlands	1
Jordan	1
Sri Lanka	1
Iraq	1
Czech Republic	1
Algeria	1
Greece	1
Palestine	1
Bosnia and Herzegovina	1
Mauritius	1

FIG.8 - HIDA VISITING RESEARCHER GRANT APPLICATIONS

Gender ratio all applicants: 100 male, 44 female, 1 Prefer not to disclose.
Of the accepted female participants, 27 are doctroal researchers and 6 are post-doctoral researchers.

FIG.9 - PARTICIPATING HOST CENTERS



HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (MARCH ROUND)

Home	Host	Project Title
Southeast University, China	KIT	Drug disease relation extraction from DailyMed using weak supervision
Internet Society, USA	CISPA	Quantifying the resilience of the African web
Institute of Computer Science at the University of Wrocław	GEOMAR	Prediction and segmentation of geochemical time-series
Technical University Berlin, Germany	AWI	Monitoring and Modelling of critical biomass in Siberian boreal forest using UAV-borne LIDAR and multispectral image data
Imperial College London, UK	Helmholtz Munich	Heterogeneous network flow and Petri nets in topological machine learning and multilayer complex network analysis
Centro de Investigaciõn Científica y de Educaciõn Superior de Ensenada, Mexico	GEOMAR	Geophysical characterization of an offshore geothermal system in the Gulf of California (Mexico)
University Hospital Essen, Germany	Helmholtz Munich	Spatial and single-cell genomic analysis of glioma
Birzeit University, Palestine	UFZ	Climatic change impacts on the water qualitative resources mnagement in Natuv Catchment / Palestine
Humboldt University Berlin, Germany	DLR	Deep learning for improved mineral quantification from planetary spectroscopic data
Max Planck Institute for Ornithology, Germany	UFZ	Measuring what we don't know in functional annotation using microbial big data
Garvan Institute of Medical Research, Australia	Helmholtz Munich	Accurate modelling of cell state transitions for the characterisation of dynamic genetic effects in single cells
University of Ibadan, Nigeria	Helmholtz Munich	Genome wide association analysis to provide insights into the genetic architecture of vascular cognitive impairment among indigenous African stroke survivors
Macquarie University, Australia	HZI	Development of an R package for the normalisation and analysis of transposon directed insertion-site sequencing (TraDIS) data
Maria Sklodowska-Curie National Research Institute of Oncology, Poland	DKFZ	Development of an alignment-free method for whole-genome methylation profiling from raw bisulfite sequencing reads
University of Miami, USA	Hereon	Hereon marine X-band radar coastal oceanography in Duck, NC
Universidade Federal do Ceará, Brazil	UFZ	Text mining and social network analysis applied to the evaluation of complex hydrosocial systems
Institute of Molecular Medicine & Experimental Immunology (IMMEI), Germany	Helmholtz Munich	Differentiation of influenza-specific T cells over the course of infection
Universitã degli Studi di Napoli Federico II, Italy	GFZ	Exploring the use of SeisBench machine learning framework for detecting the earthquake preparatory phase
University of Edinburgh, UK	Helmholtz Munich	Topological dynamics of the brain: a Conley Index & Hodge Theory view on time-varying fMRI and DTI
Ton Duc Thang University, Vietnam	Hereon	Improved hybrid framework for modeling materials degradation based on data science and artificial intelligence: case study pitting corrosion growth in aluminum constructions under maritime conditions
Ocean University of China, China	Hereon	Noise scale-separate effects on morphodynamic under a regional coupled model based on big data

HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (MARCH ROUND)

Home	Host	Project Title
Leibniz-Forschungsinstitut für Molekulare Pharmakologie, Germany	MDC	Assessment of drug-protein specificity from molecular surface embeddings
University of Groningen, the Netherlands	AWI	Transforming ecosystem data into ecosystem actions
University of South Bohemia, Czech Republic	GFZ	Application of hybrid deep learning methods and open remote sensing data for mapping global inland waters
Indian Institute of Technology Roorkee, India	UFZ	Exploring large data on soil moisture spatial fields to unravel river basins reactions and flood hazard using machine learning techniques
Indian Institute of Technology Kanpur, India	GFZ	Improving the prediction of Earth Orientation Parameters (EOP)
Max Planck Institute for Dynamics and Self Organization, Germany	KIT	Quantifying uncertainty level of wind conditions using machine-learning approach
Moore Institute for Plastic Pollution Research, USA	AWI	Integrated open web AI for the chemometric classification of Raman and FTIR microplastic spectra
University of Strasbourg, France	GFZ	Numerical evaluation on field observations of geothermal systems
Instituto Politēcnico Nacional, Mexico	UFZ	A systematic mapping of natural hazards adaptation, vulnerability, and resilience research
Queen's University, Canada	HZDR	Comminution modelling through stochastic geometry and deep neural networks
University of Padua, Italy	Helmholtz Munich	Combining graph neural networks and topology to analyze high-order structures in single-cell data with deep learning
Icahn School of Medicine at Mount Sinai, USA	Helmholtz Munich	Dynamic molecular alterations in fresh microglia across neurodegeneration
Weizmann Institute of Science, Israel	UFZ	Pattern finding and matching in omics (PatternOmics)
University of California San Diego, USA	Helmholtz Munich	Benchmarking mutational encodings for latent factor analysis of single cell multiomic data with variational autoencoders
Life and Medical Science Institute (LIMES) Bonn, Germany	Helmholtz Munich	Mapping of denoised single-cell data from a large clinical HIV cohort to reference atlases and self-constructed blood reference by transfer learning

HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (OCTOBER ROUND)

Home	Host	Project Title
National University of Sciences and Technology (NUST) Islamabad	Helmholtz Munich	Genomic data analysis for investigating virulence and zoonotic potential of mammary pathogenic E. coli (MPEC) strains isolated from mastitic dairy and machine learning approach for risk factors assessment
Tanta University	UFZ	A meta-analysis of pesticide effects on honey bee gut microbiota
University of Twente	GFZ	Machine learning based urban flood susceptibility prediction using multiple remote sensing data
University of São Paulo	UFZ	Multi-omics research using machine learning for the exploration of non-coding RNA in complex microbial communities
Max Planck Institute for Intelligent Systems	Helmholtz Munich	Extending the optimal transport-based set of tools used in single-cell genomics
University of Twente	KIT	Data-driven agent-based modeling and simulation for emergent behavior control using process mining
The University of Newcastle	UFZ	Investigating the impact of chemical additives in plastics on microbial biofilms using molecular approaches
Indian Institute of Technology (IIT) Delhi	FZJ	Investigating the non-linear relationship between groundwater and climatic extremes: a case study of Ganga basin
University of São Paulo	UFZ	BioAutoML-Fast: end-to-end multi-threaded machine learning package for life sciences
University of Ibadan	UFZ	Genetic data analyses of the diversity and structure of three edible frog species (Hoplobatrachus occipitalis, Xenopus Muelleri and Ptychadena pumilio) in Southwestern Nigeria
Warsaw University of Life Sciences	UFZ	Optimal water and nutrient retention strategies under current and future climate - a study combining integrated watershed modelling with a multi-objective genetic algorithm
State University of New York	KIT	Improving city resilience to climate and environmental change by designing effective green infrastructure
University of Grenoble Alpes	AWI	Exploring the potential of data science to unravel complex tectonic processes at the ocean bottom
Federal University Oye-Ekiti	UFZ	A bioinformatics approach to explore the environmental health risks associated with exposure to mixed hazardous e-waste chemicals
Applied Science Private University	Hereon	Using robust machine learning models to efficiently predict material compositions of novel reactive hydride composites for hydrogen storage applications
University of Oxford	CISPA	Target domain assumptions for machine learning generalisation
ETH Zürich	CISPA	Balancing the trade-off between distributional and adversarial robustness: towards an approach for test-time adaption
Universidad Autõnoma de Madrid	GFZ	Towards an early warning of cyanobacterial blooms: application of machine learning and hyperspectral imagery to discriminate changes on cyanobacterial spectral response

HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (OCTOBER ROUND)

Home	Host	Project Title
University of Ottawa	CISPA	Assessing policy options to address algorithmic and data bias in healthcare-related AI applications in the EU
German Federal Institute of Hydrology	HZDR	Deep learning-based detection and identification of plastic debris in hyperspectral data
Monash University	Hereon	Elucidating controls on earthquake statistics with simulation-based inference
Universiti Brunei Darussalam	FZJ	Deep unsupervised structured model for 3D group activity recognition
University of Bristol	GFZ	Quantitative analysis of road network components (bridges) vulnerability in flood
Institute Necker Enfants Malades (INEM) INSERM U1151	Helmholtz Munich	Novel role of class 3 PI3K in coupling of metabolic activities and gene expression for boosting healthspan
Center for Research and Advanced Studies	HZI	Frequent subgraph data mining of repurposing drugs with potential effect against SARS-CoV-2 targets through graph neural networks
Technische Universität München	AWI	Deriving permafrost vulnerability with deep learning and explainable AI
University of Science & Technology of Iran	GFZ	Machine-learning and deep learning estimation of sedimentary thermal properties for using in geothermal energy and greenhouse gas storage
University of Ghana	Hereon	Exploring the use of mangrove ecosystems as nature-based solution for coastal hazards along the eastern coast of Ghana
University of New South Wales	GFZ	A novel method to estimate flood extremes using spectrally transformed climate information
Universität Leipzig	UFZ	Using metagenomics to evaluate the biodegradation potential of glyphosate in different environments
New York University Abu Dhabi	DZNE	Epidemiological study on asthma history and cognitive functioning among older adults: a cross-sectional study of the Indonesian Family Life Survey
National University of Sciences and Technology (NUST)	GEOMAR	Marrying data science with environmental analytical chemistry to understand the fate, transport, and behavior of chemicals associated with marine microplastics
Harvard University	DESY	Towards high-throughput collection and analysis of electric field-stimulated X-ray crystallography data
University of Cagliari	UFZ	Functional traits and ecosystem services to support urban planning (FUTUR-planning)
Princeton University	HZI	Identification of immune-stimulatory RNAs in emerging virus infections
University of Douala	Hereon	Contribution of climatic and hydrological studies to the establishment of tools for adaptation to global changes for a sustainable management of the environment in coastal cities: case of Douala, Cameroon
Thuenen Institute of Sea Fisheries	UFZ	Evolving a data driven agent-based model to address future challenges of sustainable North Sea fisheries
University of Arizona	GFZ	Linking rainfall patterns to post-fire hydrological extrema across scales

HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (OCTOBER ROUND)

Home	Host	Project Title
Max Planck Institute	AWI	Data analysis techniques and machine learning for feature and information extraction in ocean physics at the polar regions
University of Liverpool	DKFZ	DNA methylation biomarker identification of pancreatic ductal adenocarcinoma metastasis using an integrated bioinformatics method
Norges teknisk-naturvitenskapelige universitet (NTNU)	FZJ	Enhancing ultra-low-dose PET/MRI using deep learning method for improved clinical interpretation
Indian Institute of Technology Roorkee	GFZ	AI-based landslide mapping using time-Series SAR data in combination with ancillary geodata for Uttarakhand Himalayas
Botswana International University of Science and Technology	UFZ	Adaptive governance for biodiversity conservation, land-use and sustainable livelihoods as a coping mechanism to climate change
The University of Queensland	Helmholtz Munich	Graph neural networks to identify cellular reprogramming factors using single cell gene expression data
University for Development Studies	KIT	An application of machine learning techniques in verifying the reliability strength of two software reliability growth models
University College London	CISPA	Gaussian processes for robust maximum moment restriction
University College Cork	GEOMAR	Geometrical feature application on 3D photogrammetric data of cold-water coral habitats
University of Cambridge	Helmholtz Munich	Predicting transcriptional perturbation response with causally aware deep learning
University Grenoble Alpes France	HZI	Modelling the estimation and distribution of epidemiologic dynamics from cycle threshold of viral infection
Aix-Marseille University	KIT	Unlocking long timescale nonadiabatic molecular dynamics with the aid of machine learning
Cochin University of Science and Technology	GEOMAR	Development of new data set at Boknis Eck time series station using model simulation, observation, data assimilation, and objective analysis
Museum für Naturkunde - Leibniz Institute for Evolution and Biodiversity Science (MfN)	AWI	Bridging the gap between short-term experiments and larger temporal (and spatial) scales
Universidad Nacional de Colombia	KIT	Uncertainty quantification of operation scheduling in power systems with renewable energy and electric vehicles, considering uncertainty cost functions and stochastic scenarios
University of Liẽge	GFZ	Developing a regional flood damage model through machine-learning techniques
McGill University	DLR	Machine learning-enabled semantic segmentation of additive manufacturing-based structures in support of data-driven solutions
Shahid Beheshti University	FZJ	Mapping individual differences of phenotypic characteristics to inter-individual variability of brain structure and function in children and adolescents: an individual-subject level approach

HELMHOLTZ VISITING RESEARCHER GRANT PROJECTS ACCEPTED IN 2022 (OCTOBER ROUND)

Home	Host	Project Title
United Arab Emirates University	UFZ	Impact of a soil extreme aridity gradient on functional adaptations of microbial communities
University Grenoble Alpes France	GFZ	Exploring continuous seismograms for hidden tectonic signatures with machine learning
Royal College of Surgeons in Ireland University of Medicine and Health Sciences	DZNE	Spatiotemporal multi-omics analysis of PD-relevant alpha-synuclein pathology
Pondicherry University	HZDR	High-throughput ab-initio electron dynamics simulations of thin films under extreme conditions
Ben-Gurion University of the Negev	Helmholtz Munich	A pseudo-SNP-based epistatic analysis for finding marginally associated genes of neurodegenerative disorders
Tsinghua University	UFZ	Unsupervised clustering of heatwaves based on perturbations in the energy balance via large ensemble model simulations
University of Ostrava	HZI	Fuzzy clustering high-dimensional (multi-)omics data with noise and outliers
University of Bucharest	AWI	Comparison between large-scale observed and simulated Antarctic sea-ice variability response to changes in atmospheric and oceanic circulation
Mines Paris	DLR	Statistical analysis and correction of a surface solar irradiance satellite retrieval model using explainable deep learning
Politecnico di Torino	DLR	Precision assessment for high definition mapping in inland waterway applications
University of Queensland	KIT	Modelling the effect of data visualisation on risky decisions
University of Alberta	FZJ	Exploring functional connectivity networks and constructing weighted cofluctuation amplitudes in fMRI brain signals
Ben Gurion University of the Negev	MDC	Interpretable deep learning in genomics
Peking University	DESY	Measurement of back-to-back azimuthal correlations in Z+jet events in pp collisions with early Run 3 data in the CMS experiment at 13.6 TeV
University of Granada	GFZ	Data-driven advancement of hydrological modelling with long-term In-Situ Observations (DAMISO)
The University of Adelaide	Hereon	Computational and data-driven analysis of electrolyte chemistries for aqueous magnesium-ion batteries
University of Groningen	UFZ	The interactions between plant metabolomics and soil microbial communities across different potato genotypes

INTERNATIONAL EXCHANGE PROGRAMS

International exchange programs continued to introduce young data scientists from strategic partner institutions to the Helmholtz universe - and helped early career Helmholtz data scientists gain international experience. HIDA facilitated two exchange programs and one internship program in 2022.

» Israel Exchange Program

HIDA organized a second round of summer exchanges with the Israel Data Science Initiative (IDSI), which coordinates the data science research centers at Israel's research universities. 19 participants, 9 from Helmholtz Centers and 10 from Israeli partner universities, took part in this year's exchange. Young scientists - from Bachelor students to Postdocs - spent six weeks working on a predefined project in the partner country. In addition, participants who had to postpone visits to their host groups due to the Corona pandemic in 2021, also traveled to Germany/Israel in 2022.

In 2023, this exchange program will become trilateral, as we will pilot the inclusion of the United Kingdom in this program next year.

» Norway Exchange Program

HIDA also launched a new international exchange program as a pilot with HIDA's partner in Norway, the Norwegian Artificial Intelligence Consortium (NORA) in 2022. In total, nine participants were chosen in two application rounds. They work on an exchange in the partner country for three month. All exchanges will be conducted until October 2023.

» Princeton University's Summer Work Program

HIDA also participated for the second time in Princeton University's Summer Work Program organized by the Princeton University's German department and their alumni. In 2022, HIDA expanded the program beyond the data sciences with the support of the talent management department at the Helmholtz Head Office. The Princeton University financially supported six-week-long stays at Helmholtz Centers for seven Bachelor students. In 2022, five students worked on data science projects at the Helmholtz Centers, one worked with a Junior PI from the Young Investigator Labs in public health and one intern joined the strategy department at the Helmholtz head office in Berlin.

IDSI EXCHANGE PROJECTS IN 2022

Participant's Home	Acad. Level	Direction	Host	Project Title
AWI	PhD	DE › IS	Keren Agay-Shay, Bar-Ilan University	Climate Change, Built Environment and Adverse Pregnancy Outcomes
DESY	PhD	DE › IS	Sarah Keren, Technion	Automated Environment Design for Promoting Collaboration of Autonomous AI Agents
DKFZ	PhD	DE › IS	Yaron Orenstein, BGU	Deep Learning in Genomics
GFZ	Postdoc	DE › IS	Asaf Weinstein, Hebrew University	Learning Optimal Regularization for Neural Network Training
DESY	PhD	DE › IS	Avigdor Gal, Technion	Assessing the Plausibility of Data in Machine Learning Pipelines
GFZ/ TU Berlin	PhD	DE › IS	Avi Ostfeld, Technion	Investigation on the Effect of Pipe Leakages on Water Quality in Water Distribution Systems (WDS)
MDC	PhD	DE › IS	Sarah Keren, Technion	Automated Environment Design for Promoting Collaboration of Autonomous AI Agents
MDC/ Charité University	PhD	DE › IS	Asaf Levy, Hebrew University	Machine Learning Based Discovery of Genes involved in Insecticidal Activity
University of Haifa	MSc › PhD	IS › DE	Marta Dembska, DLR Jena	Speech recognition in scientific laboratories
University of Haifa	MSc	IS › DE	Mehdi Saberioon, GFZ	Application of Soil Spectroscopy and Deep Learning Algorithms for Predicting Soil Properties
Hebrew University	BA	IS › DE	Clemens Alexander-Brust, DLR Jena	Multi Domain Type Inference
BGU	MSc	IS › DE	Gong Bing, FZ Jülich	Deep Learning for Temperature and Precipitation Downscaling
BGU	MSc	IS › DE	Jakob Gawlikowski, DLR Jena	Evaluating Structural Uncertainties in Neural Network Predictions
Technion	MSc	IS › DE	Bastian Rieck, Helmholtz Munich	Topological Graph Coarsening
Bar-Ilan University	MSc	IS › DE	Frederik Tilmann, GFZ	Deep Learning for Rapid Earthquake Analysis
BGU	BSc	IS › DE	Frederik Tilmann, GFZ	Deep Learning for Rapid Earthquake Analysis
Hebrew University	BSc	IS › DE	Daniel Abou-Ras, HZB	Machine Learning Applied to Multidimensional, Correlative Electron Microscopy Data
Hebrew University	BSc	IS › DE	(Erik) Ngai Ham Chan, GFZ	Quantitative Mapping of Arctic Permafrost from Satellite Time-Coverage (QMAPfroST)

NORA EXCHANGE PROJECTS IN 2022

Participant's Home	Acad. Level	Direction	Host	Project Title
FZ Jülich	PhD	DE › NO	Susanne Kunkel, Norwegian University of Life Sciences	Developing New Algorithms and Data Structures to Optimise Simulation Technologies for Spiking Neural Networks
DLR	Postdoc	DE › NO	Robert Jenssen, The Arctic University of Norway	Self-supervised Representation Learning for 3D Medical Image Data by Novel Information Theoretic Cost Functions.
DESY	PhD	DE › NO	Arnoldo Frigessi, University of Oslo	BigInsight - Developing New Methods and Algorithms for Model-based Learning
Geomar	PhD	DE › NO	Tom Michoel, University of Bergen	Uncovering Anomalies in Multibeam Data Using Causal Structure Mining
AWI	PhD	DE › NO	Stefano Nichele, Ostfold University College	Examine a Self-Organizing Neural Cellular Automaton (neural CA)
Oslomet	MA	NO › DE	Christoph Räth, DLR	Developing Mathematical Models of Eye-gaze Trajectories
Oslomet	PhD	NO › DE	Benjamin Schäfer, KIT	Investigating the Connection of Electricity Prices in Europe and Various Power Systems' Specific Data, Precipitation Levels
University of Bergen	PhD	NO › DE	Peter Sanders, KIT	Extend Techniques from Graph Neural Networks (GNN) Project to Further Combinatorial Problems
University of Oslo	PhD	NO › DE	Sebastian Krumscheid, KIT	Development of Methodologies to Quantify Different Sources of Uncertainty in Structure Learning and Causal Inference Tasks

PRINCETON UNIVERSITY'S SUMMER WORK PROGRAM IN 2022

Grad. Year	Major	Minor	Host	Center
2024	Computer Science	N.A.	Luis Samaniego, Helmholtz-Centre for Environmental Research	UFZ, Department Computational Hydrosystems
2025	Mechanical and Aerospace Engineering	Robotics & Intelligent Systems, Engineering Physics	William Smith, Helmholtz-Zentrum Berlin	HZB, EMIL - Energy Materials In-Situ Laboratory
2024	Computer Science	Applied and computational mathematics	Claudia Comito, JSC Staff - Forschungszentrum Jülich	Jülich Supercomputing Center, Division "Federated Systems and Data"
2024	Operations Research and Financial Engineering	Computer Science	Jonas Gütter, German Aerospace Center	DLR, Institute of Data Science - MLE Group
2024	Computer Science	Technology and Society, Statistics and Machine Learning, Cognitive Science	Jens Kersten, German Aerospace Center	DLR, Institute of Data Science - Applied Weband Social Media-Data Analysis
2024	Molecular Biology	Global Health Policy	E. Marie Muehe	UFZ
2023	History	N.A.	N.A.	Helmholtz Head Office Berlin / Helmholtz Leadership Academy

III | 3. Talent Scouting & Recruiting

It is an important part of HIDA's mission to strongly support the international recruitment of the most talented young scientists in the field of information and data science for all Helmholtz Centers and their university partners and to make a significant contribution to the employer branding of the association. The Helmholtz Visiting Researcher Grant and HIDA's international exchange programs contribute strongly to this goal. In addition, HIDA again reached thousands of data scientists worldwide with online recruiting efforts, making them aware of the career opportunities at Helmholtz Centers.

On its website, HIDA summarizes job opportunities in the field of information and data science at the Helmholtz Centers. The jobpage also served as landing page for HIDA's second online advertising campaign on Google Adds. The campaign was active for 116 days from September 2021 to March 2022. The ads were played out 426.000 times on Google and according to Google, users clicked the ads more than 22.000 times. During the campaign period, there were 3.553 outbound referrals from the HIDA website to job postings at Helmholtz Centers (organic website traffic included).

HIDA also increased awareness for data science careers at Helmholtz by organizing online events and job fairs:

- In spring 2022, HIDA organized a virtual career day for data scientists in health. 392 data scientists from 63 countries registered for the event and 224 visitors followed the keynotes and panel discussions from the participating centers and partner institutions and networked with them: DKFZ, HZI, FZJ, DLR, Helmholtz Munich/MUDS and CASUS.
- In September, HIDA organized a career corner as part of the Incubator Summer Academy. Here, more than 30 academy participants - mostly from Helmholtz Centers - and hiring researchers from the centers and partners joined online at the video chat platform Gathertown. Speakers from the Helmholtz Centers and partners, including the AI researcher network ELLIS and Siemens, presented career paths for data scientists and networked.
- In November 2022, HIDA organized the Helmholtz Career Day for Data Science and IT for the third time. Following a recommendation of scientists and hiring teams at the centers, the career day also addressed candidates with a background in IT fields related to data science, such as software programming, engineering and IT architecture as well as systems administration.

Please see chapter 5 for more information on these career events.

FRIENDS OF HIDA NETWORK

For the Helmholtz Information & Data Science Schools, platforms and research centers, HIDA acts as a door opener, facilitator and multiplier for cross-border and cross-sectoral cooperation. To this end, HIDA has established the Friends of HIDA network. It brings together different strategic partners internationally. Thus HIDA helps connect international data science talents with Helmholtz researchers and introduces them to the Helmholtz Centers. They also get access to HIDA's various offers in data science such as exchange programs, hackathons, career days, trainings, lectures, workshops and the diverse offerings in the HIDA Course Catalog. The partners share information about ongoing activities that are open to each other's data science communities. Moreover, the networking partners organize joint activities to promote data science skills in the communities and act as door opener for long-term research collaborations.

HIDA founded the network in late 2019. Since then it has grown to the following partners:

- **AI Campus Berlin**
- **AI Sweden**
- **Academy for Theatre and Digitality**
- **Alexander von Humboldt Institute for Internet and Society (HIIG)**
- **BIOMEDAS, Academy of the Translational Alliance of Lower Saxony (TRAIN)**
- **Data Science Research Center at Ben-Gurion University of the Negev (DSRC@BGU)**
- **German Academic Exchange Service (DAAD)**
- **Israel Data Science Initiative (IDSI)**
- **Norwegian Artificial Intelligence Research Consortium (NORA)**
- **Weizmann Artificial Intelligence Center (WAIC)**
- **Y-DATA - Yandex School of Data Analysis (YSDA)**

In addition to these partnerships, HIDA was also able to establish initial contacts with India, Canada, Denmark and the UK.

In 2022, joint activities with the Friends of HIDA included:

- AI Campus: AI Campus Berlin hosted the Helmholtz GPU Hackathon at their location this year. (Learn more: page 36)
- Academy for Theatre and Digitality: HIDA and the Academy for Theatre and Digitality organized a second round of stays for young artists at the Helmholtz Centers. (Learn more: page 44)
- DAAD: The DAAD's Postdoc-Net-AI tour included Helmholtz Centers on its two tours again this year. On these tours, international doctoral researchers and postdocs visited AI research centers throughout Germany and met with perspective employers.
- IDSI: Beyond the exchange, IDSI and the Ben-Gurion University of the Negev organized the International Archeology Challenge together with HIDA in April. (Learn more: page 36)
- In summer, HIDA and IDSI presented their partnership at the Helmholtz Innovation Summit in Tel Aviv to representatives from German and Israeli research institutions and government.

III | 4. Education & Training

One of HIDA's major goals is to provide high-quality training opportunities in the field of information and data science to all researchers within the Helmholtz Association and to foster collaborations between all community members. HIDA therefore funds and/or co-organizes courses and events with other Helmholtz platforms, institutes, or centers, and promotes training, further education, and knowledge exchange for scientists. In 2022, HIDA offered courses covering various aspects of the spectrum of data science, involving for instance programming, different software like Git or Shell, statistics, or reproducibility. The HIDA Course Catalog remains the main tool to open and offer courses to the entire Helmholtz community, as it functions as a central hub for training opportunities provided by and for the community and beyond.

HIDA COURSE FUNDING

In 2022, HIDA supported 17 workshops and courses in the field of information and data science with the HIDA Course Funding program. All funded events adhered to the main requirements of the program: They were open to researchers from the entire Helmholtz community, but also reserved a small percentage of seats for researchers not affiliated with Helmholtz. All events were organized in cooperation with other Helmholtz institutions (centers, schools, or Incubator platforms), or with international partners. Across all courses listed below, we count approximately 550 participating researchers in 2022. Events fully or partly funded through the HIDA Courses Funding:

- "Introduction to R & Statistical Models with R" with Core Facilities Statistical Consulting at Helmholtz Munich (Feb & Oct 2022)
- "Graphics with R" with Core Facilities Statistical Consulting at Helmholtz Munich (Feb & Oct 2022)
- "Shell, Git, R for Reproducible Scientific Analysis" with the Carpentries (online, Feb 2022)
- "Genomics" with the Carpentries (online, Feb 2022)
- "Ecology with Python" with the Carpentries (online, Mar 2022)
- "Introduction to Statistics" with Core Facilities Statistical Consulting at Helmholtz Munich (online, Apr & Nov 2022)
- "Mixed Models" with Core Facilities Statistical Consulting at Helmholtz Munich (online, Jun 2022)
- "Enabling Reproducibility in Data Science – Learn Why it Matters and How You Can Do it" with Helmholtz Open Science Office (online, Jun 2022)
- "RMarkdown" with Core Facilities Statistical Consulting at Helmholtz Munich (online, Jun & Nov 2022)
- "Instructor Training" with the Carpentries (online, Sep 2022)
- "Multivariate Statistics" with Core Facilities Statistical Consulting at Helmholtz Munich (online, Jul & Nov 2022)
- "Incubator Summer Academy" with Helmholtz AI, Helmholtz Imaging, HMC & HIFIS (online, Sep 2022)
  - "Reproducible Data Science" with Helmholtz AI
  - "Introduction to Napari" with Helmholtz Imaging

THE HIDA COURSE CATALOG

On the HIDA Website, the HIDA Course Catalog provides a central platform for courses and events in the area of IT, information and data science, and thus fosters community-wide sharing of training opportunities in the Helmholtz Association. On the one hand, Helmholtz researchers and employees can browse the catalog for training offers and events at the 18 centers, the five incubator platforms or our research schools. On the other hand, any member of the Helmholtz Association can effortlessly publish and advertise information and data science events organized by their institution throughout the association and beyond. In 2022, the Course Catalog offered 148 courses and events in total. Formats ranged from hackathons, workshops, talks, lecture series to courses, and career events. 8.340 people visited the Course Catalog online in 2022, and of these, 2.360 went on to the websites of the respective courses. These numbers show that the Course Catalog has become an important tool for the Helmholtz community, both, for people offering events and those interested in training opportunities.

TEACH II CONFERENCE

Within the Helmholtz community, people from various areas and with different backgrounds – researchers, training coordinators, instructors and trainers, personnel developers – offer training programs and courses to young scientists. However, developing, deploying, and managing these events requires a great set of skills and resources. To provide an exchange platform to all people involved in education within Helmholtz, HIDA organized the TEACH II Conference – Talk About Education Across Communities in Helmholtz. The virtual event was organized in cooperation with the Helmholtz Open Science Office, HIFIS, HMC and FZJ. It was participant-driven and took place for the second time in November 2022. The meeting tool Gathertown offered a virtual platform in which various workshops, talks, posters, and a keynote provided many opportunities to exchange experiences and best practices in education. Collaboration, the development of innovative teaching ideas, and sharing teaching resources were fostered. One particularly up-to-date contribution was a workshop on Mental Health First Aid – courses, whose aim is to raise awareness of the rising mental health issues among (young) researchers. The active discussions and fruitful exchange of approximately 30 participants within this online-format clearly showed the need for a regular exchange among individuals involved in education. The conference fostered connections and cooperation between participants from different Helmholtz Centers and Research Schools, and inspired participants to try out new learning methods and content.

FROM ZERO TO HERO: THE INCUBATOR SUMMER ACADEMY 2022

In September 2022, the five Helmholtz Incubator platforms HIDA, Helmholtz AI, Helmholtz Imaging, HIFIS and HMC collaboratively organized a two-week Summer Academy for Helmholtz doctoral researchers and postdocs as well as a small number of external scientists. The two main aims were to advance the research of these young scientists by offering a broad set of courses in the area of information and data science, and to foster collaborations between scientists from different research areas within and across the Helmholtz community. In addition, external young scientists were admitted to attract new talents to the Helmholtz community.

The academy started with an opening ceremony. This included an interview with the Helmholtz president Otmar D. Wiestler on "Key Skills for the Next Generation of Scientists". In addition, the director of Helmholtz AI Fabian Theis gave a keynote on "Artificial Intelligence in Biomedicine: How We Enable a Cellular View of Human Health with Big Data". The two-week program consisted of 19 courses and workshops, designed for three different levels of expertise. The consecutive structure of the program allowed participants with no prior knowledge to reach intermediate or even advanced knowledge in the course of the Incubator Summer Academy. Courses and workshops ranged from introductions to different programming languages or machine learning to events on reproducibility, metadata or statistical learning. The program furthermore included other formats like lectures held by international experts, a data challenge, as well as a career corner with representatives from within and outside Helmholtz.

More than 400 individuals registered for the Incubator Summer Academy. Most of them affiliated with at least one Helmholtz Center, while roughly 12% were external. The number of registrations shows the immense demand for training opportunities in information and data science. All courses were fully booked, and 229 participants successfully completed at least one course and received a certificate. The collaboration of the five Incubator platforms for this event strengthened the sense of community and further highlighted the importance of the Incubator for the Helmholtz Association.

MAKING RESEARCH SOFTWARE MORE SUSTAINABLE – THE EUSSI TRAINING BAZAAR

In November 2022, HIDA joined forces together with Helmholtz AI and HIFIS to take on an active role in the European Software Sustainability Institute (EuSSI) Training Bazaar. Different European training initiatives shared their goals, approaches, and experiences regarding the training for research software engineering. HIDA, Helmholtz AI and HIFIS gave an overview of their approaches. The event provided a kick-off to actively network with international training initiatives outside of Helmholtz.

III | 5. Networking Events

In 2022, HIDA has further expanded its portfolio of events. A particular highlight was the HIDA Office Launch, which finally took place. In addition, the focus of HIDA's activities was on career and networking events and new series with partners. A major goal of HIDA's events is to create contacts between scientists from the Helmholtz Centers and data scientists, partners and initiatives from all over the world. HIDA's activities also help to make Helmholtz known as an attractive employer for talents in data science. HIDA thus presents itself as an important player in the field of information and data science.

HIDA OFFICE LAUNCH

The Helmholtz Information & Data Science Academy officially opened the doors of its Berlin premises on May 31, 2022 with the event HIDA Office Launch - The Creation of a Hub for Innovation, Information & Data Science. For this purpose, HIDA invited selected guests and partners from politics, science, and business. After two years of pandemic and intensive digital work, HIDA presented itself as a dynamic, innovative hub and as a forum for training and exchange in information and data science. The event offered exchange and networking opportunities, introduced the new image film about HIDA and displayed its six research schools with an exhibition. Young investigators presented AI and data science projects from their schools and were available for discussions about the data- and information-driven future. In addition, the HIDA team provided insights into HIDA's portfolio.

Projects presented from HIDAs six research schools:

- Tabea Rettelbach from HEIBRiDS explained her research topic, which is dedicated to the climate change in polar regions and the state of Arctic permafrost soils.
- Patricia Schöntag from MarDATA showed how self-navigating underwater vehicles, equipped with data science technologies, are able to acquire more and even more accurate data and images of our oceans.
- Paul Maria Scheikl from HIDSS4Health is engineering a robotic assistant for gallbladder surgery; guests could imitate the work of a surgeon on a screen and with a video game controller.
- Ke Li from DASHH, equipped with VR googles, showed how virtual reality technology could enable the work in hard-to-reach areas, such as in a modern accelerator facility. For this, she was using a lab, built from Lego bricks.
- Max Siska and Laura Helleckes from HDS-LEE explained how scientists could conduct and analyze numerous biotech experiments simultaneously with the help of data science technologies. These bring massive improvements and are also of interest to industries.

Max Siska from HDS-LEE explains at the HIDA Office Launch how scientists could conduct numerous biotech experiments simultaneously. (Photo: Verena Brüning)

Ke Li from DASHH shows how virtual reality technology could enable the work in hard-to-reach areas. (Photo: Xenia von Polier)

CAREER EVENTS

» Data Jobs for Health@Helmholtz

On March 17, 2022, the virtual recruiting event Data Jobs for Health at Helmholtz took place for the first time. Together, DKFZ, HZI, FZJ, DLR, Helmholtz Munich/MUDS and CASUS addressed talented data scientists from Master to Postdoc, that have a background in life and health sciences. People from 63 countries registered for the event. 224 visitors followed the seven talks given by Helmholtz data scientists. The hybrid talks came from a studio in the HIDA office. Afterward, 30 Helmholtz data scientists in search of talents had 155 video chats with attendees.

During the conference program, Andreas Kosmider (Head Office Helmholtz Association) started with introducing Helmholtz, its Health Research Division, and HIDA. Afterwards, excellent speakers gave keynotes on their group's research and open positions: Keno März (Division of Intelligent Medical Systems) and Moritz Gerstung (Division AI in Oncology) from DKFZ, Yang Li (Computational Biology for Individualised Medicine) and Philipp Münch (Computational Biology of Infection Research) from HZI, Andrea Rizzi (Institute for Advanced Simulation) from FZJ, Martin Kühn and Philipp Rosauer (Institute of Software Technology) from DLR and Niki Kilbertus (Reliable Machine Learning) from Helmholtz Munich. Participants could meet the speakers or their team members in networking sessions and talk to the centers' recruiters, e.g. about open positions.

The event was promoted via Google, LinkedIn and Twitter. This increased awareness of HIDA's offerings internationally: the ads gained more than 3000 clicks. In addition, HIDA started an email campaign to approach graduate schools for data science and health in Europe. The schools passed the offer through to their students - what drew attention to HIDA and the data science jobs at Helmholtz: On the day of the event, HIDA's job page had 210 visits. On this website, HIDA collects all the data science jobs that are offered by the Helmholtz Centers.

» Helmholtz Career Day for Data Science and IT

On November 15, 2022, HIDA invited to the third Helmholtz Career Day for Data Science and IT. The joint appearance of 13 Helmholtz Centers, platforms and research schools reached data scientists and IT experts worldwide: 609 participants from 77 countries visited the online event. Its focus was on career paths in IT and data science in the six Helmholtz research fields: Energy, Earth and Environment, Health, Aeronautics, Space and Transport, Matter and Information

Julia Schnabel (Helmholtz Munich) and Thomas Jung (AWI) spoke about their research and careers at Helmholtz. In a panel on Working with IT, Data Science and Supercomputers@Helmholtz with interactive Q&A, Helmholtz scientists from FZJ, KIT and GFZ reported on career paths and opportunities. Scientists had also the opportunity to exchange ideas with the participants in short, Chatroulette-like video chats. In 159 network sessions, the visitors encountered approximately 50 data scientists and experts from Helmholtz Centers.

Andreas Kosmider and Viktoria Schwarze welcome the participants of the third Helmholtz Career Day. (Photo: HIDA)

HACKATHONS, DATATHONS AND CHALLENGES WITH HIDA

Since 2020, HIDA has successfully conducted numerous hackathons, datathons and challenges in cooperation with other Helmholtz platforms, centers and HIDA partners, no matter if virtually, hybrid or on-site. At these events, teams are developing solutions to a problem using data sets and data science methods, which will afterwards be presented and awarded. One goal of these events is the development of solutions to scientific questions from the centers, using data science methods.

» Helmholtz GPU Hackathon

The Helmholtz GPU Hackathon took place from March 29-31, 2022 in Berlin. At the hybrid event, teams of scientists accelerated their own codes on GPUs, using a programming model or machine learning system of their choice. For the Helmholtz GPU Hackathon 2022, HIDA supported HZDR, FZJ, NVIDIA and OpenACC in organizing the event and also helped to facilitate the hybrid implementation at the AI Campus in Berlin, a partner of HIDA. At the event, 27 participants collaborated in five teams from four countries. On the last day, the teams shared and discussed their results in presentations. HIDA also supported the event and its promotion via social media.

The participants of the Helmholtz GPU Hackathon. (Photo: HIDA)

» International AI Archeology Challenge with IDSI (Israel)

From April 26-27, 2022, HIDA co-organized the hackathon International AI Archaeology Challenge, together with partners from Ben-Gurion University, the Israel Data Science Initiative (IDSI), and Helmholtz Imaging (HIP). The goal of the challenge was to investigate ancient structures in the Negev Desert using modern AI methods in order to contribute to future sustainable cultivation techniques. 21 scientists in seven teams from Israel and Germany took part in the virtual challenge. Three Helmholtz Centers (DLR, HZDR, FZJ) were represented. The team of Yi Wang, Chenying Liu (Helmholtz/DLR) and Dheeraj Sharma (Banaras Hindu University) won the first price. In just two days, they developed a code that scientists at Ben Gurion University can use to identify partially obscured ancient structures on aerial photographs. The result can support scientists to figure out how the potential use of surface runoff can help to increase the global food production in the context of climate change.

» Data Challenge Help a Hematologist out

The virtual challenge Help a Hematologist out took place on September 14-23, 2022, and was part of the first Helmholtz Incubator Summer Academy - a joint event of all five Helmholtz Incubator Platforms HIDA, HMC, Helmholtz Imaging, HIFIS and Helmholtz AI. HIDA organized the event in cooperation with Helmholtz AI and the Helmholtz Institute of AI for Health. The goal of the challenge was to find intelligent domain transfer solutions for the classification of blood cells. The classification is important for the diagnosis of diseases like anemia or leukemia and is currently done manual most of the times. For one week, 23 participants in nine teams worked virtually on the task. The members came from seven centers (FZJ, HZDR, DKFZ, KIT, Hereon, DESY, HZB), mentors from the platforms and centers supported them. The teams used the new Helmholtz Data Challenges Platform for the challenge. The three best teams presented their results at the closing ceremony of the challenge and received prizes. The ceremony also served as the closing event of the Incubator Summer Academy.

CONFERENCE ATTENDANCES

» Innovation Summit Tel Aviv

At the Helmholtz Innovation Summit on June 13, 2022 in Tel Aviv, HIDA emphasized HIDA's partnership with the Israel Data Science Initiative (IDSI) by sharing an interview with Prof. Paul Feigin, Director IDSI, and Dr. Andreas Kosmider, Head of Strategic Initiatives, Helmholtz Association, and showing a film about the exchange program for doctoral researchers of both countries.

» hub.Berlin Conference

HIDA arranged the Incubator's participation at the hub.Berlin Conference in Berlin on June 23, 2022 with a masterclass on AI: "Open Data For All!? The Data Pipeline from Generation to AI Application in Science" with Dr. Wolfgang zu Castell (HMC/GFZ), Dr. Guido Juckeland (Helmholtz AI/HZDR) and Dr. Andreas Kosmider (Head of Strategic Initiatives, Helmholtz Association).

At the Helmholtz Innovation Summit, Paul Feigin, Director IDSI, and Dr. Andreas Kosmider, Head of Strategic Initiatives, Helmholtz Association, emphasized the importance of the partnership between HIDA and IDSI. (Photo: Xenia von Polier)

HIDA LECTURE SERIES

In 2021, HIDA established the HIDA Lecture Series. They are organized together with the six schools and (inter)national partners. The lectures support the exchange of information between the schools and the partners and they are promoting Helmholtz as an employer. The virtual HIDA Lectures cover all research areas of the schools and Helmholtz Centers. The event is open to the public. The international data science community and especially the doctoral researchers of Helmholtz are invited.

In 2022, HIDA continued the series successfully and implemented two lectures with Israel during the Helmholtz Incubator Summer Academy. HIDA promoted the lectures and published the videos of the events on its website. Well-known data scientists presented their research in the lectures and shared ideas with the participants:

Date	Lecture	Speaker	Participants
26.01.2022	HIDA Lectures@ HIDSS4Health	Ulf Leser, Humboldt Universität Berlin	140
23.02.2022	HIDA Lectures@ HIDSS4Health	Julia Schnabel, Helmholtz Munich	153
24.03.2022	HIDA Lectures@ MarDATA	Markus Reichstein, Max-Planck-Institut für Biogeochemie	45
27.04.2022	HIDA Lectures@ HEIBRIDS	Dirk Brockmann, HU+RKI	40
23.06.2022	HIDA Lectures@ DASHH	Pushmeet Kohli, DeepMind	115
16.09.2022	HIDA Lectures	Itzik Klein, University of Haifa, Israel	15
21.09.2022	HIDA Lectures	Uri Hershberg, University of Haifa, Israel	20
10.11.2022	HIDA Lectures@ MarDATA	Murat Eren, Universität Oldenburg (HIFMB)	68

EVENT SERIES IN COOPERATION WITH HELMHOLTZ PARTNERS

» Helmholtz Entrepreneurs Series (Helmholtz AI and HIDA)

In 2022, HIDA started the new event series Helmholtz Entrepreneurs in cooperation with Helmholtz Transfer and Helmholtz AI. The first event took place on June 22, 2022: Helmholtz Entrepreneurs: From Idea to I Did. Helmholtz researchers could join a crash course on entrepreneurship from Klara Lindner (Mobisol) and could talk with two young start-up founders, Ingmar Wolff from heliopas.ai and Lucas Steinmann from preML. The event was held for a second time and part of the Helmholtz Incubator Summer Academy on September, 20, 2022 in a similar setting. A third event with a focus on finance took place in January 2023.

» HMC Fair Fridays (HMC supported by HIDA)

In 2022, the Helmholtz Metadata Collaboration (HMC) has launched the HMC Fair Friday lecture series in cooperation with HIDA. The series aims to stimulate interdisciplinary exchange on the responsible and sustainable use of research data. It addresses stakeholders in research data management as well as scientists from all research fields of the Helmholtz Association and beyond.

Date	Lecture	Speaker	Participants
18.03.2022	Persistent Identifiers (PIDs): Sustainable Referencing and Value-added Services	Tibor Kálmán	82
29.04.2022	Organizing Scholarly Knowledge and Research Data with the Open Research Knowledge Graph	Sören Auer	66
20.05.2022	FAIR - Assessment or Improvement?	Anusuriya Devaraju	75
24.06.2022	PANGAEA - Core Trust Seal Certified Data Publisher for Earth and Environmental Science	Janine Felden	47
08.07.2022	Automating FAIR Metadata for Software and Datasets Using Open APIs	Tom Morrell	86
23.09.2022	Metadata as a Key? Open Science, Good Scientific Practice and Research Integrity	Roland Bertelmann	88
11.11.2022	Metadata and Data Management Using BEXIS2 System: A Case Study in the Jena Experiment Database	Yuanyuan Huang	26
09.12.2022	HMC FAIR Friday on FAIR for Research Software.	Leyla Jael Castro, Oliver Bertuch	76

» Reproducibility Workshops with the Helmholtz Open Science Office

In June 2022, HIDA and the Helmholtz Open Science Office co-organized a one-day workshop on "Enabling Reproducibility in Data Science". 96 people from different Helmholtz Centers, Helmholtz Research Schools and Helmholtz partners registered for the event. In two lectures and three hands-on workshops, they learned about the importance of reproducible research, suitable tools and methods, and best practice. Experts from HMC, DLR, HZDR, and the Helmholtz Open Science Office led the lectures and workshops. HIDA is planning to continue the cooperation and organize more workshops regarding reproducibility in science in 2023.

III | 6. Events at the HIDA Hub

The HIDA Hub of approximately 80 square meters offers the infrastructure for a wide range of event formats - from smaller meetings to larger events (up to 60 people). All rooms come with modern technical equipment and access to fibre optic cable and are therefore an excellent hub where data-driven minds are able to come together in the heart of Berlin (Friedrichstraße 171, 10117 Berlin). HIDA aims to promote collaboration and the interdisciplinary exchange of ideas in information and data science. To this end, the HIDA Hub is available to employees of all Helmholtz Centers, programs, working groups and committees who want to host data science events and meetings in order to bring together data scientists and to nurture the exchange of knowledge and data science methods.

Due to the Covid-19 pandemic, the HIDA Hub had limited use until spring 2022. Since then, the use has increased again. Scientists from various Helmholtz Centers used the office space. The HIDA Hub accommodated 24 events in 2022.

Meeting point Arena. (Photo: HIDA)

Listed below are the events that took place at the HIDA Hub in 2022.

- 19.01.2022: Meeting Helmholtz Open Science
- 17.03.2022: Streaming Data Jobs for Health @Helmholtz
- 16.05.2022: Visit of the AK Bildung & Wissenschaft of the FDP/DVP parliamentary group
- 31.05.2022: HIDA Office Launch
- 08.06.2022: HEIBRiDS next lecture onsite and ECDF
- 15.06.2022: Visit AWI Executive Board
- 23.06.2022: Visit of the state committee for science & research of the FDP Berlin
- 21.06.2022: Meeting Allianz AG 6 / Preliminary Hearing
- 28.06.2022: Meeting HIDA Liaison Officer
- 07.07.2022: Meeting Allianz AG 6 / Debriefing of the hearing
- 26.08.2022: Meeting of the NFDI4Earth Academy
- 07.09.2022: HMC TF Survey Retreat
- 16.09.2022: Streaming HIDA Lecture: Data-Driven Inertial Sensing
- 22.09.2022: Meeting of the VA-Forschungsbereichsplattform Gesundheit
- 28.09.2022: Meeting of the VA-Forschungsbereichsplattform Erde Umwelt
- 17.10.2022: VOICE e. V. Regionaltreffen Ost
- 19.10.2022: VA-Forschungsbereichsplattform Energie
- 24.-25.10.2022: Meeting AWI Cooperation - Norway - France
- 15.11.2022: Streaming Helmholtz Data Science Career Day
- 17.11.2022: Helmholtz Science Lunchtalk: Green Hydrogen for our Sustainable Future
- 28.11.2022: Visit of the Embassy of India - Science & Technology
- 29.11.2022: MDC-Retreat
- 30.11.2022: Strategy Meeting HIFIS
- 07.12.2022: Meeting of the VA-Forschungsbereichsplattform Information

III | 7. Communication

In 2022, HIDA has continued to expand its communication activities in order to make its and the school's numerous activities visible and to establish the HIDA as a key institution for professional development and networking in the field of information and data science. To this end, HIDA addressed its target groups through a variety of communication channels. HIDA's communication continued to provide intensive support for the recruiting and outreach activities of the schools and for its talent scouting and employer branding activities last year. The objective was to promote the Helmholtz Centers as attractive employers for national and international data science talents. In order to address these talents and promote its offerings, HIDA produced an image film as well as a film about the exchange program with Israel.

HIDA also held a string of info events at twelve Helmholtz Centers between June and October 2022, organized together with the centers. The aim of this series was to promote HIDA's offers and especially the exchange programs with its focus group doctoral and postdoctoral researchers. Through these events, HIDA was able to reach over 330 Helmholtz researchers.

WEBSITE

The HIDA website expanded to a central platform that promotes and makes cross-community education and training offers visible. It was also SEO-optimized. With the Course Catalog, HIDA provided ongoing information about data science courses and events throughout the Helmholtz Association, while the HIDA Job Board presented current job openings in information and data science at all Helmholtz Centers. Furthermore, calls for proposals from the schools as well as announcements for the HIDA exchange programs and HIDA events were advertised extensively on the website. In addition, HIDA expanded its news section with portraits of doctoral researchers and Helmholtz PIs and reports about the schools. As a new format, HIDA published interviews with international experts in the field of information and data science such as Yoshua Bengio, the world's leading expert in Deep Learning. In total, 73 articles were published in the news section so far.

In 2022, the HIDA website saw a steady increase in user interest. Website visitors in 2022 came from 163 countries (2021: 120 countries): 43% from Germany, 16% from the USA, 8% from the UK, 3% from India, 2% from Nigeria and 28% from other countries. The number of organically generated visitors kept on growing and the average time spend on the HIDA website increased to almost three minutes. This shows that an interested target group is reached by the approach on the website, providing them with information that is relevant to them. The increase of the download rate of information documents by over 124% compared to 2021 also proves this.

With almost 17.000 outbound referrals, many visitors were redirected from the HIDA website to the websites of Helmholtz Centers or Schools - a further increase compared to the previous year (2021: 15.000 outbound referrals). The website thus successfully functioned as a distribution platform and contributed to the visibility of the centers' job, networking, and training offers. This is also shown by the top 10 outbound links from the HIDA website to the institutions of the Helmholtz Association in 2022 (number of unique link clicks):

1.	**HIFIS-Events**	**3.025**
2.	**helmholtz.de**	**2.173**
3.	**FZ Jülich**	**992**
4.	**DLR**	**740**
5.	**MDC Berlin**	**601**
6.	**HDS-LEE**	**317**
7.	**HIDSS4Health**	**330**
8.	**UFZ**	**311**
9.	**MuDS**	**237**
10.	**Jobs KIT**	**219**

The HIDA Job Board generated much of the outbound traffic to the centers' websites: In 2022, it had 14.318 page views and counted 3.214 clicks on the job ads of the Helmholtz Centers. The Course Catalog also contributed to traffic from the HIDA website to the centers' websites: In 2022, there were 8.341 page views on the Course Catalog and over 2.360 clicks on the centers' course offerings.

FIG.10 - HIDA WEBSITE: PROPORTION OF VISITORS BY COUNTRY

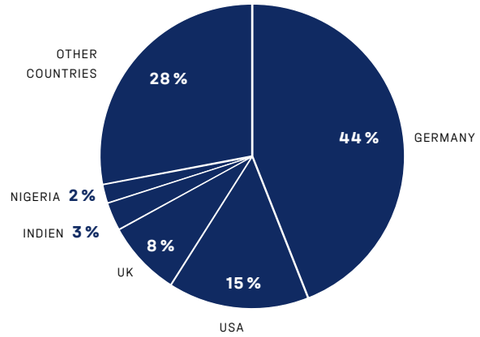


FIG.11 - HIDA WEBSITE: VISITORS IN 2022 CAME FROM 163 COUNTRIES

SOCIAL MEDIA AND NEWSLETTER

In 2022, HIDA continued to use various social media channels to provide information about its own offerings, the information and data science offerings from the Helmholtz network, and to promote events. As the user numbers show, HIDA's social media channels are well established and they are growing steadily: The Twitter channel @HIDAdigital grew to more than 3.600 followers in 2022; posts reached 925.000 impressions. In total, the HIDA Twitter profile had more than 103.000 visits last year. The HIDA LinkedIn profile has almost doubled its followers in 2022 and was followed by 2.085 people by the end of 2022. HIDAs LinkedIn posts reached more than 800.000 impressions.

In June 2022, HIDA launched a campaign on Twitter and LinkedIn with doctoral researchers from the six Helmholtz Information & Data Science Schools. The goal was to gain even greater visibility for the schools and their doctoral researchers. In the four weeks that the campaign ran, HIDA featured 20 doctoral researchers and their research projects on its social media channels. On the campaign visuals, the doctoral researchers explained what excites and motivates them most about the research in the field of information and data science at their school. The campaign reached a total of more than 33.000 views.

As new form of communication, HIDA also established the Job Alert Friday. Since July 2022, HIDA presents a hand-picked data science job opening at a Helmholtz Center every Friday on its social media channels. At the end of 2022, the traffic analysis showed that the Job Alerts became an important tool to help the centers attract qualified employees: In six months, the posts on Twitter were seen more than 22.000 times and on LinkedIn more than 9.000 times. In total, the Job Alerts stimulated more than 720 clicks on the job ads of the centers.

With its newsletter, HIDA provided regular updates on HIDA's offerings and news and shared information about ongoing activities of the Friends of HIDA to its data science community. In addition, special newsletters inform occasionally about special events or calls for proposals. The HIDA Newsletter had approximately 1.500 subscribers by the end of 2022 (900 in 2021). In the newsletter, the links to further information on offers such as courses, events, exchange programs and articles had a total of 1.640 clicks.

Twitter and LinkedIn are HIDA's social media channels with a steadily growing reach.

In June 2022, HIDA launched a campaign on Twitter and LinkedIn with doctoral researchers from the six schools.

Since July 2022, HIDA presents a hand-picked data science job opening at a Helmholtz Center every Friday.

ART MEETS SCIENCE

In 2021, HIDA launched the exchange program Art Meets Science, together with the Academy for Theatre and Digitality (Dortmund). With this program, the two partners support artists and technicians (e.g. coders, programmers, etc.) in carrying out a self-organized research stay. In total, the research project comprises five months, of which the first and fifth month are spent at the Academy in Dortmund and months two to four at one of the 18 Helmholtz Centers. HIDA supports the three month research stay at a Helmholtz Center with the HIDA Research Scholarship. With the joint project, HIDA and the Academy of Theatre and Digitality want to promote the development of formats that open up the topic of data science to the public artistically. HIDA thus aims to provide the opportunity to experiment with new methods, to promote the transfer of knowledge between science, technology and art, and to make cutting-edge research based on artificial intelligence accessible to the theater and cultural scene.

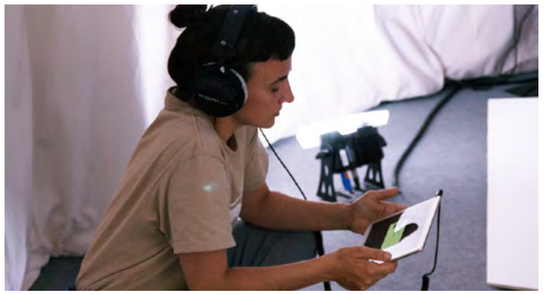
In 2022, the first two projects, (“Common Grounds” and “The (Un)Answered Question”, had their successful premieres. For the second round of the fellowship, the „Disco Earth“ project was recommended for funding. This project started in October 2022 in cooperation with GERICS (Climate Service Center Germany) and the Hereon Helmholtz Center.

» Funded Projects

Bnaya Halperin-Kaddari and Kerstin Ergenzinger. Common Grounds: Sounding out Arctic Warming

The project is realized together with Julia Boike from the Alfred-Wegener-Institute, Helmholtz Center for Polar and Marine Research (AWI).

The issue of the climate crisis is so vast and complex that its urgency is often difficult to grasp. The Arctic is currently warming at an unprecedented rate and terrestrial Arctic landscapes are changing rapidly. In the Common Grounds project, research data from the Arctic is made audible and touchable using sonification techniques. At the center of Common Grounds, the HIDA Fellows Kerstin Ergenzinger and Bnaya Halperin-Kaddari of the Sono-Choreographic Collective designed a walk-through, acoustic art installation. It is based on a dataset of 20 years of hourly weather measurements, recorded at 78° north latitude in the Svalbard archipelago in Norway. The weather data is made audible through various sonification methods, forming a polyphonic "chorus" that compresses these 20 years into a one-hour sound loop. Within this environment, a map and audio guide help create a common ground for listening - allowing visitors to sensually experience the complexities of weather data that make up the climate in a given region. The spatial sound and light environment was exhibited from October 10 to November 30 2022 at the Alfred-Wegener-Institute in Potsdam. Additional exhibitions are currently being prepared.



In the Common Grounds project, research data from the Arctic is made audible and touchable using sonification techniques.
(Photo: Kerstin Ergenzinger/Bnaya Halperin-Kaddari)

The light and sound installation of Common Grounds.
(Photo: Kerstin Ergenzinger/Bnaya Halperin-Kaddari)

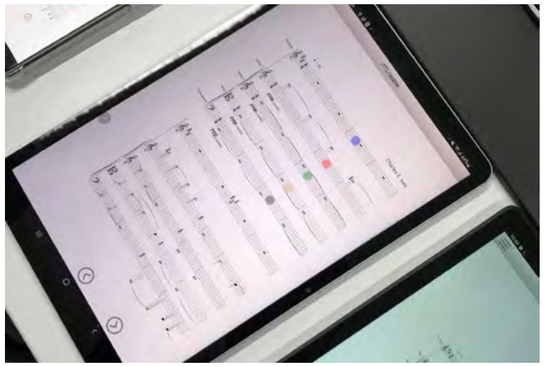
Martin Hennecke: The (Un)Answered Question - A Musical Data Science Experimental Set-up

Two working groups from different Helmholtz Centers collaborated for this project, the leading researchers were Thoralf Niendorf from the Max Delbrück Center for Molecular Medicine (MDC) and Andreas Schreiber from the German Aerospace Center (DLR). The project was also realized by a cooperation with the Saarland State Theatre.

In collaboration with scientists from DLR and MDC, the composer and HIDA Fellow Martin Hennecke has devised a special application situation for data science: The (Un)answered Question. The experimental concert was premiered at the Saarland State Theatre on November 8, 2022. For this project, artificial intelligence composed various live remixes of a piece of classical music. Based on Ralph Waldo Emerson's poem "The Sphynx" and the piece "The Unanswered Question" by American composer Charles Ives, Martin Hennecke had previously developed a prototype for the performance as part of his HIDA fellowship. At the premiere, the two interwoven works were modified through the use of artificial intelligence. Crucial to the result was a variety of audience data - including pulse and facial expression, which were captured using fitness trackers and emotion recognition via image recognition software. An algorithm then processed this data into a live remix of the original composition, which was played by the orchestra in two versions (data from the left and right halves of the audience). The result was an immersive and exclusive live experience in the sold-out "Alte Feuerwache" of the State Theatre in Saarbrücken. The concert was followed by a panel discussion in which scientists from the Berlin Ultrahigh Field Facility of the MDC and the DLR Institute for Software Technology participated and reported on their involvement in the project.

Particularly noteworthy about this Art Meets Science project was the media response. Reports about the project were published by the following news sites: Zeit Online, FAZ, FOCUS Online, Stern.de, DIE WELT, and Saarbrücker Zeitung. TV and radio stations also reported on it: the SR talked about The (Un)Answered Question on radio and TV, while the Tagesschau showed footage in its Nachtjournal and the ZDF reported on it during ZDF Logo and ZDF Heute. On 30 November 2022, the Saarland State Orchestra received the "Innovation 2022 Award" by the German Orchestra Foundation for this project.

The experimental concert The (Un)Answered Question was premiered at the Saarland State Theatre on November 8, 2022. (Photo: Xenia von Polier)



Score elements of The (Un)Answered Question are modified by live data and shown to the musicians on their tablets. (Photo: Martin Hennecke)

III | 8. HIDA Steering Board

The General Assembly of the Helmholtz Association has established HIDA-Steer - the Steering Committee of the Helmholtz Information & Data Science Academy. Top-level researchers are mandated for the steering, monitoring and strategic orientation of HIDA's activities:

HIDA-Steer had two virtual meetings in 2022, on April 8 and September 15.

Prof. Dr. Sabine Attinger
UFZ

Dr.-Ing. Manuel Dahmen
FZJ

Prof. Dr. Stephan Frickenhaus
AWI

Dr. Dr. Daniel Hübschmann
DKFZ

Dr. Uwe Konrad
HZDR

Prof. Dr. Alice McHardy
HZI

Prof. Dr. Uwe Ohler
MDC

Prof. Dr. Nina Rohringer
DESY

Prof. Dr. Julia Anne Schnabel
Helmholtz Munich

Prof. Dr. Achim Streit
KIT (SCC)

Prof. Dr. Wolfgang Wiechert
FZJ

Prof. Dr. Xiaoxiang Zhu
TUM

IV. FACTS & FIGURES ON THE HELMHOLTZ INFORMATION & DATA SCIENCE SCHOOLS

DASHH Data Science in Hamburg HELMHOLTZ Graduate School for the Structure of Matter

IV | 1. Data Science in Hamburg (DASHH) — Helmholtz Graduate School for the Structure of Matter

The Data Science in Hamburg - Helmholtz Graduate School for the Structure of Matter (DASHH) aims to educate the future generation of data and information scientists that will tackle tomorrow's scientific challenges coming along with large-scale experiments on an interdisciplinary level.

In DASHH, the Deutsches Elektronen-Synchrotron (DESY) cooperates with world-leading large-scale research facilities and other key-research institutions and universities from Hamburg and other northern German states to provide innovative training and cooperation for doctoral researchers in the field of information and data science. In using intelligent algorithms, DASHH is pioneering the development of new collaborative approaches to evaluate complex, heterogeneous data.

Research Areas: Data challenges in particle physics, structural biology, materials science, ultrafast x-ray science, accelerator science, computer science, and applied mathematics.

Partners of DASHH: DESY, Universität Hamburg (UHH), Hamburg University of Technology (TUHH), Helmut-Schmidt-University Hamburg (HSU), Helmholtz Center hereon, Helmholtz Center for Infection Research (HZI), Max Planck Institute for the Structure and Dynamics of Matter (MPSD), European XFEL (EuXFEL), Hamburg University of Applied Sciences (HAW).

APPLICANT SITUATION AND RECRUITMENT

In 2022, DASHH could welcome seven doctoral researchers. The 55 applicants came from 16 countries, 18% were female. 32 doctoral researchers are currently enrolled with a dissertation project at DASHH of which 25 are men and seven are women. Overall, 13 doctoral researchers are international, 17 are German. The international doctoral researchers are from Argentina, Italy, Romania, Belarus, China, Iran, Syria, Russia, India, Spain, and Colombia.

Additionally, two doctoral researchers at DESY, both male, one international, are associated with DASHH. They are eligible to attend to all DASHH events, attend offered courses and workshops and are also encouraged to pass the DASHH graduate program.

EVENTS AND NETWORKING

In 2022, DASHH organized 29 networking events, 21 lectures and six courses.

» 6 Courses

DASHH (co-)organized six courses. One of the highlights was the MLE Summer School '22 with more than one hundred participants, which was established by the MLE@TUHH initiative: www.mle.hamburg.

DASHH Courses

› 26.02.-08.03.2022: Dr. Theresa Schredelseker & Michael Büker - Science Communication. Write Your Own Blog (Ten participants)
› 10.-11.11.2022: Dr. Julian Golak - Hackathon. Developing New Battery Strategies (Six participants)

DASHH & PEP Courses

› 14.-17.03.2022: Dr. Matthias Mayer - Scientific Presentations (Nine participants)
› 17.-18.11.2022: Dr. Matthias Mayer - Time Management for Doctoral Candidates (Nine participants)
› 25.11.-02.12.2022: Dr. Carsten Rohr - Scientific Writing (Eleven participants)

MLE Summer School '22

› 13.-14.09.2022: Multiple Presenters & Sessions - Machine Learning in Engineering (119 participants)

» 17 Lectures

Data Science Colloquium

In 2022, DASHH continued with its monthly Data Science Colloquium where renowned scientists discuss recent data science challenges. The choice of speakers is up to the doctoral researchers. The colloquium is jointly organized by DASHH, the Center for Data and Computing in Natural Sciences (CDCS), the clusters of excellence CUI - Advanced

Imaging of Matter and Quantum Universe of the Universität Hamburg (UHH), the Department of Informatics of the UHH, the Institute of Mathematics of the Hamburg University of Technology and ahoi.digital - the Alliance of Hamburg Universities for Computer Science. This event is open to all HIDA researchers. In 2022, the Data Science Colloquium took place six times with on average 98 participants.

- 20.01.2022: Prof. Frank Noé - Deep Learning for Molecular Physics (116 participants)
- 08.02.2022: Prof. Gitta Kutyniok - Deep Learning meets Shearlets: Explainable Hybrid Solvers for Inverse Problems in Imaging Science (121 participants)
- 12.04.2022: Prof. Tatyana Krivobokova - Statistical Challenges in Protein Dynamics Modelling (78 participants)
- 23.06.2022: Dr. Pushmeet Kohli - Leveraging AI for Science (137 participants)
- 24.11.2022: Prof. Jörg Behler - Investigating Solid-Liquid Interfaces Using High-Dimensional Neural Network Potentials (62 participants)
- 08.12.2022: Prof. Michael W. Mahoney - Building Foundations for Scientific Machine Learning at Scale (72 participants)

DASHH PhD Seminar Lectures

DASHH organized eleven lectures in the form of PhD seminars, four of which were given by doctoral researchers at the end of their studies.

- 07.01.2022: Prof. Robert Meißner - Importance of Protein Conformational Sampling for Signal Interpretation in Spectroscopy (38 participants)
- 28.01.2022: Prof. Marina Tropmann-Frick - Data and Control for Accelerator Operation at DESY (33 participants)
- 20.05.2022: Dr. Johannes Hagemann - Flat-Field Correction of Dynamic Processes (47 participants)
- 03.06.2022: Prof. Frank Steinicke & Dr. Reinhard Bacher - Welcome to the Particle Accelerator Metaverses: Mixed Reality Technology for High Energy Physics Facility Operations (53 participants)
- 15.07.2022: Prof. Jochen Küpper & Prof. Michael Breuer & Prof. Philipp Neumann - Background and Tenets of Controlled Molecule/Nano Particle Imaging & Multiphysics Simulations of Turbulent Flows with High-Performance Computers & Molecular Continuum Flow Simulation (31 participants)
- 28.10.2022: Prof. Timo Gerkmann - Machine Learning for Speech Signal Processing on Hearing Devices (44 participants)
- 05.12.2022: Prof. Robin Santra - XATOM: Computing Atomic Response at High X-Ray Intensity (39 participants)

DASHH PhD Talks

- 24.06.2022: Stasis Chuchurka - Stochastic Methodology for Superradiance (40 participants)
- 08.07.2022: Yikai Kan - Relativistic Space-Charge Field Calculation by Interpolation-Based Treecode (35 participants)
- 11.11.2022: Michael Größler - Novel Iterative Phasing Algorithm for Serial Crystallography Considering Rotational Displacement Effects (37 participants)
- 25.11.2022: Georgiana Mania - Vecpar - A Multi-Purpose Framework for Efficient Parallelized Execution of Charged Particle Tracking (33 participants)

» 29 Networking Events

In 2021, DASHH organized a match-making workshop to facilitate networking between DASHH PIs and DASHH scientists. It led to promising project proposals that were advertised in 2022 and the positions are to be filled in 2023. In addition, DASHH established the Data Science for Science (DS4S) series with the CDCS and the Leibniz ScienceCampus InterACt to foster and extend scientific collaborations across the Hamburg research institutions. In 2022, seven DS4S events took place.

Monthly get together events with all DASHH doctoral researchers and associated doctoral researchers were organized throughout 2022, either online or on-site. In addition, the doctoral researchers had an annual retreat for the first time in August 2022 at the Baltic Sea to further improve networking between the DASHH researchers. There were inspiring talks with DASHH PIs and doctoral researchers, an invited talk on AI by security expert Mr. Jay Tuck, speed-dating poster sessions with all participants and two social events. The retreat was the first opportunity to have an extensive exchange after two years of pandemic and was very fruitful.

Data Science for Science (DS4S) Series

- 30.03.2022: Prof. Frank Steinicke - B(l)ending Realities - Human Imperfection as Key to the Ultimate Metaverse (63 participants)
- 13.04.2022: Prof. Adrian Mancuso - Exploiting Voluminous Data from a High Repetition Rate X-ray Free Electron Laser for Science: How More can Really Mean More When it Comes to XFEL Data (27 participants)
- 11.05.2022: Dr. Christian Feiler - Predicting the Corrosion Inhibition Efficiencies of Magnesium Dissolution Modulators using Computational Techniques (12 participants)
- 25.05.2022: Hannah Voß - Data Integration of In-House and Publicly Available Proteome Data across Tissue Types, Quantification Techniques and Experimental Setups Overcomes Cohort Size Limitations and Enables Valid Statistical Analysis for Rare Samples (22 participants)
- 08.06.2022: Prof. Jan Baumbach - Privacy-Preserving Clinical Omics Data Profiling (38 participants)
- 06.07.2022: Dr. Lorenz Adlung - May Contain Fat - A Conceptual Introduction to Systems Immunology for Data Scientists (35 participants)
- 20.07.2022: Dr. Gemma Douilhet - Programming Immune Responses in the Skin: Networks, Switches and Codes (25 participants)

DASHH PhD Seminar

- 07.01.2022: Carlos Ortiz Mahecha - Inner Non-Covalent Protein Interactions as New ML Predictor (38 participants)
- 28.01.2022: Arne Grünhagen - Data Analysis of the Optical Synchronization System of the European XFEL (33 participants)
- 20.05.2022: Thea Engler - Flat-Field Correction of Dynamic Processes (47 participants)
- 03.06.2022: Ke Li - Welcome to the Particle Accelerator Metaverses: Mixed Reality Technology for High Energy Physics Facility Operations (53 participants)
- 15.07.2022: Surya Kiran Peravali - Advanced Simulation Methodology for Optimizing Aerodynamic Lenses Used for Single-Particle Diffractive Imaging (31 participants)
- 28.10.2022: Simon Welker - Inverse Problems and Diffusion Models in Speech Processing and Imaging (44 participants)
- 09.12.2022: Laura Budewig - State-Resolved Ionization Dynamics Induced by X-Ray Free-Electron Laser Pulses (39 participants)

DASHH PhD Get Togethers

To strengthen the contact between the doctoral researchers, DASHH has organized ten networking events.

DASHH Retreat

- 22.-24.08.2022: DASHH Researchers - DASHH Retreat @ Baltic Sea (38 participants)

Further Networking Activities

- 10.-11.02.2022: DASHH Researchers & DASHH Applicants - 4th DASHH Admission Workshop (50 participants)
- 21.02.2022: DASHH Researchers - Internal Retreat DASHH (16 participants)
- 05.07.2022: DASHH Researchers & Researchers Interested in DASHH - DASHH Matchmaking Workshop - Call for Proposals 2022 (33 participants)
- 08.12.2022: DASHH Researchers & DASHH Applicants- 5th DASHH Admission Workshop (25 participants)

DASHH Summer Retreat 2022 at the Baltic Sea (Damp) in August 2022. (Photo: DASHH)

PUBLICATIONS

In 2022, DASHH doctoral researchers published 13 first author publications and 36 co-authored articles.

DASHH doctoral researchers are **highlighted**; associated doctoral researchers are marked in *italics*.

» Peer-Reviewed Journal Articles

Ai, X., Allaire, C., Calace, N., Czirkos, A., Elsing, M., Ene, I., Farkas, R., Gagnon, L.-G., Garg, R., Gessinger, P., et al. (2022). A Common Tracking Software Project. Computing and Software for Big Science 6, 8. (DASHH co-author: **Mania, G.**).

Al-Zoubi, A., **Martino, G.**, Bahnsen, F.H., Zhu, J., Schlarb, H., and Fey, G. (2022). CNN Implementation and Analysis on Xilinx Versal ACAP at European XFEL. IEEE 35th International System-on-Chip Conference (SOCC), 1–6.

Benediktovitch, A., **Chuchurka, S.,** Halavanau, A., Krušič, Š., and Rohringer, N. (2022). Modeling of 3D Paraxial X-Ray Superfluorescence Based on Stochastic Differential Equations. Optica High-Brightness Sources and Light-Driven Interactions Congress, EW6A.2.

Bieringer, S., Butter, A., Diefenbacher, S., Eren, E., Gaede, F., Hundhausen, D., Kasieczka, G., Nachman, B., Plehn, T., and Trabs, M. (2022). Calomplification - the Power of Generative Calorimeter Models. Journal of Instrumentation 17, P09028.

Budewig, L., Son, S.-K., and Santra, R. (2022). Theoretical Investigation of Orbital Alignment of X-Ray-Ionized Atoms in Exotic Electronic Configurations. Physical Review A 105.

Grott, S., **Kotobi, A.,** Reb, L.K., Weindl, C.L., Guo, R., Yin, S., Wienhold, K.S., Chen, W., Ameri, T., Schwartzkopf, M., et al. (2022). Solvent Tuning of the Active Layer Morphology of Non-Fullerene Based Organic Solar Cells. Solar RRL 6, 2101084.

Lanzieri, L., Kietzmann, P., Schmidt, T.C., and Wahlisch, M. (2022). Secure and Authorized Client-to-Client Communication for LwM2M. 21st ACM/IEEE International Conference on Information Processing in Sensor Networks (IPSN), 158–170.

Li, K., Bacher, R., Leemans, W., and Steinicke, F. (2022). Towards Robust Exocentric Mobile Robot Tele-Operation in Mixed Reality. 5th International Workshop on Virtual, Augmented, and Mixed Reality for HRI.

Li, K., Choudhuri, A., Schmidt, S., Bacher, R., Hartl, I., Leemans, W., and Steinicke, F. (2022). Taming Cyclops: Mixed Reality Head-Mounted Displays as Laser Safety Goggles for Advanced Optics Laboratories. IEEE Conference on Virtual Reality and 3D User Interfaces Abstracts and Workshops (VRW), 544–545.

Margenberg, N., Kärtner, F., and Bause, M. (2022). Ultrabroadband Simulation of Nonlinear Optical Processes with Finite Element Time Domain Methods. Conference on Lasers and Electro-Optics (CLEO), 1–2.

Martino, G., Aderhold, S., Bellandi, A., Benwell, A., Branlard, J., Doolittle, L., Eichler, A., Fey, G., Gonnella, D., Hoobler, S., et al. (2022). Anomaly Detection Based Quench Detection System for CW Operation of SRF Cavities. 31st International Linear Accelerator Conference (LINAC), 775–777.

Martino, G., and Fey, G. (2022). Runtime Monitoring of c-LTL Specifications on FPGAs Using HLS. 18th International Conference on Synthesis, Modeling, Analysis and Simulation Methods and Applications to Circuit Design (SMACD), 1–4.

Puhlfürß, T., Montgomery, L., and Maalej, W. (2022). An Exploratory Study of Documentation Strategies for Product Features in Popular GitHub Projects. IEEE International Conference on Software Maintenance and Evolution (ICSME), 379–383.

Schütte, M., Eichler, A., Schlarb, H., Lichtenberg, G., and Werner, H. (2022). Convex Synthesis of Robust Distributed Controllers for the Optical Synchronization System at European XFEL. IEEE Conference on Control Technology and Applications (CCTA), 1061–1067.

Srinivasan, V., Brognaro, H., Prabhu, P.R., de Souza, E.E., Guenther, S., Reinke, P., Lane, T., Ginn, H., Han, H., Ewert, W., et al. (2022). Antiviral Activity of Natural Phenolic Compounds in Complex at an Allosteric Site of SARS-CoV-2 Papain-Like Protease. Communications Biology 5, 805. (DASHH co-author: **Größler, M.**).

Tumasyan, A., Adam, W., Andrejkovic, J.W., Bergauer, T., Chatterjee, S., Damanakis, K., Dragicevic, M., Del Valle, A.E., Fruhwirth, R., Jeitler, M., et al. (2022). Search for Higgs Boson Pair Production in the Four b Quark Final State in Proton-Proton Collisions at √s = 13 TeV. Physical Review Letters 129, 081802. (DASHH co-authors: **Rübenach, J., Bayat Makou, M.**).

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Welker, S., Chapman, H.N., and Gerkmann, T. (2022). Blind Drifting: Diffusion Models with a Linear SDE Drift Term for Blind Image Restoration Tasks. The Symbiosis of Deep Learning and Differential Equations II (DLDE).

Welker, S., Peer, T., Chapman, H.N., and Gerkmann, T. (2022). Deep Iterative Phase Retrieval for Ptychography. IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), 1591-1595.

Welker, S., Richter, J., and Gerkmann, T. (2022). Speech Enhancement with Score-Based Generative Models in the Complex STFT Domain. ISCA Interspeech, 2928-2932.

CONFERENCE CONTRIBUTIONS

National

» 26 Posters

- 21.-28.01.2022, European XFEL Users' Meeting 2022, DESY Photon Science Users' Meeting 2022 (Hamburg), "Flat-Field Correction of Highly-Dynamic Processes", Thea Engler (DASHH doctoral researcher).
- 21.-28.01.2022, European XFEL Users' Meeting 2022, DESY Photon Science Users' Meeting 2022 (Hamburg), "Spectral Learning for (Co-) Vibrational Calculations of Weakly-Bound Molecules", Yahya Saleh (DASHH doctoral researcher).
- 21.-28.01.2022, European XFEL Users' Meeting 2022, DESY Photon Science Users' Meeting 2022 (Hamburg), "Self-Optimizing of Reconstruction Parameters Enables Online View for Holographic in-situ Experiments", Johannes Dora (DASHH doctoral researcher).
- 21.-28.01.2022, European XFEL Users' Meeting 2022, DESY Photon Science Users' Meeting 2022 (Hamburg), "Dynamic Structure Investigation of Biomolecules with Supervised and Unsupervised Machine Learning", Amir Kotobi (DASHH doctoral researcher).
- 28.03.-01.04.2022, 14th International Conference on Synchrotron Radiation Instrumentation (Hamburg), "Ptychography for Phase Retrieval in Nuclear Resonance Scattering", Ankita Negi (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Dynamic Structure Investigation and Spectra Prediction of Near Edge X-Ray Absorption Spectroscopy Fine Structure (NEXAFS) Implementing Supervised and Unsupervised Machine Learning Techniques", Amir Kotobi (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Simulation of Capillarity-Driven Flow Dynamics of Water in Nanoporous Silica (MCM-41)", Lars Dammann (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Taming Cyclops: Mixed Reality Head-Mounted Displays as Laser Safety Goggles for High-energy Optics Laboratories", Ke Li (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Predictive Maintenance for the Optical Synchronisation System at the European XFEL", Arne Grünhagen (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Combination of Machine Learning with Finite Element Time Domain Methods for the Ultrabroadband Simulation of Nonlinear Optical Processes", Nils Margenberg (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Spectral Learning for (Co-) Vibrational Calculations of Weakly-Bound Molecules", Yahya Saleh (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Metadata-Based Analysis of Image Quality for Single Particle Cryo-EM", Anna Theresa Cavasin (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Benchmarking Noise Models for Quantum Computing", Tom Weber (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Descriptors Based on the Fragment Molecular Orbital Method for Machine Learning Prediction of X-Ray Absorption in Proteins", Carlos Andrés Ortiz Mahecha (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Deep Iterative Phase Retrieval for Ptychography", Simon Welker (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Phase Retrieval from Crystals with Rotational Displacement", Michael Größler (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Flat-Field Correction of Highly-Dynamic Processes", Thea Engler (DASHH doctoral researcher).
- 15.-19.08.2022, 14th International Workshop on Boosted Object Phenomenology, Reconstruction, Measurements and Searches in HEP (Hamburg), "Calomplification: The Power of Generative Calorimeter Models", Sebastian Guido Bieringer (DASHH doctoral researcher).
- 04.-09.09.2022, DPG Meeting of the Division of Metal- and Materials Physics (Regensburg), "Freezing and Melting of Water in Nanopores: A Temperature-Dependent X-Ray Scattering Study", Lars Dammann (DASHH doctoral researcher).
- 05.-07.09.2022, German Conference for Research with Synchrotron Radiation, Neutrons and Ion Beams at Large Facilities (Berlin), "Ptychography for Phase Retrieval in Nuclear Resonance Scattering", Ankita Negi (DASHH doctoral researcher).
- 07.-09.09.2022, 10th MT Accelerator Research & Development ST3 Meeting (Berlin), "Towards Detecting Ageing Precursors on the European XFEL Beam Control Hardware", Leandro Lanzieri Rodriguez (DASHH doctoral researcher).
- 13.-14.09.2022, MLE Summer School '22 (Hamburg), "Dynamic Structure Investigation and Spectra Prediction of Peptides using Machine Learning Techniques", Amir Kotobi (DASHH doctoral researcher).
- 13.-14.09.2022, MLE Summer School '22 (Hamburg), "DNN-MG: A Neural Network Multigrid Solver for the Navier-Stokes Equations", Nils Margenberg (DASHH doctoral researcher).
- 13.-14.09.2022, MLE Summer School '22 (Hamburg), "Energy Decomposition Based on the Fragment Molecular Orbital Method for Machine Learning X-Ray Absorption in Proteins", Carlos Andrés Ortiz Mahecha (DASHH doctoral researcher).
- 15.-17.09.2022, 35th Chemnitz Finite Element Symposium (Herrsching), "The Neural Network Multigrid Solver for the Navier-Stokes Equations and its Application to 3D Simulation", Nils Margenberg (DASHH doctoral researcher).
- 05.-07.10.2022, CFEL Symposium (Timmendorfer Strand), "New Computational Methods for Serial Crystallography at X-Ray Free Electron Lasers", Michael Größler (DASHH doctoral researcher).

» 17 Talks

- 14.-18.03.2022, DBG-Frühjahrstagung Atomic, Molecular, Quantum Optics and Photonics Section (SAMOP, Erlangen), "Spectral Learning for (Co-) Vibrational Calculations of Weakly-Bound Molecules", Yahya Saleh (DASHH doctoral researcher).
- 21.-25.03.2022, DPG-Frühjahrstagung 2022 (Heidelberg), "Adding Errors to the Quantum Circuit Model", Tom Weber (DASHH doctoral researcher).
- 21.-25.03.2022, DPG-Frühjahrstagung 2022 (Heidelberg), "Search for the Standard Model Higgs Boson in Association with a Bottom-Quark Pair (bbH)", Maryam Bayat Makou (DASHH doctoral researcher).
- 21.-25.03.2022, DPG-Frühjahrstagung 2022 (Heidelberg), "Clustering and Tracking in Dense Environments with the ITkSearch for the Standard Model Higgs Boson in Association with a Bottom-Quark Pair (bbH)", Nicola de Biase (Associated DASHH doctoral researcher).
- 21.-25.03.2022, DPG-Frühjahrstagung 2022 (Heidelberg), "Search for Heavy Higgs Bosons Decaying to Top Quark Pairs Using the CMS Experiment", Jonas Rübenach (DASHH doctoral researcher).
- 26.-28.04.2022, CDCS Opening Symposium 2022 (Hamburg), "Statistics of Generative Calorimeter Models", Sebastian Guido Bieringer (DASHH doctoral researcher).
- 14.05.2022, CFEL Science Seminar (Hamburg), "Theoretical Investigation of Orbital Alignment of X-Ray-Ionized Atoms in Exotic Electronic Configurations", Laura Budewig (DASHH doctoral researcher).
- 16.-18.05.2022, COST Action CA20129 - 1st Annual MultIChem Conference (Boppard am Rhein), "Dynamic Structure Investigation and Spectra Prediction of Peptides by Machine Learning Techniques", Amir Kotobi (DASHH doctoral researcher).
- 13.-17.06.2022, Hausdorff Center for Mathematics Workshop: Synergies between Data Science and PDE Analysis (Bonn), "Deep Spectral Methods for Solving Variational Problems Arising from Differential Equations", Yahya Saleh (DASHH doctoral researcher).
- 15.-19.08.2022, 92nd Annual Meeting of the International Association of Applied Mathematics and Mechanics (Aachen), "Deep Spectral Methods for Solving Variational Problems Arising from Differential Equations", Yahya Saleh (DASHH doctoral researcher).
- 17.08.2022, INET Seminar (Hamburg), "Monitoring of Ageing Precursors on the XFEL", Leandro Lanzieri (DASHH doctoral researcher).
- 04.-09.09.2022, DPG Meeting of the Condensed Matter Section (Regensburg), "Flat-Field Correction of Highly-Dynamic Processes", Thea Engler (DASHH doctoral researcher).
- 07.-09.09.2022, 10th MT Accelerator Research & Development ST3 Meeting (Berlin), "Adaptive Computing Accelerator Platform (ACAP) First Experience and Vitis Tool Chain", Gianluca Martino (DASHH doctoral researcher).
- 13.-14.09.2022, MLE Summer School '22 (Hamburg), "Detecting Faults, Failures, and Anomalies with Machine Learning", Gianluca Martino (DASHH doctoral researcher).
- 13.-14.09.2022, MLE Summer School '22 (Hamburg), "Active and Spectral Learning in Quantum Molecular Physics", Yahya Saleh (DASHH doctoral researcher).
- 25.11.2022, 5th Round Table on Deep Learning at DESY 2022 (Hamburg), "Modelling Quantum States using Normalizing Flows", Alvaro Fernandez Corral (DASHH doctoral researcher).
- 15.12.2022, ITP Seminars - Phenomenology (Heidelberg), "Different Algorithms for Bayesian Neural Networks", Sebastian Guido Bieringer (DASHH doctoral researcher).

International

» 16 Posters

- 28.02.-01.04.2022, HERCULES European School (Grenoble, France), "Lensless X-Ray Microscopy at the Photon Limit", Thea Engler (DASHH doctoral researcher).
- 07.03.2022, International Workshop on Virtual, Augmented, and Mixed-Reality for Human-Robot Interactions (Sapporo, Japan), "Towards Robust Exocentric Mobile Robot Tele-Operation in Mixed Reality", Ke Li (DASHH doctoral researcher).
- 12.-16.03.2022, IEEE Conference on Virtual Reality and 3D User Interfaces (Online), "Taming Cyclops: Mixed Reality Head-Mounted Displays as Laser Safety Goggles for Advanced Optics Laboratories", Ke Li (DASHH doctoral researcher).
- 15.-20.05.2022, Conference on Lasers and Electro-Optics: Applications and Technology (California, USA), "Ultrabroadband Simulation of Nonlinear Optical Processes with Finite Element Time Domain Methods", Nils Margenberg (DASHH doctoral researcher).
- 22.-27.05.2022, IEEE International Conference on Acoustics, Speech and Signal Processing (Singapore), "Deep Iterative Phase Retrieval for Ptychography", Simon Welker (DASHH doctoral researcher).
- 03.-11.06.2022, International School of Crystallography (Erice, Italy), Poster, "Phase Reconstruction of Protein Crystals with Rotational Displacement", Michael Größler (DASHH doctoral researcher).
- 25.-29.06.2022, Molecular Simulation 2022: Present, Past and Future (Erice, Italy), "Dynamic Structure Investigation and Spectra Prediction of Peptides Using Machine Learning Techniques", Amir Kotobi (DASHH doctoral researcher).
- 27.06.-01.07.2022, 14th European Conference on Atoms Molecules and Photons (Vilnius, Lithuania), "Schwinger Bosons for Density Matrices: Permutation Symmetry and Entanglement", Vladislav Sukharnikov (DASHH doctoral researcher).
- 27.06.-01.07.2022, 14th European Conference on Atoms Molecules and Photons (Vilnius, Lithuania), "Stochastic Methodology for Superradiance Based on Positive P Representation", Stasis Chuchurka (DASHH doctoral researcher).
- 12.-17.07.2022, 13th International Particle Accelerator Conference 2022 (Bangkok, Thailand), "Relativistic Space-Charge Force Calculation by Interpolation-Based Treecode", Yi-Kai Kan (DASHH doctoral researcher).
- 21.-26.08.2022, 29th General Conference of the Condensed Matter Division of the European Physical Society (Manchester, United Kingdom), "Simulation of Imbibition-Induced Strain in Oriented Nanoporous Silica (MCM-41) on the Single Pore Scale", Lars Dammann (DASHH doctoral researcher).
- 22.-25.08.2022, PSI-K 2022 Conference (Lausanne, Switzerland), "Energy Decomposition Analysis Based on a Fragment Molecular Orbital Method for Machine Learning X-Ray Absorption in Proteins", Carlos Andrés Ortiz Mahecha (DASHH doctoral researcher).
- 18.-22.09.2022, Interspeech 2022 (Incheon, Korea), "Speech Enhancement with Score-Based Generative Models in the Complex STFT Domain", Simon Welker (DASHH doctoral researcher).
- 17.-21.10.2022, International Symposium on Mixed and Augmented Reality (Singapore), "Mixed Reality Tunneling Effects for Stereoscopic Untethered Video-See-Through Head-Mounted Displays", Ke Li (DASHH doctoral researcher).
- 17.-21.10.2022, International Symposium on Mixed and Augmented Reality (Singapore), "Stereoscopic Video See-Through Head-Mounted Displays for Laser Safety: An Empirical Evaluation at Advanced Optics Laboratories", Ke Li (DASHH doctoral researcher).
- 09.12.2022, NeurIPS Workshop 2022 "The Symbiosis of Deep Learning and Differential Equations II" (New Orleans, USA, and online), "Blind Drifting: Diffusion Models with a Linear SDE Drift Term for Blind Image Restoration Tasks" (virtual), Simon Welker (DASHH doctoral researcher).

» 12 Talks

- 13.-18.02.2022, 42nd EAS - Meeting Extreme Atomic Systems (Riezlern/Kleinwalsertal, Austria), "Stochastic Methodology for Light-Matter Interaction", Stasis Chuchurka (DASHH doctoral researcher).
- 04.-06.05.2022, International Conference on Information Processing in Sensor Networks (Milano, Italy), "Secure and Authorized Client-to-Client Communication for LwM2M", Leandro Lanzieri (DASHH doctoral researcher).
- 09.-13.05.2022, 5th Inter-experiment Machine Learning Workshop (Geneva, Switzerland), "The Power of Generative Calorimeter Models", Sebastian Guido Bieringer (DASHH doctoral researcher).
- 31.05.-02.06.2022, Connecting the Dots 2022 (Princeton, USA), "Vecpar - A Portable Parallelization Library", Georgiana Mania (DASHH doctoral researcher).
- 12.-16.06.2022, 9th International Charge Density Meeting (Aarhus, Denmark), "Experimentally Constrained Wave Function Method", Stasis Chuchurka (DASHH doctoral researcher).
- 22.-24.06.2022, 33rd Canadian Materials Science Conference (Toronto, Canada), "Dynamic Structure Investigation and Spectra Prediction of Near Edge X-Ray Absorption Spectroscopy Fine Structure (NEXAFS) Implementing", Amir Kotobi (DASHH doctoral researcher).
- 03.-06.07.2022, International Conference on Synthesis, Modeling, Analysis and Simulation Methods and Applications to Circuit Design (SMACD) 2022 (Villasimius, Italy), "Runtime Monitoring of c-LTL Specifications on FPGAs Using HLS", Gianluca Martino (DASHH doctoral researcher).
- 28.08.-02.09.2022, International Linear Accelerator Conference (LINAC) 2022 (Liverpool, United Kingdom), "Anomaly Detection Based Quench Detection System for CW Operation of SRF Cavities", Gianluca Martino (DASHH doctoral researcher).
- 29.08.-02.09.2022, Computational Methods in Applied Mathematics (Vienna, Austria), "Spectral Learning for Solving the Schrödinger Equation for Molecules", Yahya Saleh (DASHH doctoral researcher).
- 04.-07.10.2022, 38th IEEE International Conference on Software Maintenance and Evolution (Limassol, Cyprus), "An Exploratory Study of Documentation Strategies for Product Features in Popular GitHub Projects", Tim Puhlfürß (DASHH doctoral researcher).
- 09.-13.10.2022, Low Level RF Workshop 2022 (Brugg, Switzerland), "FPGA-Based Hardware Acceleration of Machine Learning Algorithms for Particle Accelerators", Gianluca Martino (DASHH doctoral researcher).
- 01.-03.11.2022, ML4Jets2022 (New Jersey, USA), "Estimating Uncertainties for Trained Neural Networks", Sebastian Guido Bieringer (DASHH doctoral researcher).

FURTHER NEWS FROM DASHH

» DASHH International Advisory Panel

In March 2022, DASHH welcomed the six members of its International Advisory Panel (IAP): Prof. Holger Gohlke (Heinrich Heine University Düsseldorf & Forschungszentrum Jülich, Germany, panel chair), Prof. Tatyana Krivobokova (University of Vienna, Austria), Prof. Tilmann Rabl (University of Potsdam & Hasso Plattner Institute Potsdam, Germany), Dr. Daniel Ratner (SLAC National Accelerator Lab, Stanford, USA), Prof. Matteo Sonza Reorda (Politecnico di Torino, Turin, Italy), and Dr. Sofia Vallecorsa (CERN, Geneva, Switzerland). Discussions on the future of the graduate school followed in September 2022 as DASHH could welcome the IAP member in Hamburg for a two-day retreat.

» DASHH PhD News

The DASHH doctoral researchers are working on projects ranging from photon science to particle physics. Their profiles and projects can be found on the DASHH website: www.dashh.org/people/doctoral_candidates/index_eng.html

- In March 2022, the DASHH doctoral candidates Tom Weber and Theresa Cavasin presented their research at the Match Days 2022 in Hamburg with a focus on "Big Data in Science". The Match Days are regularly organized by mint:match, a platform for career orientation for pupils about to finish their school education, and the NAT initiative.
- Arne Grünhagen was awarded a poster prize at the CDCS Symposium in April 2022 for his poster entitled "Predictive Maintenance for the Optical Synchronization System at the European XFEL".
- Ke LI presented her project at the HIDA Office Launch in May 2022.
- In May 2022, Gianluca Martino had a collaboration visit at the SLAC National Accelerators Laboratory in California. He gave a talk there, entitled "LCLS-II SRF fault displays for human-in-the-loop anomaly detection" and introducing work on integrating displays for SRF faults in the LCLS-II LLRF system.
- The first MLE Summer School of the Machine Learning in Engineering initiative of the TUHH took place in September 2022. The DASHH doctoral researchers, Gianluca Martino and Yahya Saleh, presented their work as use cases at this summer school.

- In December 2022, Simon Welker's conference contribution "Blind Drifting: Diffusion models with a linear SDE drift term for blind image restoration tasks" was presented at the virtual NeurIPS 2022 Workshop – The Symbiosis of Deep Learning and Differential Equations (DLDE) as a spotlight work.
- Throughout the year, several DASHH doctoral candidates successfully applied for international exchange and Helmholtz Trainee Network programs organized by HIDA: Ke Li – Israel Exchange, Sebastian Bieringer – Norway Exchange, Amir Kotobi & Carlos Ortiz Mahecha – Helmholtz Trainee Network.

» DASHH PI & Scientist News

- In 2022, 80 DASHH PIs and 44 DASHH scientists were involved in DASHH. DASHH welcomed four new PIs in 2022: Prof. Ricardo Usbeck (UHH), Prof. Köhler-Bußmeier (HAW), Prof. Jun.-Prof. Katharina Sophie Isleif (HSU), and Prof. Robin Wilke (HAW).
- In February 2022, a study on X-ray multiphoton-induced Coulomb explosion images complex single molecules was published in Nature Physics. DASHH PI Prof. Robin Santra led the theoretical part of the work.
- In April 2022, the DESY team of Markus Ilchen and DASHH PI Prof. Sadia Bari and Swedish colleagues received research funding by the Röntgen Ångström Cluster (RÅC) as a Swedish-German science collaboration. www.desy.de/news/news_search/index_eng.html?openDirectAnchor=2275&two_columns=0
- In May 2022, DASHH PI Prof. Annika Eichler was appointed for a W2 professorship at the TUHH fostering the research field of data analysis and controls of accelerator systems. www.desy.de/news/news_search/index_eng.html?openDirectAnchor=2287&two_columns=0
- In June 2022, DASHH PI Prof. Henry Chapman received the 2021 Gregori Aminoff Prize for Crystallography by the Royal Swedish Academy of Sciences. www.desy.de/news/news_search/index_eng.html?openDirectAnchor=2318&two_columns=0
- In November 2022, DASHH PI Dr. Alke Meents was awarded the Bjørn Wiik Prize 2022 for his outstanding achievements in his COVID-19 drug research. www.desy.de/news/news_search/index_eng.html?openDirectAnchor=2442&two_columns=1
- In December 2022, DASHH PI Prof. Franz Kärtner was awarded the Laser Instrumentation Award by the Institute of Electrical and Electronics Engineers (IEEE) for his efforts in synchronizing large research facilities with femtosecond precision as the IEEE Photonics Society explained.

» Communication

DASHH has a website (www.dashh.org) and maintains social media accounts on LinkedIn and Twitter. It is also encouraging international researchers to learn more about the school and opportunities via the DAAD website. Mailing lists are announcing the DASHH Data Science Colloquium und the Data Science for Science (DS4S) lecture series.

DASHH established a blog for all doctoral and postdoctoral researchers within Helmholtz and partner organizations to train and encourage science communication in data science fields as part of the transferable skills. Everyone is welcome to join, add blog articles or comment on existing ones: www.hida-blogs.org/.

HDSLEE HELMHOLTZ School for Data Science in Life · Earth · Energy

IV | 2. Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE)

The Helmholtz School for Data Science in Life, Earth and Energy (HDS-LEE) offers a structured doctoral program that aims at excellent graduates of mathematics, computer science, natural sciences and engineering from all over the world. The doctoral researchers at HDS-LEE are trained in all essential areas of information and data sciences as well as in communication and other key qualifications. The training components of the program are strengthened by individually tailored training measures, e.g. at the Jülich Supercomputing Center (JSC).

Research Areas: Data science in the life & medical sciences, earth sciences, and energy systems/materials

Partners of HDS-LEE: RWTH Aachen University, University Hospital Aachen, University of Cologne, German Aerospace Center (DLR), Max-Planck-Institut für Eisenforschung, Forschungszentrum Jülich (FZJ)

APPLICANT SITUATION AND RECRUITMENT

In 2021, a recruiting campaign started to hire the second cohort of doctoral researchers with 435 applicants from 40 nations. During 2022, most vacancies were filled and advertisements expired. Nevertheless, 271 people from 38 nations applied to eleven open positions advertised through the recruiting portal at FZJ (October 12, 2022). A high proportion of applicants was international (90%) and came mostly from Iran (24%), India (15%) and Pakistan (15%). The proportion of women was 28%.

HDS-LEE was able to record immense increase. The number of doctoral researchers grew from 26 to 46. The current 46 PhD positions at HDS-LEE are held by people from 16 nations, 28 of them are Germans. Ten women are among the doctoral researchers. 18 other doctoral researchers are associate members, including four women. Of the associated researchers, 14 come from FZJ, three from RWTH Aachen University, one from University of Cologne and one from University Bonn. In 2022, four doctoral researchers finished their theses; one successfully defended his dissertation and received his doctoral degrees. This results in six submitted dissertations; three were successfully defended in 2021 and 2022.

EVENTS AND NETWORKING

In 2022, HDS-LEE organized 42 events online and onsite: six networking events, 20 lectures and 17 courses.

» 17 Courses

EU Regional School Courses (RWTH)

The EU Regional School is open to doctoral researchers from universities in Germany, Belgium, and the Netherlands. There are four courses per term. It is a series of three-hour "short courses" on various topics in computational science, like fluid mechanics, computer science, molecular dynamics, contact mechanics, or reduced-order modeling. It is attended by a cross-section of doctoral researchers and organized by the International Research Training Group „Hierarchical and Hybrid Approaches in Modern Inverse Problems" (IRTG 2379).

- 19.05.2022: Paolo Bientinesi, Ph.D. – High-Performance Matrix Computations: It's not all about Libraries
- 14.07.2022: Prof. Dr. Roger Sauer – Nonlinear Finite Element Methods

The group of HDS-LEE doctoral researchers at the annual internal retreat in Monschau. (Photo: HDS-LEE)

- 15.09.2022: Prof. Dr. Patrick Anderson- Advances in Single and Multi-Component Computational Rheology
- 15.12.2022: Prof. Martin J. Gander - Time Parallel Time Integration

Lectures on Data Science, Methods & Applications (HDS-LEE)

The Lectures on Data Science, Methods & Applications aim to teach and train the doctoral researchers in all essential elements of data science and information. The doctoral researchers are introduced to the respective disciplines and data science methods, get an insight and apply what they have learned in hands-on sessions. It is organized by HDS-LEE. www.hds-lee.de/events/lectures-on-data-science/

- 14.01.2022: Prof. Ira Assent - Unsupervised Learning
- 12.10.2022: Prof. Harrie-Jan Hendricks-Franssen - Data Assimilation
- 17.11.2022: Dr. Achim Basermann and Dr. Michael Denker - Data Science, Data Management and Scientific Workflows

Transferable Skill Courses (HDS-LEE)

Transferable skill courses aim to foster the professional skills and personal development essential to the successful completion of doctoral projects. The courses are open to the entire group of HDS-LEE doctoral researchers and are organized in cooperation with the Jülich Center for Doctoral Researchers and Supervisors (JuDocS), a center for transferable skills training for doctoral researchers at FZJ. In HDS-LEE, four transferable skill courses are mandatory: "Good Scientific Practice", "Management of a Doctoral Project", "Scientific Writing", and "Academic Presentation".

Additional courses were offered in 2022: "Career Planning Training" and "Efficient Literature Search and Management". The "Career Planning Training" was organized in cooperation with the career center at FZJ, the course "Efficient Literature Search and Management" in cooperation with the central library at FZJ.

Furthermore, a mental health course was offered, with a particular focus on communication with supervisors.

- 26.01.-27.01.2022 and 06.-07.12.2022: Career Planning Training
- 22.-23.03.2022 and 08.-09.11.2022: Management of a Doctoral Project
- 03.03.2022: Managing a Constructive Relationship between Doctoral Reseachers and their Supervisors, in cooperation with HIDSS4Health
- 19.-20.05.2022: Scientific Presentation
- 02.-03.06.2022: Scientific Writing
- 30.09.2022: Good Scientific Practice
- 01.-02.12.2022: Efficient Literature Search and Management

» 20 Lectures

HDS-LEE Seminar Series

In the HDS-LEE Seminar Series, data science experts from the application areas Life, Earth and Energy are invited to present the current state of their research to other interested researchers. The doctoral researchers have the chance to meet experts in the individual research fields. www.hds-lee.de/events/seminar-series

- 30.11.2022: Prof. Sebastian Trimpe - Gaussian Process Regression in Learning Control

SSD Seminar Series (SSD, JARA-CSD)

Experts are invited to present their research in a seminar series, operating on a semester-based schedule. The aim is to invite speakers relevant to the SSD (School for Simulation and Data Science - a cooperation of RWTH Aachen and FZJ), but potentially also for a wider audience. Such seminars provide opportunities for learning about state-of-the-art research, and for interaction and discussion with top experts. The seminar series invites up to 20 speakers per year. A combination of national and international guest speakers is anticipated.

- 10.01.2022: Dr. Patrick Simon Stumpf - Digital Twins in Biomedical Research - Towards a Systems-Level Model of Human Disease
- 17.01.2022: Dr. Daniel Caviedes-Voullième - Performance Portability for Earth System Modeling: Who, Why, How?
- 20.01.2022: Prof. Christian Rohde - Compressible Two-Phase Flow across Scale using Sharp and Diffuse Interface Ideas
- 24.01.2022: Prof. Susanne Buiter - Geodynamic Experiments on the Formation of Plate Margins during Continental Break-Up
- 31.01.2022: Binbin Lin, M. Sc. and Dr. Daniel Utt and Setareh Medghalchi, M. Sc. - Computational and Experimental Methods in Material Science
- 16.06.2022: Jun.-Prof. Abhishek Khetan - Solid State Batteries: What's the Hype all about?
- 23.05.2022: Prof. Karsten Urban - The Reduced Basis Method in Space and Time: Challenges, Limits and Perspectives
- 13.06.2022: Daniel Bogdoll, M.Sc - How to Fail a Startup after Graduation
- 20.06.2022: Prof. Karol Miller - Patient-Specific Solution of the Electrocorticography Forward Problem in Deforming Brain
- 27.06.2022: Prof. Britta Nestler - Accelerated Microstructure Design by High Performance Materials Simulations
- 11.07.2022: Prof. Surya Kalidindi - A new AI/ML Framework for Materials Innovation
- 19.08.2022: Prof. Hanyu Gao - Computational Modelling for Chemical Process and Reaction Design
- 24.10.2022: Dr. Anna-Lena Gerner - Arbeiten mit Daten in der Versicherungsbranche
- 07.11.2022: Dr. Tim Gerrits - Scientific Visualization of Complex and High Dimensional Data: Dealing with Tensor Fields and Vector Field Ensembles
- 14.11.2022: Dr. Sebastian Stinner - Using CES for more Sustainability
- 05.12.2022: Mātē Koch - Environments - Large Scale Simulation for Analysing Complex Situations
- 12.12.2022: Prof. Dr. David Bommes - Hexahedral Mesh Generation with Integer-Grid Maps
- 19.12.2022: Atilla Sezen, M.Sc. - Entry as CES Graduate in Plant Engineering Lifecycle Services

Charlemagne Distinguished Lecture (SSD, JARA-CSD)

The AICES doctoral researchers organize the prestigious Charlemagne Distinguished Lecture as part of the SSD Seminar Series. For inspiration for their own scientific achievements, the researchers invite persons, who have achieved impressive accomplishments throughout their career.

- 12.10.2022: Prof. Dr. Wolfgang Dahmen - Predictive Science and Deep Learning - an Odd Couple?

» 5 Networking events

The weekly virtual coffee breaks were well attended in 2022 and used as a platform to get feedback on the current situation of the doctoral researchers. The coffee break was initiated in 2020 to enable an informal exchange between the doctoral researchers and to have the possibility to have regular contact to the coordinator team. In addition, a virtual women lunch enables the exchange between female doctoral researchers: They network, learn about programs for female scientists and get to know other female experts in their field.

The discussion group meetings received great interest in 2022. In these informal meetings, doctoral researchers present their work and answer questions. The aim is to exchange knowledge and build cooperation between the doctoral researchers.

The Presentation Club continued its work in 2022. It allows doctoral researchers to practice giving presentations and giving feedback.

In 2022, the annual internal retreat took place onsite for the first time. It was held as hybrid event in Monschau with talks and team building activities (20.-22.06.2022) www.hds-lee.de/events/internal-retreat/. The retreat is a platform where doctoral researchers inform each other about their latest research results and open issues. It is a forum for knowledge transfer and information exchange. The doctoral researchers give presentations on current research topics (both results and open issues). Additionally, an internal poster session was realized in April 2022 to strengthen the group networking.

- 29.04.2022: Poster event
- 20.-22.06.2022: Annual internal retreat
- 29.06.2022: Doctoral seminar: Discussion groups on video presentations
- 01.09.2022: Doctoral seminar: Discussion groups on video presentations
- 02.08.2022: Presentation Club
- Weekly Coffee Break
- Monthly Women Lunch

PUBLICATIONS

In 2022, 25 first author publications and 17 co-authored publications were published as peer-reviewed journal articles or conference proceedings. Two conference proceedings were awarded. HDS-LEE doctoral researchers gave 48 talks at conferences and they were involved in six talks given by collaborating scientist of their projects. One talk was awarded at a conference. HDS-LEE doctoral researchers presented their projects in 28 posters at conferences and were involved in the work of two other posters presented at conferences.

HDS-LEE doctoral researchers are **highlighted**, associated doctoral researchers are marked in *italics*.

» Doctoral Theses

E. Cramer, (2022). Normalizing Flow-Based Scenario Generation for Energy System Optimization, RWTH Aachen University, Dissertation, defended

J. Kruse, (2022). Machine Learning of Power Grid Frequency Dynamics and Control: Prediction, Explanation and Stochastic Modelling, University of Cologne, Dissertation, submitted

G. Santarpia, (2022). RepOdor: A Manually-Curated, Comprehensive Repository of Odorants and their Olfactory Receptors, RWTH Aachen University, Dissertation, submitted

Alper Yegenoglu, (2022). Gradient-Free Optimization of Artificial and Biological Networks Using Learning to Learn, RWTH Aachen University, Dissertation, submitted

» Peer-reviewed Journal Articles and Conference Proceedings

C. Betancourt, *T.T. Stomberg, A.-K. Edrich, A. Patnala,* M.G. Schultz, R. Roscher, J. Kowalski, and S. Stadtler, (2022) Global, High-resolution Mapping of Tropospheric Ozone – Explainable Machine Learning and Impact of Uncertainties. Geoscientific Model Development, 15(11): p. 4331-4354.

L. Beumer and I. Niemeyer (2022). Developing a Big Data Framework for Processing Sentinel-2 Data in the Context of Nuclear Safeguards. ESARDA Bulletin - The International Journal of Nuclear Safeguards and Non-proliferation. 64(1).

L. Boledi, B. Terschanski, S. Elgeti, and J. Kowalski. A Level-set Based Space-time Finite Element Approach to the Modelling of Solidification and Melting Processes. Journal of Computational Physics. 457.

P.C. Bottcher, D. Witthaut, and *L.R. Gorjão* (2022). Dynamic Stability of Electric Power Grids: Tracking the Interplay of the Network Structure, Transmission Losses, and Voltage Dynamics. Chaos, 32(5): p. 053117.

E. Cramer, *L.R. Gorjão*, A. Mitsos, B. Schäfer, D. Witthaut, and M. Dahmen (2022). Validation Methods for Energy Time Series Scenarios from Deep Generative Models. IEEE Access (Institute of Electrical and Electronics Engineers), 10. 8194-8207.

E. Cramer, A. Mitsos, R. Tempone, and M. Dahmen (2022). Principal Component Density Estimation for Scenario Generation Using Normalizing Flows. Data-Centric Engineering, 3.

E. Cramer, L. Paeleke, A. Mitsos, and M. Dahmen (2022). Normalizing Flow-based Day-ahead Wind Power Scenario Generation for Profitable and Reliable Delivery Commitments by Wind Farm Operators. Computers & Chemical Engineering, 166.

J. Ebert, **D.T. Doncevic,** R. Kloß, and S. Kesselheim (2022). Hearts Gym: Learning Reinforcement Learning as a Team Event. Proceedings of the 3rd Teaching Machine Learning and Artificial Intelligence Workshop (PMLR), 2022 (accepted).

C. Fricke, **D. Wolff,** M. Kemmerling, and S. Elgeti (2022). Investigation of Reinforcement Learning for Shape Optimization of Profile Extrusion Die Flow Channels. Advances in Computational Science and Engineering 2022 (accepted).

C. Gerloff, K. Konrad, D. Bzdok, C. Busing, and V. Reindl (2022). Interacting Brains Revisited: A Cross-brain Network Neuroscience Perspective. Human Brain Mapping, 43(14): p. 4458-4474.

C. Gerloff, K. Konrad, J. Kruppa, M. Schulte-Rüther, and V. Reindl (2022). Autism Spectrum Disorder Classification Based on Interpersonal Neural Synchrony: Can Classification be Improved by Dyadic Neural Biomarkers Using Unsupervised Graph Representation Learning? Medical Image Computing and Computer Assisted Intervention – MICCAI: 5th International Workshop on Machine Learning in Clinical Neuroimaging (conference proceedings).

S.H.M. Germscheid, A. Mitsos, and M. Dahmen (2022). Demand Response Potential of Industrial Processes Considering Uncertain Short-term Electricity Prices. AIChE Journal (American Institute of Chemical Engineers), 68(11).

L.R. Gorjão, L. Vanfretti, D. Witthaut, C. Beck, and B. Schafer (2022). Phase and Amplitude Synchronization in Power-Grid Frequency Fluctuations in the Nordic Grid. IEEE Access (Institute of Electrical and Electronics Engineers), 10: p. 18065-18073.

Y. Guo, F. Dietrich, T. Bertalan, **D.T. Doncevic,** M. Dahmen, I.G. Kevrekidis, and Q. Li (2022). Personalized Algorithm Generation: A Case Study in Learning ODE Integrators. SIAM Journal on Scientific Computing, 44(4): p. A1911-A1933.

L.M. Helleckes, J. Hemmerich, W. Wiechert, E. von Lieres, and A. Grünberger (2022). Machine Learning in Bioprocess Development: From Promise to Practice. Trends in Biotechnology (S0167-7799(22)00281-5).

L.M. Helleckes, C. Muller, T. Griesbach, V. Waffenschmidt, M. Moch, M. Osthege, W. Wiechert, and M. Oldiges (2022). Explore or Exploit? A Model-based Screening Strategy for PETase Secretion by Corynebacterium Glutamicum. Biotechnology and Bioengineering, 2022.

L.M. Helleckes, M. Osthege, W. Wiechert, E. von Lieres, and M. Oldiges (2022). Bayesian Calibration, Process Modeling and Uncertainty Quantification in Biotechnology. PLoS Computational Biology, 18(3): p. e1009223.

C. Idzik, D. Hilger, N. Hosters, M. Kemmerling, P. Niemietz, L. Ortjohann, J. Sasse, A. Serafeim, J. Wang, **D. Wolff,** and G. Hirt (2022). Decision Support for the Optimization of Continuous Processes Using Digital Shadows, in Internet of Production: Fundamentals, Applications and Proceedings.

J. Kruse, B. Schäfer, and D. Witthaut (2022). Secondary Control Activation Analysed and Predicted with Explainable AI. Electric Power Systems Research, 212.

C. Müller, P.J. Bakkes, P. Lenz, V. Waffenschmidt, *L.M. Helleckes,* K.E. Jaeger, W. Wiechert, A. Knapp, R. Freudl, and M. Oldiges (2022). Accelerated Strain Construction and Characterization of C. Glutamicum Protein Secretion by Laboratory automation. Applied Microbiology and Biotechnology, 106(12): p. 4481-4497.

S. Pütz, B. Schäfer, D. Witthaut, and **J. Kruse** (2022). Revealing Interactions between HVDC Cross-area Flows and Frequency Stability with Explainable AI. Energy Informatics Academy Conference 2022 (accepted).

V. Reindl, A. Schippers, K. Tenbrock, A.K. Job, *C. Gerloff,* A. Lohaus, N. Heinrichs, and K. Konrad (2022). Caregiving Quality Modulates Neuroendocrine and Immunological Markers in Young Children in Foster Care Who Have Experienced Early Adversity. Journal of Child Psychology and Psychiatry, 63(5): p. 535-543.

M. Röhrig-Zöllner, J. Thies, and A. Basermann (2022). Performance of the Low-Rank TT-SVD for Large Dense Tensors on Modern MultiCore CPUs. SIAM Journal on Scientific Computing, Society for Industrial & Applied Mathematics (SIAM), 44(4): p. C287-C309.

M. Rüttgers, S. Jeon, S. Lee, and D. You (2022). Prediction of Typhoon Track and Intensity Using a Generative Adversarial Network with Observational and Meteorological Data. IEEE Access (Institute of Electrical and Electronics Engineers), 10: p. 48434-48446.

M. Rüttgers, M. Waldmann, W. Schröder, and A. Lintermann (2022). A Machine-learning-based Method for Automatizing Lattice-Boltzmann Simulations of Respiratory Flows. Applied Intelligence, 52(8): p. 9080-9100.

K. Ruzaeva, K. Nöh, and B. Berkels (2022). A Hybrid Multi-Object Segmentation Framework with Model-Based B-Splines for Microbial Single Cell Analysis. IEEE (Institute of Electrical and Electronics Engineers) 19th International Symposium on Biomedical Imaging (ISBI).

C.C. Sachs, **K. Ruzaeva,** *J. Seiffarth,* W. Wiechert, B. Berkels, K. Nöh, and A. Bateman (2022). CellSium: Versatile Cell Simulator for Microcolony Ground Truth Generation. Bioinformatics Advances, 2(1).

M. Einollahzadeh Samadi, S. Kiefer, S.J. Fritsch, J. Bickenbach, and A. Schuppert (2022). A Training Strategy for Hybrid Models to Break the Curse of Dimensionality. PLoS One, 17(9): p. e0274569.

T. Scherr, *J. Seiffarth,* B. Wollenhaupt, O. Neumann, M.P. Schilling, D. Kohlheyer, H. Scharr, K. Noh, and R. Mikut (2022). MicrobeSEG: A Deep Learning Software Tool with OMERO Data Management for Efficient and Accurate Cell Segmentation. PLoS One, 17(11): p. e0277601.

S. Schito, R. Zuchowski, D. Bergen, D. Strohmeier, B. Wollenhaupt, P. Menke, *J. Seiffarth,* K. Noh, D. Kohlheyer, M. Bott, W. Wiechert, M. Baumgart, and S. Noack (2022). Communities of Niche-optimized Strains (CoNoS) - Design and Creation of Stable, Genome-reduced Co-cultures. Metabolic Engineering, 73: p. 91–103.

J.C. Schulze, **D.T. Doncevic,** and A. Mitsos (2022). Identification of MIMO Wiener-type Koopman Models for Data-driven Model Reduction Using Deep Learning. Computers & Chemical Engineering, 161.

K. Sharafutdinov, J.S. Bhat, S.J. Fritsch, K. Nikulina, *M. Einollahzadeh Samadi,* R. Polzin, H. Mayer, G. Marx, J. Bickenbach, and A. Schuppert (2022). Application of Convex Hull Analysis for the Evaluation of Data Heterogeneity between Patient Populations of Different Origin and Implications of Hospital Bias in Downstream Machine-learning-based Data Processing: A Comparison of 4 Critical-care patient Datasets. Frontiers in Big Data, 5.

N. Swainston, C. Kettner, S. Schnell, S. Lauterbach, H. Dienhart, J. Range, *S. Malzacher,* J.-D. Spöring, D. Rother, M.F. Pinto, P. Martins, C. Lagerman, A. Bommarius, A. Vang Høst, J. Woodley, S. Ngubane, T. Kudanga, F. Bergmann, J. Rohwer, D. Iglezakis, A. Weidemann, U. Wittig (2022). EnzymeML: Seamless Data Flow and Modelling of Enzymatic Data. Accepted in Nature Methods.

M. Waldmann, *M. Rüttgers,* A. Lintermann, and W. Schröder (2022). Virtual Surgeries of Nasal Cavities Using a Coupled Lattice-Boltzmann–Level-Set Approach. Journal of Engineering and Science in Medical Diagnostics and Therapy, 5(3).

F. Wellmann, S. Virgo, D. Escallon, M. de la Varga, A. Jüstel, F.M. Wagner, J. Kowalski, *H. Zhao,* R. Fehling, and Q. Chen (2022). Open AR-Sandbox: A Haptic Interface for Geoscience Education and Outreach. Geosphere, 18(2): p. 732–749.

A. Yegenoglu, A. Subramoney, T. Hater, C. Jimenez-Romero, W. Klijn, A. Perez Martin, M. van der Vlag, M. Herty, A. Morrison, and S. Diaz-Pier (2022). Exploring Parameter and Hyper-Parameter Spaces of Neuroscience Models on High Performance Computers with Learning to Learn. Frontiers in Computational Neuroscience, 16: p. 885207.

H. Zhao and J. Kowalski (2022). Bayesian Active Learning for Parameter Calibration of Landslide Run-out Models. Landslides, 19(8): p. 2033–2045.

D. Wolff, C. Fricke, M. Kemmerling, and S. Elgeti (2022). Towards Shape Optimization of Flow Channels in Profile Extrusion Dies Using Reinforcement Learning. Proceedings in Applied Mathematics and Mechanics, 2022 (accepted).

K. Ruzaeva, K. Kusters, W. Wiechert, B. Berkels, M. Oldiges, and K. Nöh (2022). Automated Characterization of Catalytically Active Inclusion Body Production in Biotechnological Screening Systems. International Conference of the IEEE Engineering in Medicine & Biology Society (EMBC), p. 3874–3877.

L. Beumer and I. Niemeyer (2022). A Deep Learning Approach for Safeguards-relevant Change Detection using Sentinel-2 Imagery. Proceedings of the Institute of Nuclear Materials Management 63rd Annual Meeting.

L. Beumer and I. Niemeyer (2022). Change Detection of Nuclear Facilities - Automatic Classification of Sentinel-1 & 2 Data Using Deep Learning. Proceedings of the Symposium on International Safeguards: Reflecting on the Past and Anticipating the Future.

K. Ruzaeva, J.-C. Cohrs, K. Nöh, and B. Berkels (2022). Cell Tracking for Live-cell Microscopy Using an Activity-prioritized Assignment Strategy IPAS: IEEE (Institute of Electrical and Electronics Engineers) International Image Processing Applications and Systems, 2022 (in press, accepted at IEEE IPAS).

» Conference Posters and Talks

C. Aujoulat and A. Matuszyńska (2022). Graph Theory as a Driver for Multi-omic Mechanistic Model Construction Applied to Tomato Glandular Trichomes. International Study Group for Systems Biology Conference (ISGSB), Innsbruck (poster).

D. Chatterjee, P. Bigalke, S. Schnitt, C. Acquistapace, H. Deneke, and S. Crewell (2022). Representation Learning of Cloud Systems Using Energy-based Deep Learning Neural Networks. European Centre for Medium-Range Weather Forecasts-European Space Agency Workshop on Machine Learning for Earth Observation and Prediction (poster).

D. Chatterjee, H. Deneke, and S. Crewell (2022). Understanding Cloud Systems Structure and Organization Using a Machine's Self-learning Capability. 2nd Workshop on Cloud Organization (poster).

M. Einollahzadeh Samadi, S. Kiefer, S. Fritsch, J. Bickenbach, and A. Schuppert (2022). A Training Strategy for Hybrid Models to the Break Curse of Dimensionality: An Application in Mortality Estimation for a Cohort of COVID-19 Patients 2022: 21st International Conference in System Biology ICSB, Berlin (poster + flash talk).

M. Einollahzadeh Samadi and A. Schuppert (2022). Mechanisms of Disease Progression in Critically Ill COVID-19 Patients during ICU Stay 2022: Third International Summer Institute on Network Physiology (ISINP) hosted by Lake Como School of Advanced Studies (poster).

E. Cramer, R. Tempone, A. Mitsos, and M. Dahmen (2022). Nonlinear Isometric Manifold Learning for Injective Normalizing Flows. Stochastic Numerics Workshop @ KAUST, Tuwal Saudi-Arabia (poster).

C. Gerloff, K. Konrad, J. Kruppa, M. Schulte-Rüther, and V. Reindl (2022). Autism Spectrum Disorder Classification Based on Interpersonal Neural Synchrony: Can Classification be Improved by Dyadic Neural Biomarkers Using Unsupervised Graph Representation Learning? Medical Image Computing and Computer Assisted Intervention – MICCAI; 5th International Workshop on Machine Learning in Clinical Neuroimaging, Singapore, Singapore (poster).

J. Guzman and A. Schuppert (2022). Hybrid Models for Cellular Signaling: Meso-scale Pathway Identification. International Conference on Systems Biology (ICSB) (flash talk + poster).

C. Ben Hammouda, N. Ben Rached, R. Tempone, and **S. Wiechert** (2022). Efficient Importance Sampling via Optimal Control for Stochastic Reaction Networks. Stochastic Numerics and Statistical Learning: Theory and Applications Workshop in KAUST Saudi Arabia (poster).

J. Hassan, J. Beck, R. Hahn, and E. von Lieres (2022). Hybrid Chromatography Modelling with Mechanistic Transport Equations and Machine Learned Adsorption Models. DECHEMA Jahrestagung, Aachen, Germany (poster).

J.F. Jadebeck, M. Beyß, M. Weitzel, S. Azzouzi, P. Droste, W. Wiechert, and K. Nöh (2022). FluxML: An Open Standard for Reproducible Modeling in 13C Metabolic Flux Analysis. Computational Modeling in Biology Network (COMBINE – Satellite Event ov ICSB) (poster).

J. Kruse, B. Schäfer, and D. Witthaut (2022). Explainable AI for Power Grid Frequency Stability and Control. 11th DACH+ Conference on Energy Informatics, Freiburg, Germany (poster).

S. Malzacher, P. Warmelink, J. Lohmann, F. Engelmann, J. Range, J. Pleiss, and D. Rother (2022). BioCatHub, a Platform for FAIR Data Acquisiton in Biocatalysis. 2022: Biocat conference (poster + lightning talk).

C. Neubacher, P. Franke, A. Heinlein, A. Klawonn, A. Kindler-Scharr, and A.C. Lange (2022). Coupling Regional Air Quality Simulations of EURAD-IM with Street Canyon Observations – A Machine Learning Approach. European Geosciences Union (EGU), Wien (poster).

C. Neubacher, P. Franke, A. Heinlein, A. Klawonn, A. Kindler-Scharr, and A.C. Lange (2022). Coupling Regional Air Quality Simulations of EURAD-IM with Street Canyon Observations - A Machine Learning Approach. ECMWF ESA workshop on ML for Earth Observation and Prediction, Reading, UK (poster).

B. Oloruntoba (2022). Pan-African High-Resolution Simulations for Agriculture Using Terrestrial Systems Modelling and Data Assimilation. Kirkham Conference (Soil Physics Conference), Skukuza, Kruger National Park South Africa (poster).

A. Patnala, S. Stadtler, M.G. Schultz, and J. Gall (2022). Generating Views Using Atmospheric Correction for Contrastive Self-supervised Learning on Multi-spectral Images. 1st AI4EO (Artificial Intelligence for Earth Observation – Reasoning, Uncertainties, Ethics and Beyond) Symposium of the International AI Future Lab, Ottobrunn (poster).

K. Ruzaeva and K. Nöh, and B. Berkels (2022). A Hybrid Multi-object Segmentation Framework with Model-based B-splines for Single Cell Analysis, ISBI: IEEE International Symposium on Biomedical Imaging (poster).

A. Saxena, N. Polin, B. Berkels, D. Raabe, B. Gault, C. Freysoldt, and J. Neugebauer (2022). A Materials Informatics Framework to Discover Patterns in Atom Probe Tomography Data, Young researcher's Workshop on Machine Learning for Materials, Treiste, Italy (poster).

S. Schnitt, *D. Chatterjee,* P. Bigalke, and S. Crewell (2022). Shallow Convective Organization in the Trades as Seen by Self-learning Artificial Intelligence. 2nd Workshop on Cloud Organization (poster).

M.G. Schultz, C. Betancourt, B. Gong, F. Kleinert, L.H. Leufen, A. Patnala, and S. Stadtler (2022). On the Potential of Transformer Networks for Air Quality Forecasting. Transformers for Environmental Science (ESST), Magdeburg (poster).

J. Seiffarth, B.Wollenhaupt, D. Kohlheyer, H. Scharr, and Katharina Nöh (2022). Understanding Microbial Communities: The Microfluidic Live-Cell Microscopy Toolbox. 2022: 24th EMBL PhD Symposium "The Spectra of Life: Dimensional Breadth in Biological Research", Heidelberg, Germany (poster).

A. Simson, M.S. Boxberg, and J. Kowalski (2022). Enriched Metadata for Hybrid Data Compilations with Applications to Cryosphere Research. Helmholtz Metadata Collaboration (HMC) conference, online (virtual poster).

V.K. Srivastav, A. Kranz, and B. Usadel (2022). The Plantome Database: An Integrated Resource for Plant Phenomics Experimental Data. PhD Workshop Topic 7: Towards a Sustainable Bioeconomy - Resources, Utilization, Engineering and AgroEcosystems (poster).

F. Terhag, P. Knechtges, A. Basermann, and R. Tempone (2022). Parameter-Free Uncertainty Estimates for Volume Predictions in Heart MRIs. Stochastic Numerics and Statistical Learning: Theory and Applications Workshop, Thuwal, Saudi Arabia (poster).

K.J. van der Weg, E. Merdivan, M. Piraud, and H. Gohlke (2022). Improved Classification of Protein Function by a Localized 3D Protein Descriptor and Deep Learning. Helmholtz PhD Workshop Topic 7: Towards a Sustainable Bioeconomy, Leipzig (poster).

K.J. van der Weg, E. Merdivan, M. Piraud, and H. Gohlke (2022). Improved Classification of Protein Function by a Localized 3D Protein Descriptor and Deep Learning. 11th NIC Symposium of the John von Neumann Institute for Computing (NIC), Juelich (poster).

J. Wasmer, R. Mozumder, P. Rüßmann, I. Assent, and S. Blügel (2022). Benchmark Study of Symmetry-adapted ML-DFT Models for Magnetically Doped Topological Insulators. Psi-k (6th general conference for the worldwide Psi-k community), Lausanne, Switzerland (poster).

P. Ackermann, L.H.J. Fleitmann, J. Schilling, J. Kleinekorte, *J.G. Rittig,* F. vom Lehm, A. Schweidtmann, H. Pitsch, K. Leonard, A. Mitsos, A. Bardow, and M. Dahmen (2022). Molecular Design of Spark-Ignition Engine Fuels for Maximal Engine Efficiency. 10th International Fuel Science Conference, Aachen, Germany (talk).

P. Ackermann, L.H.J. Fleitmann, J. Schilling, J. Kleinekorte, *J.G. Rittig,* F. vom Lehm, A. Schweidtmann, H. Pitsch, K. Leonard, A. Mitsos, A. Bardow, and M. Dahmen (2022). Molecular Design of Spark-ignition Fuels by Combining Predictive Thermodynamics and Machine Learning. 32nd European Symposium on Computer-Aided Process Engineering (ESCAPE-32), Toulouse, France (talk).

M.S. Boxberg, **A. Simson,** Q. Chen, and J. Kowalski (2022). Investigation of Ice with Geophysical Measurements during the Transit of Cryobots. European Geosciences Union (EGU), Vienna (short talk).

C. Ben Hammouda, N. Ben Rached, R. Tempone, and S. Wiechert (2022). Efficient Importance Sampling via Optimal Control for Stochastic Reaction Networks. UQ hybrid Seminar (talk).

C. Ben Hammouda, N. Ben Rached, R. Tempone, and **S. Wiechert** (2022). Efficient Importance Sampling via Optimal Control for Stochastic Reaction Networks. SIAM Conference on Uncertainty Quantification; hybrid in Atlanta, Georgia, U.S. (talk).

C. Ben Hammouda, N. Ben Rached, R. Tempone, and **S. Wiechert** (2022). Efficient Importance Sampling via Optimal Control for Stochastic Reaction Networks. 15th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing (MCQMC) (talk).

C. Ben Hammouda, N. Ben Rached, R. Tempone, and **S. Wiechert** (2022). Efficient Importance Sampling via Optimal Control for Stochastic Reaction Networks. GAMM (Gesellschaft für Angewandte Mathematik und Mechanik) (talk).

L. Beumer (2022). Data Science in Nuclear Verification – Extracting Verification-relevant Information from Geospatial Big Data. The European Safeguards Research and Development Association (ESARDA) Annual Meeting (talk).

L. Beumer (2022). Deep Learning for Understanding Satellite Imagery in Support of Safeguards. FONAS (Forschungsverbund Naturwissenschaft, Abrüstung und internationale Sicherheit) Jahrestagung (talk).

L. Boledi, S. Elgeti, and J. Kowalski (2022). Computational Multiphysics Modelling to Predict the Performance of Melting Probes in Ice. The 8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress) (talk).

D. Carta, *M. Zimmer,* T. Pesch, and A. Benigni (2022). Bad Data Detection and Handling in ICT Platform for Energy. 12th IEEE International Workshop on Applied Measurements for Power Systems (talk).

D. Chatterjee, H. Deneke, and S. Crewell (2022). Can Satellite Images Provide Supervision for Cloud Systems Characterization? European Geoscience Union (talk).

D. Chatterjee, H. Deneke, and S. Crewell (2022). Utilizing the Self-learning Capability of a Deep Neural Network and Continuous Monitoring of Geostationary Satellite to Understand Clouds Structure and Organization. European Centre for Medium-Range Weather Forecasts Machine Learning Workshop (talk).

D. Chatterjee, H. Deneke, and S. Crewell (2022). Understanding Cloud Regimes from What they Look like Rather than from What they are: A Bottom-up Approach Based on Deep Learning. The European Organization for the Exploitation of Meteorological Satellites Meteorological Satellite Conference (talk).

A. Demirci, M. Stricker, N. Merkert, D. Weygand, and S. Sandfeld (2022). Statistical Analysis and Machine Learning Of Discrete Dislocation Dynamics Simulations: Initial Structures, Cross-Slip, And Microstructure Evolution. GAMM (Gesellschaft für Angewandte Mathematik und Mechanik), Aachen, Germany (talk).

A. Demirci, M. Stricker, N. Merkert, D. Weygand, and S. Sandfeld (2022). Statistical and Machine Learning Analysis of the Effects of the Cross-slip on the Microstructure Evolution in Discrete Dislocation Dynamics Simulations. Materials Science and Engineering Congress (MSE), Darmstadt, Germany (talk).

A.-K. Edrich, A. Yildiz, R. Roscher, and J. Kowalski (2022). A Modular and Scalable Workflow for Data-driven Modelling of Shallow Landslide susceptibility. European Geosciences Union (EGU) General Assembly (talk).

S. Elgeti, S. Hube, J. Lee, and **D. Wolff** (2022). Intelligent Numerical Design of Components and their Production Processes. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS) (keynote lecture).

S.H.M. Germscheid, M. Dahmen, and A. Mitsos (2022). Lastverschiebungspotenzial Industrieller Prozesse bei Kombinierter Day-Ahead- und Intraday-Strommarktteilnahme. Jahrestreffen der ProcessNet-Fachgemeinschaft Prozess-, Apparate- und Anlagentechnik - PAAT. Frankfurt am Main, Germany (talk).

V. Grimm, A. Heinlein, and A. Klawonn (2022). Physics-Aware Convolutional Neural Networks for Computational Fluid Dynamics Simulations. ECCOMAS 2022 - 8th European Congress on Computational Methods in Applied Sciences and Engineering, Oslo, Norway (talk).

V. Grimm, A. Heinlein, and A. Klawonn (2022). Physics-Aware Convolutional Neural Networks for Computational Fluid Dynamics Simulations. GAMM – 92nd Annual Meeting, Gesellschaft für Angewandte Mathematik und Mechanik, Aachen, Germany (talk).

V. Grimm, A. Heinlein, and A. Klawonn (2022). Physics-Aware Convolutional Neural Networks for Computational Fluid Dynamics Simulations. GACM 2022 – 9th Colloquium on Computational Mechanics, Essen, Germany (talk).

J. Hassan, J. Beck, R. Hahn, J. Schmoelder, and E. von Lieres (2022). Hybrid Process Modelling Combining Mechanistic Equations with Machine Learning. 35th International Symposium on Preparative and Process Chromatography, Baltimore, USA (talk).

J. Hassan, J. Schmoelder, and E. von Lieres (2022). Hybrid Chromatography Modelling with Mechanistic Transport Equations and Machine Learned Adsorption Models. 17th SoCSS Conference, Karlsruhe, Germany (talk).

L.M. Helleckes, T. Griesbach, C. Müller, M. Osthege, B. Geinitz, E. von Lieres, W. Wiechert, and M. Oldiges (2022). Explore or Exploit? A Model-based Screening Strategy for Autonomous Microbial Phenotyping. Recent Advances in Fermentation Technology 14, Orlando (Florida, US) (talk).

L.M. Helleckes, T. Griesbach, C. Müller, M. Osthege, W. Wiechert, and M. Oldiges (2022). Accelerated Microbial Phenotyping: How Process Modelling and a Decision Policy Can Enhance High-Throughput Screening of PETase-Secreting *Corynebacterium glutamicum* Variants. BioProScale, Berlin (talk).

L.M. Helleckes, D. Puchta, H. Czech, C. Müller, H. Morschett, W. Wiechert, and M. Oldiges (2022). From Frozen Working Cell Bank to Final Product Assay – Closing the Loop of Autonomous High-Throughput Strain Characterization. Himmelfahrtstagung, Mainz (talk).

J.F. Jadebeck, M.G. Gollub, A. Theorell, and K. Nöh (2022). Integrating 13C Labeling and Thermodynamic Data for Thermodynamically Consistent Bayesian Metabolic Flux Analysis (T13C-MFA). The 21st International Conference on Systems Biology (ICSB) (talk).

C.A. Köhler (2022). Describing Provenance for the Analysis of Electrophysiological Activity Data. Training Session Enabling Multilevel Data Integration: Turning Data to Knowledge during the INCF Assembly, Online. (talk).

J. Kruse, B. Schäfer, and D. Witthaut (2022). Secondary Control Activation Analysed and Predicted with Explainable AI. Power System Computation Conference (Porto, Portugal) (talk).

A. Mohan, *M. Rüttgers,* W. Schröder, and A. Lintermann (2022). Shape Optimization for Respiratory Flows through Reinforcement Learning. Society for Computational Fluid Dynamics of the Nose and Airway (SCONA), Oklahoma, USA (talk).

K. Patakchi Yousefi and S. Kollet (2022). Closing the Gap between Models and Observations: Deep Learning from Mismatches. European Geosciences Union (EGU) General Assembly 2022, Vienna, Austria (talk).

J.G. Rittig, K. Ben Hicham, A.M. Schweidtmann, M. Dahmen, and A. Mitsos (2022). Predicting Temperature-Dependent Activity Coefficients of Ionic Liquid-Solute Systems through Graph-Based Machine Learning. AIChE (American Institute of Chemical Engineers) Annual Meeting, Phoenix, United States of America (talk).

J.G. Rittig, M. Ritzert, A.M. Schweidtmann, S. Winkler, J.M. Weber, P. Morsch, K.A. Heufer, M. Grohe, A. Mitsos, and M. Dahmen (2022). Computer-Aided Fuel Design with Generative Graph Machine Learning. AIChE (American Institute of Chemical Engineers) Annual Meeting, Phoenix, United States of America (talk).

G. Santarpia (2022). RepOdor, a Manually-Curated, Comprehensive Repository of Odorant Molecules and their Receptors. 18th Annual Meeting of the Bioinformatics Italian Society – Bioinformatics for Unraveling Brain Complexity Workshop (invited talk).

A. Saxena and N. Polin (2022). A Machine Learning Framework to Discover Patterns in Atom Probe Tomography Data, BiGmax Workshop – Atom Probe Tomography & Microscopy, Nanjing, China (online) (talk).

A. Saxena, N. Polin, B. Berkels, D. Raabe, B. Gault, C. Freysoldt, and J. Neugebauer (2022). A Materials Informatics Framework for Microstructure Evaluation in Atom Probe Tomography Data, BiGmax Workshop, Bochum, Germany (talk).

A. Saxena, N. Polin, B. Berkels, D. Raabe, B. Gault, C. Freysoldt, and J. Neugebauer (2022). A Materials Informatics Framework to Discover Patterns in Atom Probe Tomography Data. Deutsche Physikalische Gesellschaft (DPG) meeting, Regensburg, Germany (talk).

J. Seiffarth, B. Wollenhaupt, T. Scherr, O. Neumann, D. Kohlheyer, H. Scharr, R. Mikut, and K. Nöh (2022). Deep Learning Meets Microbial Live-Cell Imaging: Powerful Analysis Workflows from Annotation to Prediction. Helmholtz Imaging Conference, Berlin (talk).

T.T. Stomberg (2022). XAI am Projektbeispiel der Wildnisflächenklassifizierung über KI. Künstliche Intelligenz im Naturschutz (Bundesamt für Naturschutz) (talk).

S.M. Subbiah Pillai, N. Ben Rached, A.L. Haji-Ali, and R. Tempone (2022). Importance Sampling for McKean-Vlasov Stochastic Differential Equation. Special Session Talk at the 15th International Conference on Monte Carlo and Quasi Monte Carlo Methods in Scientific Computing (MCQMC), Johannes Kepler University Linz (talk).

V. Travnikova, N. Dirkes, H. Lubjuhn, D. Wolff, E. von Lieres, and M. Behr (2022). Physics-Informed Neural Networks for Predicting Flow Fields in Bioreactors. GAMM (Gesellschaft für Angewandte Mathematik und Mechanik), Aachen (talk).

K.J. van der Weg, E. Merdivan, M. Piraud, and H. Gohlke (2022). TopEC: Improved Classification of Protein Function by a Localized 3D Protein Descriptor and Deep Learning. German conference on Cheminformatics, Garmisch-Partenkirchen, Germany (talk).

K.J. van der Weg, E. Merdivan, M. Piraud, and H. Gohlke (2022). TopEC: Improved Classification of Protein Function by a Localized 3D Protein Descriptor and Deep Learning. International conference on chemical structures, Noordwijkerhout, Netherlands (talk).

D. Wolff, C. Fricke, M. Kemmerling, and S. Elgeti (2022). Shape Optimization of Flow Channels in Profile Extrusion Dies Using Reinforcement Learning. 92nd Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM) (talk).

D. Wolff, C. Fricke, M. Kemmerling, and S. Elgeti (2022). Reinforcement Learning for Spline-Based Shape Optimization of Flow Channels in Profile Extrusion Dies. 9th GACM Colloquium on Computational Mechanics (GACM) (talk).

D. Wolff, K. Key, E. von Lieres, and S. Elgeti (2022). Physics-informed Neural Networks as Reduced Simulation Models for Bioreactor and Crystallisation Modeling. 8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS) (talk).

A. Yegenoglu (2022). Introduction into the L2L Framework, Bernstein Workshop (online) (talk).

B. Winkels, J. Hofmann, A. Yildiz, *A.-K. Edrich,* H. Schüttrumpf, and J. Kowalski (2022). Quantifying Rainfall Forecast Uncertainty and Error Propagation in Flash Flood and Landslide Prediction Models. European Geosciences Union (EGU) General Assembly (talk – co-author).

I. Steldermann, J. Kowalski, and M. Torrilhon (2022). Moment Approximations for Shallow Flow. International Conference on Hyperbolic Problems: Theory, Numerics and Applications (HYP), Málaga (talk + poster).

T.T. Stomberg, I. Weber, M. Schmitt, and R. Roscher (2022). Jungle-Net: Using Explainable Machine Learning to Gain New Insights into the Appearance of Wilderness in Satellite Imagery. ISPRS Annals of the Photogrammetry, Remote Sensing and Spatial Information Sciences Congress, Nice (talk + poster).

FURTHER NEWS FROM HDS-LEE

» New Partner

HDS-LEE has grown and extends the list of cooperation partners with the University Hospital Aachen. Contact person is Prof. Andreas Schuppert. He has gained particular recognition in recent years for his predictions on intensive care bed occupancy in the COVID-19 pandemic. Thus, HDS-LEE increases its expertise in the field of computational biomedicine.

» Further Activities

D. T. Doncevic published the teaching strategy of the HDS-LEE Hearts Gym Hackathon that took place in 2021, at the Teaching Workshop at the ECML Conference in the paper and talk together with the Helmholtz AI team at FZJ: J. Ebert, D. T. Doncevic, R. Kloß, S. Kesselheim. Hearts Gym: Learning Reinforcement Learning as a Team Event.
www.arxiv.org/abs/2209.05466

» Awards

- L. Beumer received the "Student Paper Award" as "Division Finalist Cyber and Emerging Technology" at INMM 63rd Annual Meeting for the conference proceedings in 2022: L. Beumer and I. Niemeyer, A Deep Learning Approach for Safeguards-relevant Change Detection using Sentinel-2 Imagery.
- L. Helleckes received the 2nd lecture award at BioProScale 2022 for her talk: L.M. Helleckes, T. Griesbach, C. Müller, M. Osthege, W. Wiechert, and M. Oldiges, Accelerated Microbial Phenotyping: How Process Modelling and a Decision Policy Can Enhance High-Throughput Screening of PETase-Secreting Corynebacterium glutamicum Variants.
- K. Ruzaeva received the "Best session paper award" at IEEE IPAS 2022 for the peer-reviewed conference proceedings article: Ruzaeva, K., Cohrs J.-C., Kasahara, K., Kohlheyer, D., Nöh, K., Berkels, B., Cell Tracking for Live-cell Microscopy Using an Activity-prioritized Assignment Strategy (in press).
- H. Zhao received the Borchers-Plakette for finishing doctoral study with "summa cum laude" in 2022.

» Acquired AI and Data Science Projects

Scientists at HDS-LEE have acquired new large-scale AI and data science projects.

- HDS-LEE PI Prof. Martin Grohe (RWTH) received an Advanced Grant of the European Research Council (ERC AdG) for his project "Symmetry and Similarity" for five years (started October 2022). The goal of the ERC project is to develop a theory of graph similarity and to demonstrate its use for problems of practical relevance. This will be done in close connection to HDS-LEE projects.

- The International Research Training Group (IRTG 2379) „Hierarchical and Hybrid Approaches in Modern Inverse Problems" is funded by the German Research Foundation (DFG) and started in October 2018. In November 2022, it was approved for a second phase. It is a cooperation between RWTH Aachen University and the University of Texas at Austin with the following HDS-LEE PIs involved in this program: Prof. Marek Behr, Prof. Alexander Mitsos, Jun.-Prof. Benjamin Berkels, Prof. Julia Kowalski, Prof. Raūl Tempone, and the associated PIs Prof. Abigail Morrison, Prof. Michael Herty, Prof. Stefanie Elgeti. The doctoral theses address modern inverse problems and introduce a new innovative approach to the education of future scientists and engineers. They focus on the challenges posed by the interplay of four specific topics: geometry, data, models, and applications. The training program is open to HDS-LEE doctoral researchers and a regular exchange takes place.

- In the Rhine-Ruhr region, funding has been supplied to plan the establishment of the "Rhine-Ruhr Center for Scientific Data Competence (DKZ.2R)" with Prof. Stefan Sandfeld in the lead (associated PI in HDS-LEE, FZJ). The goals are to support (cultural) change in the handling of research data and the application of current data science and high-performance computing methods and in particular the combination of these methods. Measures include research and scientific transfer as well as outreach, networking, learning, and education. One focus is on training and education of experts at all levels in data literacy in terms of methods and domains with HDS-LEE as one major part. The data competence center is a consortium with research groups at the FZJ, Fraunhofer Institute for Intelligent Analysis and Information Systems, and the Universities of Aachen, Bochum, Bonn, Cologne, Duisburg-Essen, and Düsseldorf as well as the University of Applied Sciences Bonn-Rhein-Sieg. BMBF funding is two-stage: a five month concept phase followed by a three years implementation phase. After the first application phase, the concept phase is funded, starting November 2022.

- The project "LOKI - Integrated Early Warning System for Local Recognition, Prevention, and Control for Epidemic Outbreaks", funded by the Helmholtz Initiative and Networking Fund, was launched in July 2022 as an initiative to mitigate the consequences of epidemiologically relevant outbreaks of infections. In LOKI, four Helmholtz centers - FZJ, Helmholtz Center for Infection Research (HZI), Helmholtz Center for Information Security (CISPA), and German Aerospace Center (DLR) - are collaborating, supported by the Robert-Koch-Institute (RKI) and the Academy for Public Health Services (AÖGW), under the lead of Prof. Michael Meyer-Hermann (HZI). With Prof. Alexander Mitsos (FZJ), Prof. Wolfgang Wiechert (FZJ), and Dr.-Ing. Achim Basermann (DLR), three HDS-LEE PIs are involved in the successful proposal. The aim of LOKI is to provide the local health authorities (LHA) with a platform for early detection, prevention, and mitigation of epidemics with pandemic potential (e.g., SARS, MERS, COVID-19) and recurring outbreaks (e.g., seasonal influenza, measles). In LOKI, data streams from various sources are integrated in a privacy-preserving manner. Data-driven outbreak detection and model-based conditional forecasting are combined and run in fully automated evaluation workflows on HPC resources. An interactive web application allows the customized simulation of user-driven scenarios, empowering LHAs to perform "what-if"-scenario calculations to test non-pharmaceutical interventions and to plan and optimize policy measures.

- HDS-LEE Scientific Director Prof. Wolfgang Wiechert is involved in a Helmholtz Enterprise Spin-off Program named "MiBioLab - Automated Bioprocess Development", funded by Helmholtz in a second phase starting in 2023. The aim is to develop an automated microbioreactor platform to accelerate the development of sustainable bioprocesses. In 2017, the lab got a first funding from the Helmholtz Association to build a Helmholtz Innovation Lab. The goal was to apply the technology in joint research projects with industrial companies. This was the starting point of the Microbial Bioprocess Lab (MiBioLab) as a contract research organization. A digital twin of the lab robotic facility and on-line data processing plays a central role in MiBioLab. Laura Helleckes, a doctoral researcher of MiBioLab, was associated in HDS-LEE in 2021. HDS-LEE will highly profit from the platform and the generated high throughput experimental data.

- The project EMSIG (Event Driven Microscopy for Smart Microfluidic Single-Cell Analysis) is a follow-up project of SATOMI that deals with microfluidic live-cell imaging (MLCI) that provides spatio-temporal insights into population heterogeneity ensuing from a single cell. For becoming a versatile screening tool, MLCI must master the challenge of robust real-time analysis, capable to autonomously detect rare events in hundreds of parallel experiments and to follow their temporal evolution. Using deep-learning empowered image analysis, EMSIG brings live-event detection capabilities to MLCI, to facilitate the reactive optimization of biological event resolution in real-time. EMSIG is funded by the Helmholtz Initiative and Networking Fund, part of the Helmholtz Imaging Platform (HIP), and will start in May 2023 with the following PIs at FZJ: Dr. Dietrich Kohlheyer, Dr. Hanno Scharr (HDS-LEE PI), Dr. Erenus Yildiz (FZJ), Dr. Katharina Nöh (part of the group of HDS-LEE PI Prof. Wolfgang Wiechert, project coordinator), and Prof. Ralf Mikut from KIT who is HIDSS4Health PI and director.

- HDS-LEE PI Prof. Björn Usadel (FZJ) is part of NFDI FAIRagro that is a community-driven initiative within the National Research Data Infrastructure (NFDI) funded by DFG (from 2023-2028). This NFDI consortium is an initiative of NFDI4Agri and focuses on the development of sustainable crop production and agroecosystems. FAIRagro works on an interoperable and scalable research data infrastructure for agrosystems research. It is a consortium of research groups at Leibniz Centre for Agricultural Landscape Research (ZALF), Federal Research Centre for Cultivated Plants (JKI), Information Centre for Life Sciences (ZB MED), Kuratorium für Technik und Bauwesen in der Landwirtschaft (KTBL), Senckenberg Leibniz Institution for Biodiversity and Earth System Research (SGN), Leibniz Institute for Information Infrastructure (FIZ Karlsruhe), Leibniz Institute of Plant Genetics and Crop Plant Research (IPK), University of Bonn, Thünen Institute, and World Agricultural Systems Center of Technical University Munich.

- HDS-LEE PI Prof. Harry Vereecken together with the PIs Prof. Harrie-Jan Hendricks-Franssen, and Prof. Stefan Kollet (FZJ) is part of the Collaborative Research Centers "DETECT - Regional Climate Change: Disentangling the Role of Land Use and Water Management" funded by

DFG from January 2022 - December 2025 with Prof. Dr. Kusche (University of Bonn) in the lead and project partners from FZJ, University of Göttingen and Cologne, ABC/J Geoverbund, and Deutscher Wetterdienst. As existing climate models fail to explain observed patterns of hydrological change sufficiently, in DETECT scientists aim to close this gap in understanding by better comprehending the origin of patterns. Therefore, they will build a modeling framework that explains past observations as realistically as possible, accounts for potential drivers of change that may have been understudied in the past, and can predict future changes. In DETECT, data science (in particular, data assimilation, machine learning and artificial intelligence, and big data analytics) plays an eminent role and methodological developments as pursued in HDS-LEE are of interest for DETECT. In addition, DETECT offers interesting and challenging applications for data scientists.

› The group of HDS-LEE PI Andreas Schuppert (UKA) participates in the BMBF-funded Consortium "Epidemic Hospital Resource Demand - Modeling Incidence, Bedoccupancy, Staffing and Supply Chains - PROGNOSIS" within the BMBF-Program "Strengthening the Modelling Competence on Spreading of Severe Infectious Diseases" funded for three years (May 2022 - April 2025). The focus is to develop a model enabling short- and long-term prognosis based on hybrid ensemble-models of multiple infections on the health care system from hospitalization to ECMO therapies in combination with a simulator for the required logistics management in hospitals. Partners are TU Dresden, University Leipzig, RWTH Aachen, University Münster, and University Augsburg with the associated partners DIVI und ECDC.

› Based on prior work on virtual patients in intensive care, the group of HDS-LEE PI Andreas Schuppert (UKA) is member of the EU-funded CSA "EDITH: Ecosystem for digital twins in healthcare" that started in October 2022. EDITH aims to develop a European roadmap to establish an ecosystem for Digital Twins in Health Care to support the health care systems as well as biomedical research.

› The project "Data- and Knowledge-driven Engineering of Transaminases" led by the HDS-LEE PI Prof. Holger Gohlke aims to develop novel and extend existing physics- and machine learning-based software for the data- and knowledge-driven engineering of transaminases. The collaboration provides a unique opportunity: It combines the expertise of the Gohlke group in developing and applying computational methods in knowledge-driven enzyme engineering, with the expertise of evoxx technologies GmbH. The company is specialized on TAms and the company's acquired data from previous engineering campaigns, as well as the available capacity to generate new data for training and validation of computational approaches. In particular, the project aims to improve TAms (thermo) stability in conditions required for substrate solubilization, activity and selectivity (or promiscuity) towards its substrate, and enantioselectivity towards its product. The results from this project will be included into the HDS-LEE projects of Karel van der Weg and Martin ben Ahmed. It is funded by evoxx technologies GmbH for three years (April 2022 - May 2025).

› In Aachen, the European Digital Innovation Hub (EDIH) Rheinland will be established starting from January 2023 and funded by the European Commission. The European Digital Innovation Hubs (EDIH) will act as central contact points to support companies in responding dynamically to digital challenges and becoming more competitive. EDIH Rheinland focuses on advanced simulation, artificial intelligence, big data, data analytics, data processing, cyber-physical systems, and internet of things, modeling, and digital twins. Several research groups from RWTH Aachen work together: CSD, CATS, AIA, and ITC. The HDS-LEE Prof. Marek Behr will be the contact point for further cooperation of this Innovation Hub with HDS-LEE.

» Communication & Marketing

HDS-LEE has a website (www.hds-lee.de) and is also active on Twitter and uses advertising services. Local recruiting services at FZJ and RWTH were used.

HDS-LEE presented itself at the "Helmholtz Virtual Career Day for Data Science and IT" in November 2022 with a virtual booth. There were 18 talks with interested master's students, doctoral researchers and postdocs from all over the world.

A mailing list (Hds-lee-newsletter@fz-juelich.de) informs about open positions at HDS-LEE, a second mailing list is for scientists that are interested in talks and workshops organized by the school (Hds-lee-event@fz-juelich.de).

HEIBRIDS
HELMHOLTZ EINSTEIN INTERNATIONAL BERLIN RESEARCH SCHOOL IN DATA SCIENCE

IV | 3. HEIBRiDS - Helmholtz Einstein International Research School on Data Science

The Helmholtz Einstein International Research School on Data Science (HEIBRiDS) brings together six Helmholtz Centers and four university partners from the Einstein Center Digital Future (ECDF). The goal of HEIBRiDS is to train a new generation of researchers: skilled data scientists, who understand the demands and challenges of the disciplines in which data science has become indispensable.

Research areas: Data management, machine/deep learning, imaging, mathematical modelling, high-throughput data analytics, molecular medicine, astrophysics, polar and marine research, aerospace, materials science, and geosciences

Partners of HEIBRiDS: Alfred Wegener Institute for Polar and Marine Research (AWI), Deutsches Elektronen-Synchrotron (DESY), the German Aerospace Center (DLR), German Research Centre for Geosciences (GFZ), Helmholtz Zentrum Berlin for Materials and Energy (HZB), Max-Delbrück Center for Molecular Medicine (MDC), Freie Universität Berlin (FU), Humboldt-Universität Berlin (HU), Technische Universität Berlin (TU), Charitē-Universitätsmedizin Berlin.

Six out of the seven new doctoral researchers of HEIBRiDS (Photo: Felix Noak)

APPLICANT SITUATION AND RECRUITMENT

In 2022, HEIBRiDS recruited the fourth cohort of seven doctoral researchers (three female, four international). They started their projects between July and October 2022. The School received 84 applications from 24 nationalities. In addition, four new doctoral researchers (one female, two international) became associated to HEIBRiDS.

Two HEIBRiDS researchers from the first cohort have successfully defended their thesis. Two additional researchers have submitted their thesis and are in the process of planning their defense.

EVENTS AND NETWORKING

In 2022, HEIBRiDS organized two events, 13 seminars and 15 lectures.

» 2 Events

› 29.-31.03.2022, HEIBRiDS Spring School, online. The HEIBRiDS Spring School included a seminar on "Quantum Computing" and an interactive workshop on "Data Science Career outside Academia".
www.heibrids.berlin/events-training/spring-schools/heibrids-spring-school-2022/

› 12.-14.10.2022, HEIBRiDS mid-term evaluation, in-person.

HEIBRiDS underwent a successful mid-term evaluation. The written report was submitted end of August and the on-site evaluation took place on 12-14 October. The feedback from the panel of nine external reviewers was that HEIBRiDS has been true to its mission of educating young researchers on the interface of data science and domain expertise. The continuation of the school was strongly recommended.

HEIBRiDS mid-term evaluation, October 2022 (Photo: Felix Noak)

» 13 PhD Seminars

The HEIBRiDS PhD Seminar takes place every second Wednesday in summer and winter semesters. Every seminar starts with a round table, where each doctoral researcher gives a short update on what they have been working on. Following this, one of the doctoral researchers gives a more detailed presentation with slides on their recent research.

» 15 HEIBRiDS Lectures on Applying Data Science

This biweekly lecture is open to the public. Data science experts from academia and industry are invited to give insights into their work. The HEIBRiDS Lecture Series attracts 25-40 attendants per event.
www.heibrids.berlin/events-training/lecture-series/

- 05.01.2022: Sheeba Samuel (University of Jena) – Reproducible Research: Responding to 6W and 1H Questions of Data Provenance
- 19.01.2022: Claudia Draxl (HU Berlin) – Similarity of Materials and Data-Quality Assessment by Unsupervised Learning
- 02.02.2022: Fereshta Yazdani (Lufthansa Industry Solutions) – Artificial Intelligence: A Cross-sectional Technology with Algorithmic Prejudices
- 16.02.2022: Kerstin Ritter (Charitē Universitätsmedizin) – Machine Learning in Clinical Neuroimaging
- 27.04.2022: Dirk Brockmann (HU Berlin) – The Data Donation Project – How Wearable Sensors Can Help in Dealing with the COVID-19 Crisis
- 11.05.2022: Christoph Gröger (Bosch) – There Is No AI Without Data: Industry Experiences on the Data Challenges of AI
- 25.05.2022: Alexandra Grebe de Baron (Bayer) – The Real-World Data Store, a Data Product to Accelerate Evidence Generation
- 08.06.2022: Jochen Schiller (FU Berlin) – Security Aspects in the Internet of Things – Think of Risks and Side Effects in Advance!
- 22.06.2022: Holger Schwarz (University of Stuttgart) – Enterprise Data Landscapes: Data Lakes and Data Marketplaces
- 06.07.2022: Laleh Haghverdi (MDC) – Dimension-reduction and Data Visualization; Applications and Challenges in Single-cell Biology
- 20.07.2022: Klemens Böhm (KIT) – Energy Status Data – Towards a Better Energy Footprint with Informatics Methods
- 19.10.2022: Johann-Christoph Freytag (HU Berlin) – Processing of (Scientific) Data in the Age of Data Science
- 02.11.2022: Pat Reed (Cornell University) – MultiSector Dynamics: Advancing the Science of Complex Adaptive Human-Earth Systems
- 16.11.2022: Ruth Fong (Princeton University) – Directions in Interpretability
- 30.11.2022: Henning Sprekeler (TU Berlin) – Data Science and Machine Learning in Neuroscience

PUBLICATIONS

In 2022, 21 first author publications and five co-authored articles were published by HEIBRiDS doctoral researchers.

Doctoral researchers from HEIBRiDS are **highlighted**. Associated HEIBRiDS doctoral researchers are in *italics*. Co-first authorship is labeled ǂ.

» Doctoral Theses

Agarwal S. (2022). Unraveling the Interior Evolution of Terrestrial Planets through Machine Learning. Technische Universität Berlin.

Münchmeyer J. (2022). Machine Learning for Fast and Accurate Assessment of Earthquake Source Parameters. Implications for Rupture Predictability and Early Warning. Humboldt Universität zu Berlin.

» Peer-reviewed Journal Articles and Conference Proceedings

Kirschbaum, T., Petit, T., Dzubiella, J., and Bande A. (2022). Effects of Oxidative Adsorbates and Cluster Formation on the Electronic Structure of Nanodiamonds. J. Comput. Chem. 43, 13, 923-929.

Pfalz, G., Diekmann, B., Freytag, J.-C., Sryrkh, L., Subetto, D.A., and Biskaborn, B.K. (2022). Improving Age-depth Correlations by Using the LANDO Model Ensemble. Geochronology, 4, 269-295.

Ghosh, B., Garg, S., and Motagh, M. (2022). Automatic Flood Detections from Sentinel-1 Data Using Deep Learning Architectures. ISPRS Ann. Photogramm. Remote Sens. Spatial Inf. Sci., V-3-2022, 201-208.

Singh, K., , J., Weber, L., Leser U., and Bande, A. (2022). Graph Neural Networks for Learning Molecular Excitation Spectra. J. Chem. Theory Comp., 18, 7, 4408-4417.

Woollam ǂ, J., **Münchmeyer ǂ, J.,** Tilmann, F., Rietbrock, A., Lange, D., Bornstein, T., Diehl, T., Giunchi, C., Haslinger, F., Jozinović, D., Michelini, A., Saul, J., and Soto, H. (2022). SeisBench – A Toolbox for Machine Learning in Seismology. Seismological Research Letters, 93, 3, 1695-1709.

Münchmeyer, J., Lesera, U., and Tilmann, F. (2022). A Probabilistic View on Rupture Predictability: All Earthquakes Evolve Similarly. Geophysical Research Letters, 49, 13, e2022GL098344.

Lilienkamp, H., von Specht, S., Weatherill, G., Caire, G., and Cotton, F. (2022). Ground-Motion Modeling as an Image Processing Task: Introducing a Neural Network Based, Fully Data-Driven, and Nonergodic Approach. Bull. Seismol. Soc. Am. 112, 1565-1582.

Tillmann, P., Jäger, K., Karsenti, A., Kreinin, L., and Becker, C. (2022). Model-chain Validation for Estimating the Energy Yield of Bifacial Perovskite/Silicon Tandem Solar Cells. Sol. RRL, 202200079.

Vlot, A.H.C., Maghsudi, S., and Ohler, U. (2022). Cluster-independent Marker Feature Identification from Single-cell Omics Data Using SEMITONES. Nucleic Acids Research, gkac639.

Miranda, N., Freytag, J-C., Nordin, J., Biswas, R., Brinnel, V., Fremling, C., ... and van Santen, J. (2022). SNGuess: A Method for the Selection of Young Extragalactic Transients. Astronomy & Astrophysics, 665, A99.

Weber, L., Sänger, M., Garda, S., Barth, F., Alt, C., and Leser, U. (2022). Chemical-Protein Relation Extraction with Ensembles of Carefully Tuned Pretrained Language Models. Database, baak098.

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FURTHER NEWS FROM HEIBRIDS

- Two HEIBRiDS doctoral researchers and two associated HEIBRiDS doctoral researchers have participated in the HIDA Israel Exchange Program: Lusinē Nazaretyan has been granted funding for a six-week stay at the Hebrew University of Jerusalem. Hermann Stolte, Peter Hirsch and Ivo Daniel have been granted funding for a six-week stay at Technion - Israel Institute of Technology.
- HEIBRiDS doctoral researcher Femke van Geffen has been granted funding for a three-month stay at the Department of SAR Technology, DLR in Munich, with the HIDA Trainee Network Network.
- The Helmholtz AI project Artificial Intelligence for X-ray Absorption Spectroscopy has been granted to HEIBRiDS PI Annika Bande (lead PI) and HEIBRiDS doctoral researcher Kanishka Singh from HZB, and researchers from Hereon. The core of this project is to utilize molecular graphs in combination with the probabilistic analysis of molecular motifs for a supervised machine learning prediction trained on data obtained for smaller building blocks of the huge molecules of interest.
- HEIBRiDS doctoral researcher Jannes Münchmeyer received an Outstanding Student and PhD candidate Presentation (OSPP) Award at the General Assembly of the European Geoscience Union in Vienna in May 2022. www.egu.eu/awards-medals/ospp-award/2022/jannes-munchmeyer

HiDSS 4HEALTH | HELMHOLTZ INFORMATION & DATA SCIENCE SCHOOL FOR HEALTH

IV | 4. Helmholtz Information & Data Science School for Health - HIDSS4Health

The goal of the Helmholtz Information & Data Science School for Health (HIDSS4Health) is to train and promote the best young talents at the interface between data science and health. HIDSS4Health offers a structured doctoral program with close integration into an interdisciplinary network of leading scientists from both, the data and life sciences.

Research Areas: Imaging & diagnostics, surgery & intervention 4.0, models for personalized medicine.

Partners of HIDSS4Health: Karlsruhe Institute of Technology (KIT), German Cancer Research Center Heidelberg (DKFZ), and Heidelberg University

APPLICANT SITUATION AND RECRUITMENT

In 2022, HIDSS4Health recruited the fourth kohort of doctoral researchers. Out of 152 applications (56 from women, 123 international), seven applicants (one female, three international) have been selected for the doctoral researcher positions. In addition, one associated doctoral researcher joined the school. At the end of the reporting period of 2022, the school has 44 active doctoral researchers, of which 37 are fully funded by the School and seven are associated doctoral researchers from the partner institutions.

EVENTS AND NETWORKING

In 2022, HIDSS4Health hosted ten networking events, nine courses and 30 lectures. In various formats, the school was fostering the exchange between HIDSS4Health members.

» 10 Networking events

Networking events serve as contact points for doctoral researchers and other researchers or partners from industry. The main objective is to provide the doctoral researchers with an opportunity for scientific exchange, for cooperation with peers and for networking.

- 01.-03.02.2022: 1. AI HERO hackathon, online. Doctoral researchers attended for solving challenges in model development, training and optimization. Participants joined teams in order to create solutions for two different use cases, concerning health and energy. The Hackathon had been organized by Helmholtz AI, HIP, HMC, HIDSS4Health and HIDA.
- 04.05.2022: Extraordinary General Assembly, online. Introduction and discussion regarding the future concept of the school in preparation of the school's evaluation in November 2022.
- 15.07.2022: Networking meeting, in-person. Kick-off event for a series with talks from doctoral researchers and external guests.
- 08.09.2022: Doctoral Researcher General Assembly (DRGA), in-person. Organizational aspects of the school and funding opportunities of the doctoral researchers were discussed; representatives for the General Assembly and the Steering Committee were elected.
- 12.-14.09.2022: HIDSS4Health Retreat, in-person. Retreat for the doctoral researchers to network, get to know each other and discuss their projects and possible collaborations.
- 27.10.2022: General Assembly, online. Assembly of the HIDSS4Health "parliament", consisting of all PIs, two postdocs and one selected doctoral researcher per cohort. Here, the current state of the school was discussed and members of the Steering Committee and new PI candidates were elected.
- 24.-25.11.2022: Evaluation of HIDSS4Health, in-person. Poster presentations and talks by doctoral researchers and HIDSS4Health PIs for an external reviewer panel and internal members.

» 9 Courses

HIDSS4Health organizes courses in cooperation with partner schools, like BioInterfaces International Graduate School (BIF-IGS), International Helmholtz Research School of Biophysics and Soft Matter (IHRS Biosoft) or the Incubator platform Helmholtz AI, based on required skills and interests of the doctoral researchers. The offered courses cover a broad spectrum of topics and convey skills that might be valuable in the context of scientific work and personal development. In 2022, HIDSS4Health organized and conducted nine courses:

- 19.-21.01.2022: Introduction to Machine Learning (39 participants)
- 19.-20.01.2022: Communicating Science (11 participants)
- 03.03.2022: Communicating with your Supervisor (9 participants)
- 02.-04.04.2022: Scientific Writing held from the Papermill (14 participants)
- 11.04.2022: Docker / Container (14 participants)
- 27.04.-27.02.2022: Introduction to Cell Biology (32 participants)
- 15.06.-20.07.2022: Mental Health First Aid (15 participants)
- 29.08.-02.09.2022: Python from Zero to Data Science (26 participants)
- 29.09.-07.10.2022: Introduction to Statistics (41 participants)

» 30 Lectures

11 Lectures "Data Science & Health"

All lectures were given online and were open for people affiliated with Helmholtz or universities. The average number of participants in each lecture was 37; approximately 29% were from HIDSS4Health, 52% from Helmholtz and 8% from other scientific organizations. On average, 25% of the participants were female.

- 11.01.2022: Annika Reinke (DKFZ) – Next-generation Biomedical Image Analysis Competitions (37 participants)
- 18.01.2022: Michael Gertz (Heidelberg University) – Trends and Topics in Text Analysis (38 participants)
- 01.02.2022: Oliver Stegle (DKFZ) – Machine Learning for Genomics (42 participants)
- 08.02.2022: Carsten Dachsbacher (KIT) – Introduction to Visual Data Science (31 participants)
- 15.02.2022: Bogdan Savchynskyy (Heidelberg University) – Combinatorial Optimization Techniques for Bioimaging (16 participants)
- 25.10.2022: Leonardo Ayala (DKFZ) – Optical Imaging Concepts Enabled by Deep Learning (42 participants)
- 08.11.2022: Junyan Lu (Uni Klinikum Heidelberg) – Multi-omics Data Integration for Precision Medicine (45 participants)
- 15.11.2022: Alexander Schug (FZJ) – Data Inference in Molecular Biology: From Mutual Information to Alpha Fold (51 participants)
- 06.12.2022: Pascal Friederich (KIT) – Bayesian Optimization for Autonomous Experiments (41 participants)
- 13.12.2022: Ullrich Köthe (Uni Heidelberg) – Bayesian Inference with Invertible Neural Networks (39 participants)
- 20.12.2022: Mark Ladd (DKFZ) – Imaging Physics in Oncology (5 participants)

10 Lectures "Advanced Topics in Data Science & Health"

The lectures were held online by the doctoral researchers and postdocs of HIDSS4Health and were open to all HIDSS4Health doctoral researchers. The average number of participants was 16 to 25.

- 27.04.22: Verena Bitto (DKFZ) – Statistics Done Wrong (25 participants)
- 04.05.2022: Stefan Haller (UHEI) – Lagrange Decomposition for Combinatorial Optimization Problems (20 participants)
- 04.05.2022: Alexandra Walter (KIT) – Optimization of Artificial Neural Networks: Mathematics behind Stochastic Gradient Descent (19 participants)
- 11.05.2022: Elaine Zaunseder (UHEI) – The Needle in the Haystack – How to Handle Imbalanced Medical Data (23 participants)
- 11.05.2022: Philipp Toussaint (KIT) – Explainable AI – Methods for Interpretability and Explainability in ML and DL (24 participants)
- 18.05.2022: Philipp Wimmer (UHEI) – Visualization of Scientific Data with Paraview (23 participants)
- 18.05.2022: Paul Maria Scheikl (KIT) – Reinforcement Learning for Surgical Robotics (23 participants)
- 25.05.2022: Vahdaneh Kiani (UHEI) – Introduction to Medical Image Registration (17 participants)
- 25.05.2022: Alejandra Jayme (UHEI) – Hypernetworks for CNN or Bayesian Neural Networks (17 participants)
- 01.06.2022: Julian Herold (KIT) – Is Attention All You Need? (Intro to Transformers) (16 participants)

2 Lectures held by HIDSS4Health SAB members

- 26.01.2022: Ulrich Leser – HIDA@HIDSS4Health lecture
- 23.02.2022: Julia Schnabel – HIDA@HIDSS4Health lecture

7 Lectures on Imaging – "From Organisms to Molecules"

The lectures were held online and were open to people affiliated with Helmholtz or universities. The average number of participants in each lecture was 72; approximately 6% were from HIDSS4Health, 78% from Helmholtz and 17% from other scientific organizations.

- 28.04.2022: Mark Ladd (DKFZ) – Imaging Physics in Medicine (125 participants)
- 12.05.2022: Lukas Klein (DKFZ), Paul Jäger (DKFZ) – Analyzing Medical Images Using Machine Learning (103 participants)
- 02.06.2022: Michael Wagner (KIT) – Optical Coherence Tomography in Biofilm Research – Visualization and Characterization of the Mesoscopic Biofilm Structure (73 participants)
- 23.06.2022: Rudolf Merkel (FZJ) – Basics of Light Microscopy for the Study of Cells (57 participants)
- 30.06.2022: Gerd Ulrich Nienhaus (KIT) – Advanced Fluorescence Microscopy (53 participants)
- 07.07.2022: Lennart Hilbert (KIT) – Microscopy Assessment of DNA-based Information Processing in Biological and Artificial Systems (56 participants)
- 14.07.2022: Carsten Sachse (FZJ) – Imaging Biological Molecules by Electron Cryo-Microscopy (cryo-EM) (36 participants)

PUBLICATIONS

In 2022, doctoral researchers from HIDSS4Health have published 13 first author publications and 8 co-authored publications.

Doctoral researchers from HIDSS4Health are **highlighted**. Co-first authorship is labeled *. Associates are *italicized*.

» Peer-reviewed journal articles and conference proceedings

Beyene, M., Toussaint, P. A., Thiebes, S., Schlesner, M., Brors, B., & Sunyaev, A. (2022). A Scoping Review of Distributed Ledger Technology in Genomics: Thematic Analysis and Directions for Future Research. Journal of the American Medical Informatics Association.

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T. Scherr, **K. Löffler,** M. P. Schilling, O. Neumann, R. Mikut. Tuning a Distance-Prediction-Based Cell Segmentation, International Symposium on Biomedical Imaging, ISBI 2022; 28.03.2022–31.03.2022, Kolkata, India.

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Kumpost, V.; Hilbert, L.; Mikut, R., Intrinsic Noise Facilitates Population Synchronization of Uncoupled Cellular Oscillators to External Signals, 13th Conference on Dynamical Systems Applied to Biology and Natural Sciences; 08.02.2022–11.02.2022.

Patricia Vieten, Kris K Dreher, Niklas Holzwarth, **Melanie Schellenberg,** Jan-Hinrich Nölke, Alexander Seitel, Janek Gröhl, Zoë Rachel, Andrei Siea, Thomas Held, Sebastian Adeberg, Jürgen Debus, Lena Maier-Hein, Deep Learning-based Semantic Segmentation of Clinically Relevant Tissue Structures Leveraging Multispectral Photoacoustic Images, SPIE Photonics West; 22.01.22 – 27.01.22.

Tom Rix, Marco Hübner, Kris K Dreher, Jan-Hinrich Nölke, Leonardo Ayala, **Melanie Schellenberg, Jan Sellner, Silvia Seidlitz,** Alexander Studier-Fischer, Beat Müller-Stich, Felix Nickel, Alexander Seitel, Lena Maier-Hein, Deep Learning for Spectral Image Synthesis, SPIE Photonics West; 22.01.22 – 27.01.22.

Julian Herold, Eric Behle, Jakob Josenbauer, Alexander Schug, Machine Learning Based Optimization to Simulate Tumor Development, Biophysical Society Annual Meeting; 19.02.2022–23.02.2022 .

Eric Behle, **Julian Herold,** Jakob Josenbauer, Alexander Schug. Large-scale Simulation of Tumor Spheroid Invasion Dynamics, Biophysical Society Annual Meeting; 19.02.2022–23.02.2022.

Roitberg, A., Peng, K., **Marinov, Z., Seibold, C.,** Schneider, D., & Stiefelhagen, R., A Comparative Analysis of Decision-Level Fusion for Multimodal Driver Behaviour Understanding, Intelligent Vehicles 2022 – IV2022; 5-9.6.2022.

Sarfraz, S., Koulakis, M., **Seibold, C.,** & Stiefelhagen, R., Hierarchical Nearest Neighbor Graph Embedding for Efficient Dimensionality Reduction, IEEE/CVF Conference on Computer Vision and Pattern Recognition – CVPR2022; 21-24.6.2022.

Alexandra Walter, Kristina Giske, Philipp Hoegen, Sebastian Adeberg, Jürgen Debus, Oliver Jäkel, and Martin Frank, Quality Measures of CTV Delineation for Irradiation Planning of Head and Neck Cancers for Conformity with Expert Guidelines, 2022 Medical Image Understanding and Analysis Conference, Cambridge, 27 – 29 July 2022.

Schölch, L., Steinhäuser, J., Beichter, M., **Seibold, C.,** Yang, K., Knaeble, M., ... & Stiefelhagen, R., Towards Automatic Parsing of Structured Visual Content through the Use of Synthetic Data, 26th International Conference on Pattern Recognition (ICPR); 21-25.8.2022.

Eric Behle, **Julian Herold,** Alexander Schug, In Silico Tumor Invasion, DPG Spring Meeting, Condensed Matter Section; 04.09.2022–09.09.2022.

Julian Herold, Eric Behle, Jacopo Ferruzzi, Alexander Schug, Machine Learning Based Parametrization of Tumor Simulations, Physics of Cancer Symposium, 04.09.2022–09.09.2022.

Reiß, S., **Seibold, C.,** Freytag, A., Rodner, E., & Stiefelhagen, R., Graph-Constrained Contrastive Regularization for Semi-weakly Volumetric Segmentation, European Conference on Computer Vision – ECCV 2022; 23-27.10.2022.

ORAL PRESENTATIONS

Pia Stammer, Lucas Burigo, Oliver Jäkel, Martin Frank and Niklas Wahl, Using Importance Sampling to Speed up Non-intrusive Uncertainty Quantification for Monte Carlo Simulations, MCQMC 2022 – 15th International Conference on Monte Carlo and Quasi-Monte Carlo Methods in Scientific Computing; 17.07.2022-22.07.2022.

Pia Stammer, Jonas Kusch, A Robust Collision Source Method for Rank Adaptive Dynamical Low-rank Approximation in Radiation Therapy, GIMC SIMAI Young 2022; 29.09.2022-30.09.2022.

Warsinsky, Simon, Schmidt-Kraepelin, M., Thiebes, S., Wagner, M., & Sunyaev, A., Gamified Expert Annotation Systems: Meta-Requirements and Tentative Design, International Conference on Design Science Research in Information Systems and Technology in St. Petersburg, FL, USA; 01-03.06.2022.

Paul Maria Scheikl, Franziska Mathis-Ullrich, Surgical Robot Reinforcement Learning in Simulated Soft-Body Environments, SOFA Symposium; 15.11.2022

Lidia Al-Zogbi, Yanzhou Wang, Yinoussa Adagolodjo, **Paul Maria Scheikl,** Guanyun Liu, Pedro Lopes Da Frota Moreira, Franziska Mathis-Ullrich, Junichi Tokuda Iulian Iordachita, Axel Krieger, Simulating Flexible Bevel-Tipped Needle Insertion into Multi-Layer Tissue in SOFA, SOFA Symposium; 15.11.2022.

Silvia Seidlitz, Jan Sellner, Jan Odenthal, Berkin Özdemir, Alexander Studier-Fischer, Samuel Knödler, Leonardo Ayala, Tim J. Adler, Hannes G. Kenngott, Minu Tizabi, Martin Wagner, Felix Nickel, Beat P. Müller-Stich, Lena Maier-Hein, Robust Deep Learning-based Organ Segmentation in Hyperspectral Imaging, International Conference on Information Processing in Computer-Assisted Interventions 2022 (IPCAI 2022); 07.06.2022-08.06.2022.

Leonardo Ayala, Tim J. Adler, **Silvia Seidlitz,** Sebastian Wirkert, Christina Engels, Alexander Seitel, **Jan Sellner,** Alexey Aksenov, Matthias Bodenbach, Pia Bader, Sebastian Baron, Anant Vemuri, Manuel Wiesenfarth, Nicholas Schreck, Diana Mindroc, Minu Tizabi, Sebastian Pirmann, Brittaney Everitt, Annette Kopp-Schneider, Dogu Teber, Lena Maier-Hein, Spectral Imaging Enables Contrast Agent-free Real-time Ischemia Monitoring in Laparoscopic Surgery. International Conference on Information Processing in Computer-Assisted Interventions 2022 (IPCAI 2022); 07.06.2022-08.06.2022.

FURTHER NEWS FROM HIDSS4HEALTH

» Awards

The following prizes were awarded to the school's members:

- The doctoral researcher Constantin Seibold and PI Rainer Stiefelhagen won the Teaching Award KIT - Best practical course of the Computer Science Faculty for SS21 for their excellent lectures and teaching.
- The doctoral researcher Paul Maria Scheikl and PI Franziska Mathis-Ullrich won the Simulation Open Framework Architecture (SOFA) Award 2022. www.sofa-framework.org/about/news/two-winners-of-the-sofa-awards-2022/
- The doctoral researcher Zdravko Marinov and PI Rainer Stiefelhagen achieved the 5th place at the AutoPET MICCAI 2022 Challenge.
- The doctoral researchers Constantin Seibold, Zdravko Marinov, Alexander Jaus and their data science PI Rainer Stiefelhagen received the Top Three Winner Award on Single Metric (GPU) at the MICCAI PARSE 2022 Challenge.
- The doctoral researcher Constantin Seibold supervised by PI Rainer Stiefelhagen obtained the Medical Image Computing and Computer Assisted Intervention (MICCAI) Student Travel Award.
- The doctoral researcher Katharina Löffler and PI Ralf Mikut won the first place at the ISBI Cell Tracking Challenge.
- The doctoral researcher Simon Warsinsky and PI Ali Sunyaev obtained the i4health Collaboration Research Exchange Grant. Thus, Simon Warsinsky visited the UCL in London for a research stay.

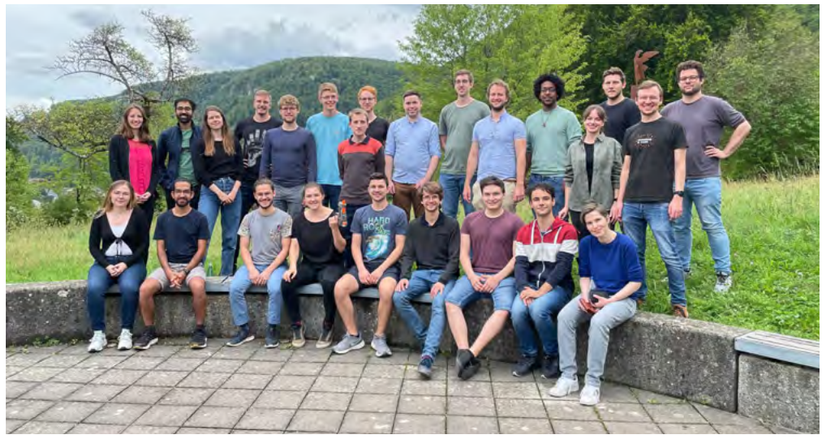
» Science Communication activities

HIDSS4Health is active on twitter, LinkedIn and has a mailing list. Its members participate in various media activities, e.g.:

- Zaunseder, E., Podcast on Machine Learning in Newborn Screening: https://soundcloud.com/user-109006120/machine-learning-in-newborn-screening?utm_source=clipboard&utm_medium=text&utm_campaign=social_sharing

» Miscellaneous

Doctoral researchers from HIDSS4Health in total supervised five Bachelor and nine Master theses in 2022.



Doctoral researchers of the HIDSS4Health. (Photo: HIDSS4Health)

MarDATA HELMHOLTZ School for Marine Data Science

IV | 5. Helmholtz School for Marine Data Science (MarDATA)

The Helmholtz School for Marine Data Science (MarDATA) aims to define, educate and establish the profile of marine data scientists. Therefore, it enables young researchers with a strong computer science background to apply their skills to multidisciplinary marine sciences and supports their doctoral research through a comprehensive training program.

Research Areas: Information technology, computer science, mathematics, marine research, supercomputing, modelling, (bio) informatics, robotics, statistics, big data methodologies

Partners of MarDATA: Helmholtz Centre for Ocean Research Kiel (GEOMAR), Alfred Wegener Institute for Polar and Marine Research (AWI), Christian-Albrechts-University zu Kiel (CAU) University of Bremen, Constructor University Bremen (formally known as Jacobs University Bremen)

APPLICANT SITUATION AND RECRUITMENT

In 2022, MarDATA finished the recruitment of the second cohort of doctoral researcher, MarDATA received a total of 223 applications in 2022. Out of the 11 advertised projects, 10 were able to hire a candidate. Successful applicants started until the end of 2022 and were from Germany, India, Iran, Kazakhstan, Portugal and Pakistan. 36 % of the MarDATA doctoral researchers are female. As first MarDATA doctoral researcher, Dr. Carola Trahms, has successfully defended her thesis in December 2022.

EVENTS AND NETWORKING

In 2022, MarDATA organized nine lectures, three workshops and 17 events.

» 9 Lectures

MarDATA Online Lecture Series (MOLS)

MarDATA Online Lecture Series is the central platform for lectures initiated and organized by MarDATA. It includes recurring elements (e.g. Introduction to Marine Sciences) and lectures that address the current needs of doctoral researchers.

- 13.01.2022: Prof. Thorsten Reusch (GEOMAR) – An Introduction to Marine Biology
- 20.01.2022: Prof. Isabella Peters (CAU) – Altmetrics & Science 2.0
- 26.01.2022: Prof. Arne Biastoch (GEOMAR) – Ocean General Circulation Modelling
- 10.02.2022: Prof. Tal Dagan (CAU) – An Introduction to Bioinformatic
- 17.02.2022: Uta Krebs-Kanzow (AWI) – An Introduction to Climate Science
- 03.03.2022: Prof. Angelika Humbert (AWI) – Satellite Remote Sensing
- 31.03.2022: Daniyal Kazempour (CAU) – Unsupervised Learning with High Dimensional Data
- 21.11.2022: Prof. Thomas Slawig (CAU) – Optimization Methods
- 01.12.2022: Prof. Thorsten Dickhaus (Bremen University) – Emperical Orthogonal Functions (EOF) Methods

» Workshops

MarDATA Workshops

MarDATA workshops are largely demand-driven, but also cover central aspects of the daily scientific routine of doctoral researchers. In contrast to the lectures, the workshops always include hands-on training. MarDATA workshops are usually held by external trainers and/or in cooperation with other (Helmholtz) initiatives.

- 21.-22.06.2022: Crash Course on Semantics and Knowledge Representation, online, in cooperation with Helmholtz Metadata Collaboration Platform (10 participants)
- 30.06.2022: Am I Just Stressed or am I Already Sick? – A Mental Health Workshop, online
- 14.-15.07.2022: Visual Communication of Science, online

» 17 Events

MarDATA Special Events

MarDATA special events cover a broad range of topics and formats. They include networking events, career development and internal MarDATA meetings.

- 12.01.2022: PI/Supervisor Onboarding, online
- 13.01.2022: MarDATA: Lessons Learned by the 1st Cohort, online
- 24.02.2022: Women in Data Science, Seminar Series (speaker: Prof. Robin Teigland), online
- 02.03.2022: MarDATA General Assembly, online
- 24.03.2022: HIDA Lecture @ MarDATA (Prof. Markus Reichstein), online
- 26.04.2022: MarDATA Meets Industry (networking), online
- 24.08.2022: MarDATA Meets Industry (on-site networking), in person
- 19.-21.09.2022: MarDATA Retreat, in person
- 22.09.2022: MarDATA PhD Assembly, in person
- 10.11.2022: HIDA Lecture @ MarDATA (Prof. A. Murat Eren), online
- Weekly: MarDATA Weekly, only for doctoral researchers

Events with MarDATA Participation

MarDATA is cooperation partner in various initiatives. In this role, the school supports also external events, e.g. the weekly Digital Science Monday @ GEOMAR.

- 27.06.2022: MarDATA Project Intro by Armin Bernstetter & Josē Kling
- 11.07.2022: MarDATA Project Intro by Patricia Schöntag & Tobias Ziolkowski
- 24.10.2022: MarDATA Project Intro by Yvonne Jenniges & Hameed Moqadam
- 14.11.2022: MarDATA Project Intro by Yannick Wölker & Christian Kanarski
- 15.11.2022: Helmholtz Data Science Career Day
- 15.12.2022: Helmholtz AI Walk-in Consulting @ GEOMAR

Conference Sessions organized/chaired by MarDATA doctoral researchers:

- AGU Fall Meeting 2022: Interpretable Machine Learning for Marine Sciences, Chicago, USA

From left to right: Yvonne Jenniges (2nd cohort MarDATA, AWI/University Bremen), Yannick Wölker (2nd cohort MarDATA, GEOMAR/CAU) and Dr. Carola Trahms (MarDATA Alumni) at the AGU 2022 Fall Meeting in Chicago, USA. (Photo: Yvonne Jenniges)

MarDATA members at the MarDATA retreat in 2022. (Photo: Sarah Kaehlert, GEOMAR)

PUBLICATIONS

In 2022, MarDATA doctoral researchers published ten first author publications and two co-authored articles.

Doctoral researchers are **highlighted**; MarDATA has (so far) no associated doctoral researchers.

» Doctoral Thesis

Trahms C. (2022) Marine Data Fusion for Analyzing Spatio-Temporal Ocean Region Connectivity

» Peer-reviewed Journal Publications

Contzen, J., Dickhaus, T., and Lohmann, G. (2022). Variability and Extremes: Statistical Validation of the Alfred Wegener Institute Earth System Model (AWI-ESM), Geosci. Model Dev., 15, pp. 1803–1820.

Humbert, A., Christmann, J., Hugh, F.J., Helm, V., **Höyns, L.S.,** Hofstede, C., Müller, R., Neckel, N., Nicholls, K.W., Schultz, T., Steinhage, D., Wolovick, M., and Zeising, O. (2022). On the Evolution of an Ice Shelf Melt Channel at the Base of Filchner Ice Shelf, from Observations and Viscoelastic Modeling, The Cryosphere, 16 (10), pp. 4107–4139.

Mbani, B., Schoening, T., Gazis, IZ., Koch, R., and Greinert, J. (2022). Implementation of an Automated Workflow for Image-based Seafloor Classification with Examples from Manganese-nodule Covered Seabed Areas in the Central Pacific, Ocean. Sci. Rep., 12, 15338.

Zainab, T., Karstens, J., and Landsiedel, O. (2022). Cross-domain Fusion in Smart Seafloor Sensor Networks, Informatik Spektrum, 45, pp. 290–294.

Ziolkowski, T., Koschmider, A., Kröger, P., and Devey, C. (2022). Outlier Quantification for Multibeam Data, Informatik Spektrum, 45, pp. 218–222.

» Conference Papers & Proceedings

Dinkel, V., Buchwald, S.Z., Stoof-Leichsenring, K., Hütt, M.-T., Nürnberg, D., and Herzschuh, U. (2022). Paleometagenomic Network Analysis of Ancient DNA from Bering Sea Sediments to Examine Past Ecological Communities, EGU General Assembly 2022, Vienna, Austria, 23–27 May 2022, EGU22-12176.

Landt-Hayen, M., Kröger, P., Claus, M., and Rath, W. (2022). Layer-wise Relevance Propagation for Echo State Networks Applied to Earth System Variability, In Proceedings of the 3rd International Conference on Machine Learning Techniques (MLTEC 2022), Zurich, Switzerland, vol. 12, no. 20, pp. 115–130.

Schöntag, P., Nakath, D., Röhrl, S., and Köser, K. (2022). Towards Cross Domain Transfer Learning for Underwater Correspondence Search In: Sclaroff, S., Distante, C., Leo, M., Farinella, G.M., Tombari, F. (eds) Image Analysis and Processing – ICIAP 2022. Lecture Notes in Computer Science, vol 13233. Springer, Cham.

Tavares de Sousa, N., **Trahms,** C., Kröger, P., Renz, M., Schubert, R., and Biastoch, A. (2022) Tracking the Evolution of Water Flow Patterns Based on Spatio-temporal Particle Flow Clusters, 23rd IEEE International Conference on Mobile Data Management (MDM), pp. 246–253.

von See, T. B., Meurer, T., and Greinert, J. (2022). Chemical Plume Tracking Using an AUV with UKF Based Extremum Seeking, IFAC-PapersOnLine, 55(31), pp. 178–183.

Ziolkowski, T., Koschmider, A., Schubert, R., and Renz, M. (2022). Process Mining for Time Series Data. In: Augusto A., Gill A., Bork D., Nurcan S., Reinhartz-Berger I., and Schmidt R. (eds) Enterprise, Business-Process and Information Systems Modeling. BPMDS EMMSAD 2022. Lecture Notes in Business Information Processing.

» Conference Talks

Höyns, L.-S., Kleiner, T., Rademacher, A., Rückamp, M., Wolovick, M., and Humbert, A. (2022). Basal Properties of the WAIS from Inverse Modeling Including Effective Pressure, WAIS Workshop 2022, 26–29 September 2022.

Kinzel, L., Fromm, T., Schlindwein, V., and Maass, P. (2022). Unsupervised Deep Representation Learning for Icequake Detection at Neumayer Station, Antarctica, AG Seismologie, 26–30 September 2022.

Landt-Hayen, M., Kröger, P., Claus, M., and Rath, W. (2022). Layer-wise Relevance Propagation for Echo State Networks Applied to Earth System Variability, American Geophysical Union (AGU) Fall Meeting, 12.–16. December 2022.

Mohn, H. (2022). SWIFT-AI: Implicit Neural Representations for Stratospheric Ozone Chemistry, Climate Informatics 22, 09–13 May 2022.

Mohn, H., Kreyling, D., Wohltmann, I., Lehmann, R., Maass, P., and Markus, R (2022). SWIFT-AI: Significant Speed-up in Modelling the Stratospheric Ozone Layer, European Geosciences Union (EGU) General Assembly, 23–27 May 2022.

FURTHER NEWS FROM MARDATA

» MarDATA on Tour

During the annual Fall Meeting of the American Geophysical Union (AGU22), doctoral researchers from MarDATA led their own session titled "Interpretable Machine Learning for Marine Sciences". Yvonne Jenniges (2nd cohort MarDATA), Carola Trahms (now MarDATA Alumni), Maike Sonnewald (Princeton University), and Dani Jones (NERC) participated. The focus of the session was to find quantitative ways to objectively compare existing results from marine research with results from marine data science methods - one of the central themes of MarDATA. The session was dealing with the question: How can the integration of innovative computational science methods in marine science contribute to real added value? What knowledge and which tools are needed to get more interpretable, explainable and trustworthy results?

» Further activities

› Two MarData doctoral researchers delivered presentations on Womens Day 2022 at CAU: Maria-Theresia Pelz (former Verwega), "Methodenentwicklung zur Verbesserung von Ozeanmodellen" and Carola Trahms, "Data Science meets 'other Sciences' - Adventures of an Interdisciplinary PhD Student".

› Two MarDATA doctoral researchers are NFDI4Earth Academy Fellows: Lena Happ (AWI) and Sweety Mohanty (GEOMAR). The NFDI4Earth Academy is a network of early career scientists interested in bridging Earth System and Data Sciences beyond institutional borders. It is coordinated by Technical University Dresden and funded by the German Research Foundation DFG.

› One MarDATA doctoral researcher was granted a 3-month research stay at Hereon under the HIDA Trainee Network Program: Narveen Kumnar Parameswaran.

MUDS Munich School for Data Science HELMHOLTZ · TUM · LMU

IV | 6. MUDS – Munich School for Data Science

The Munich School for Data Science (MUDS) trains the next generation of data scientists at the interface of data science and four different sciences: biomedicine, plasma physics, earth observation, and robotics. It aims to strengthen the domain-driven research within the Helmholtz Association by teaching methodological skills in data science in an interdisciplinary and application-oriented fashion.

Research areas: Data science with a focus on biomedicine, plasma physics, earth observation, and robotics

Partners: German Research Center for Environmental Health (Helmholtz Munich), Max-Planck-Institute for Plasma Physics (IPP), German Aerospace Center (DLR), Ludwig-Maximilians-Universität München (LMU), Technical University of Munich, Leibniz Computing Centre (LRZ) and Max Planck Computing & Data Facility (MPCDF).

APPLICANT SITUATION AND RECRUITMENT

In 2022, MUDS recruited its fourth cohort of doctoral researchers with two calls for applications and interviews. In these rounds, MUDS received a total of 304 applications from 41 different nationalities, 47 candidates were interviewed (18 female, 35 international). 24 matches between candidates and projects were found. Two candidates were recruited in the alternative, year-round recruiting process. 22 recruited researchers are in associate status, two newly recruited researchers are funded by MUDS.

EVENTS AND NETWORKING

In 2022, MUDS organized two lectures, eight events and 31 seminars and courses.

» 8 Events

Recruiting Events

MUDS has two rounds of applications per year. Selected applicants of each round are invited for a four-day online interview symposium that offers PI project presentations, candidate presentations, individual PI/candidate interviews, and networking among applicants and current MUDS doctoral researchers.

- 15.02.-18.02.2022: MUDS recruiting event winter, virtual (49 participants)
- 28.06.-01.07.2022: MUDS recruiting event summer, virtual (43 participants)

Networking Events

- 17.02.2022 & 30.06.2022: Virtual get togethers and poster sessions on the virtual platform gather-town with MUDS doctoral researchers and applicants (22 & 18 participants)
- 05.07.2022: MUDS Networking Event, in-person. Get together for doctoral researchers for scientific networking across different institutions & domains (54 participants)
- 28. - 30.09.2022: MUDS Retreat, in-person. Annual retreat with PhD talks, poster sessions, networking & get together with industry (ROCHE). Three keynote speakers: Michael Bronstein (University of Oxford, Twitter), Esther Puyol-Anton (HeartFlow, King's College London), Mikhail Langovoy (KIT) (91 participants)
- 30.11.2022: Meet the Data Scientist, in-person. Data scientists from industry talk about their daily work, how they interact with colleagues and clients, and present several use cases of data science in practice (11 participants)
- 12.12.2022: MUDS Welcome Event & Teambuilding Workshop for the class of 2022, in-person. Welcome and introduction to PhD administrative matters, Q&A with MUDS office, teambuilding workshop, joined dinner with current doctoral researchers (55 participants)

» 2 Lectures

- 13.-24.06.2022: Life Science Course, virtual. Covers basic life science/biology concepts and experimental methods, tailored for doctoral researchers with a more theoretical/computational background (11 participants).
- 07.-18.11.2022: Data Science Block Course, in-person. Covers data science-related topics (25 participants).

» 31 Seminars and Courses

Seminar Series

Biweekly seminars with progress reports by MUDS doctoral researchers, also with guest speakers invited by the doctoral researchers. 23 progress reports by MUDS doctoral researchers (virtual), number of participants varies

- 12.10.2022: Seminar by guest speaker Andreas Meyer (University College London), Reading the T-Cell Receptor Code, followed by a meet the speaker-session, virtual (40 participants)

Transferable Skill Courses

In addition to the courses offered by the local graduate programs of the MUDS doctoral researchers, MUDS offered the following courses, to complement as per demand by the doctoral researchers:

- 02.02.2022 & 09.02.2022: Stress Release Workshop, virtual. Course on strategies to help dealing with stress and anxiety and increase concentration (13 participants)
- 12.-13.05.2022: Presentation Skills Course, in-person. Course on how to present research, shared course with an LMU PhD program (4 participants)
- 15.07.2022: Scientific Writing Course, in-person. Course on how to communicate research clearly and effectively (12 participants)
- 19.-20.09.2022: Scientific Writing Course, virtual. Course on how to communicate research clearly and effectively, shared course with LMU PhD program (3 participants)
- 25.10. & 28.10.2022: Presentation Skills Course, in-person. Course on how to present research (10 participants)

Members of the Munich School for Data Science (MUDS). (Photo: MUDS)

PUBLICATIONS

In 2022, 21 first author publications and 20 co-authored articles were published by MUDS doctoral researchers.

Doctoral researchers from MUDS are **highlighted**. Co-first authorship is labeled *. Associated doctoral researchers are marked in *italics*.

» Peer-reviewed Journal Articles and Conference Proceedings

Arruda A., Zeggini E. (2022). Shared Genetic Aetiology of Type 2 Diabetes and Ostheoarthritis. Osteoarthritis and Cartilage, Vol. 30,1, S340.

Bercea, C.I., Wiestler, B., Rueckert, D., Albarqouni, S. (2022). Federated Disentangled Representation Learning for Unsupervised Brain Anomaly Detection. Nat Mach Intell 4, 685-695.

Castelblanco, A., Rivera, E., Solano, J., Tengana, L., Lopez, C., Ochoa, M. (2022). Dynamic Face Authentication Systems: Deep Learning Verification for Camera Close-Up and Head Rotations Paradigms. Computers&Security Vol 115.

Ito-Kureha, T., Leoni, C., Borland, K., *Cantini, G.,* Bataclan, M., Metzger, R.N., Ammann, G., Krug, A.B., Marsico, A., Kaiser, S., Canzar, S., Feske, S., Monticelli, S., König, J., Heissmeyer, V. (2022). The Function of Wtap in N^6-adenosine Methylation of mRNAs Controls T Cell Ceceptor Signaling and Survival of T Cells. Nat Immunol 23, 1208-1221.

Noack, F., Vangelisti, S., Raffl, G., Carido, M., Diwakar, *J., Chong, F.,* Bonev, B. (2022). Multimodal Profiling of the Transcriptional Regulatory Landscape of the Developing Mouse Cortex Identifies Neurog2 as a Key Epigenome Remodeler. Nature neuroscience, 25(2), 154–167.

Fritz, C., **Dorigatti, E.,** Rügamer, D. (2022) Combining Graph Neural Networks and Spatio-temporal Disease Models to Improve the Prediction of Weekly COVD-19 Cases in Germany. Scientific Reports 12, 3930.

Savoldi, A., Morra, M., Castelli, A., Mirandola, M., Berkell, M., Smet, M., Konnova, A., Rossi, E., Cataudella, S., De Nardo, P., Gentilotti, E., Gupta, A., Fasan, D., Gibbin, E., Puviani, F.C., Hasenauer, J., *Gusinow, R.,* Tami, A., Kumar-Singh, S., Malhotra-Kumar, S., mAb ORCHESTRA Working Group, Tacconelli, E. (2022). Clinical Impact of Monoclonal Antibodies in the Treatment of High-Risk Patients with SARS-CoV-2 Breakthrough Infections: The ORCHESTRA Prospective Cohort Study. Biomedicines 2022, 10, 2063.

Hu, Y., *Rehawi, G.,* Moyon, L., Gerstner, N., Ogris, C., Knauer-Arloth, J., Bittner, F., Marsico, A., & Mueller, N. S. (2022). Network Embedding Across Multiple Tissues and Data Modalities Elucidates the Context of Host Factors Important for COVID-19 Infection. Frontiers in Genetics, 13, 909714.

Spath S., Roan F., Presnell S.R., **Höllbacher B.,** Ziegler S.F. (2022). Profiling of Tregs Across Tissues Reveals Plasticity in ST2 Expression and Hierarchies in Tissue-specific Phenotypes. Iscience Vol. 25, Issue 9, 16 Sept 2022, 104998.

Lamm, L., Righetto, R. D., Wietrzynski, W., Pöge, M., Martinez-Sanchez, A., Peng, T., & Engel, B. D. (2022). MemBrain: A Deep Learning-aided Pipeline for Detection of Membrane Proteins in Cryo-electron Tomograms. Computer Methods and Programs in Biomedicine, 224, 106990.

Loureiro, H., Becker, T., Bauer-Mehren, A. (2022). A longitudinal Early-indicator of Overall Survival Based on Prognostic Scores. Pharmacoepidemiology and Drug Safety. Vol 31. John Wiley & Sons, Ltd; 2022:559

Padovani F, **Mairhörmann B.,** Falter-Braun P., Lengefeld J., Schmoller K.M. (2022). Segmentation, Tracking and Cell Cycle Analysis of Live-cell Imaging Data with Cell-ACDC. BMC Biology 20, 174.

Palla G., Spitzer H., Klein M., Fischer D., Schaar A.C., Kuemmerle L.B., Rybakov S., Ibarra I.L., Holmberg O., Virshup I., Lotfollahi M., **Richter S.,** Theis F.J. (2022). Squidpy: a Scalable Framework for Spatial Omics Analysis. Nature Methods 19, 171–187.

Palla G., Fischer D.S., Revev A., Theis F.J. (2022). Spatial Components of Molecular Tissue Biology. Nature Biotechnology 40, 308–318.

Ratajczak F., Joblin, M., Ringsquandl, M., & Hildebrandt, M. (2022). Task-driven Knowledge Graph Filtering Improves Prioritizing Drugs for Repurposing. BMC Bioinformatics, 23(1), 84.

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Koller, C., Kauermann, G., Zhu, X.X., AI4EO: Learning from Human Uncertainty. Living Planet Syposium (LPS), Bonn, Germany. 23-27 May 2022.

Loureiro, H., A longitudinal early-indicator of overall survival based on prognostic scores. International Conference on Pharmacoepidemiology (ICPE), Copenhagen, Denmark, 24-28 August 2022.

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Spieker, V. Towards a Patient Specific Template for Respiratory Motion Estimation Using Groupwise Learning-Based Registration. ISMRM Workshop on Motion Detection & Correction. Oxford, UK, 30 August - 02 September 2022.

FURTHER NEWS FROM MUDS

» Awards

Prof. Dr. Dr. Fabian Theis, speaker and founding member of MUDS, was awarded the Gottfried Wilhelm Leibniz Prize, the most important research prize in Germany.

Furthermore, MUDS doctoral researchers received the following awards and fellowships in 2022:

- Christoph Koller received the Best Poster Award at Symposium of the International Future Lab AI4EO 2022.
- Valentin Koch received funding for his project from the Funding & Innovation Call for his ongoing project.
- Jianxiang Feng was award finalist as part of a team at DLR KUKA Innovation of KUKA GmbH: www.kuka.com/de-de/future-production/konzernforschung/kuka-innovation-award/kuka-innovation-award-2023 .
- Salome Kazeminia has achieved 2nd place in the Best Scientific Image Contest 2022 of Helmholtz Imaging: www.instagram.com/p/CkabDoOI8vX/?utm_source=ig_web_copy_link .
- Sophia Wagner, Simon Wengert and Felix Drost joined the Joachim Herz Add on-Fellowship.
- Mara Stadler was granted a DAAD fellowship for a research stay in the USA.
- Lorenz Lamm is now a fellow of the Boehringer Ingelheim Fonds.

» Internships

- Simon Geisler did a four-month internship at DeepMind, London.
- Sophia Wagner was hosted as an intern at EKFZ Dresden in the lab of Jakob Kather.

» Miscellaneous

In 2022, several events on career, responsible research and diversity were offered by and to the MUDS community:

- The InPharma Career Symposium took place in June at Max-Planck-Institute in Planegg.
- The Responsible Research Symposium Sustainable World, co-organized by MUDS, took place in September in Martinsried.
- Laura Martens and Ana Arruda co-organize the STEM-Tisch, a monthly event to support and empower women and gender minorities at Helmholtz Munich who are practicing, studying or are interested in the fields of STEM (Science, Technology, Engineering and Mathematics).
- Helmholtz Graduate School of Environmental Health (HELENA) invited MUDS doctoral researchers to events on diversity: Webinar "Everything's equal isn't it? - Understanding why we're not there yet", and the workshop "Gender and Research Programs"

» Further Cooperations

MUDS has a total of seven PhD projects in industry collaborations with the following partners: ROCHE (5), Boehringer Ingelheim (1), Jura BioINC (1).

Three more will start in 2023.

» Science Communication

- MUDS has a website (www.mu-ds.de) and a twitter account (@MunichDS). For recruiting, advertisement services are used as well as social media campaigns on Facebook, Instagram and LinkedIn.
- Robert Köberl participated at the "Simons Workshop" on stellarator optimisation at IPP Greifswald and at the "Data Science Mini-Workshop" at TU-Graz.
- Jianxiang Feng co-organized a workshop at IROS2022 (https://probabilisticrobotics.github.io/).
- Sugandha Doda co-organized the Helmholtz AI "CountMeIn Challenge" hackathon.
- MUDS participated at the "Helmholtz Virtual Career Day for Data Science and IT" on November 15, 2022 with a virtual booth.
- MUDS participated in a twitter campaign organized by HIDA in June 2022 to highlight its diversity and scientific profiles of its doctoral researchers.

V. OUTLOOK

For HIDA, the year 2023 is marked by the transition from the set-up phase to the regular operation phase: after the first graduations in the HIDSS, a larger group of doctoral researchers will now receive their degrees, which means that the first cohort of fellows will have completed the entire course program. HIDA's exchange programs will now settle into their planned mode after the real start of the post-pandemic phase last year, and the partnerships will stabilize and generate added value through the further expansion of reciprocal activities. The assessments of HIDSS, which started as early as 2022, and especially the assessment of HIDA in June 2023, represent an important milestone in its further development.

With an elaborate future concept, HIDA will position itself for this new phase and lay the foundation for its further development. The focus will be on sharpening the mission and profile, and in particular on the targeted further development of HIDA's central offerings and the interactions of the HIDSS. In this context, an important goal is to continue to broadly disseminate the HIDA offerings to the community in order to provide increasing added value to all centers in their efforts to establish information and data science as a crucial foundation of scientific activities in all fields. In particular, HIDA is going to strengthen interaction with the programs and research areas as structuring and unifying elements of the Helmholtz Association.

Specifically, in 2023 HIDA will establish its regular events such as the Career Day for Data Science and IT and the Summer Academy and build on the success of previous years. Real encounters can and will be the focus again. Likewise, further development of processes, particularly in the area of exchange programs, is planned in order to meet the increasing interest and further expand exchanges. HIDA will continue to intensively promote Helmholtz as a leading player in the field of information and data science through communication initiatives.

We are looking forward to the highlights of HIDA's 2023 program. Please save the dates:

Date	Event
12.01.2023	Helmholtz Entrepreneurs Workshop
24.-25.01.2023	Evaluation MarDATA
14.-15.02.2023	Evaluation HDS-LEE
23.03.2023	TechTalk with KI Park about Synthetic Data
15.-16.05.2023	Evaluation MUDS
01.-02.06.2023	Evaluation DASHH
07.-08.06.2023	Evaluation HIDA
19.-30.09.2023	Helmholtz Incubator Summer Academy
05.11.2023	Helmholtz Career Day for Data Science and IT

VI. RESPONSIBILITY FOR REPORT & HIDA MAIN CONTACT

The members of the Steering Committee of the Helmholtz Information & Data Science Academy (HIDA-Steer) checked and approved this report in February 2023.

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CORRECT AS OF MARCH 2023

The illustration is based on a data set containing signals from 22 different regions of the human brain.

CHRISTIAN GERLOFF from HDS-LEE applies artificial intelligence and machine learning methods to the neurosciences to gain a better understanding of the human brain.

This image is an example of an artistic implementation of research data used by the doctoral researchers of the six Helmholtz Data Science Schools in the fields of Energy, Earth and Environment, Health, Key Technologies, Structure of Matter, and Aeronautics, Space and Transport.