UNIVERSITÄT PADERBORN

Paderborn Center for Parallel Computing

PROJECTS
FACTS
RESEARCH
HPC
TEACHING
PEOPLE

ANNUAL REPORT 2020/21/22

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Paderborn Center for Parallel Computing

PREFACE

It is my great pleasure to present the latest PC2 research and service report for the period July 2019 - December 2022.

The evolution of PC2 and the world situation during this period has been, there is no other way to put it, spectacular. While the world was reeling from the first severe pandemic in many decades beginning in early 2020, which had serious implications for global supply chains in addition to the health consequences of contact and travel restrictions, the University and its partners were working on the realization of the Noctua research building, which broke ground in the Fall of 2019. Delivering a complex technical building like an HPC data center in the midst of a pandemic with an ambitious schedule, even in normal times, required the highest level of commitment from all involved. It is thanks to the high level of commitment of the university management, construction department, BLB, specialist planners and executing companies that the new construction of the data center was successfully completed with minimal delays despite the adverse circumstances and that the building was handed over for use in November 2021. This report provides you with a detailed insight into the technical infrastructure of the building, and we cordially invite you to visit the site to gain a more in-depth impression.

The period under review also saw the long-awaited call for proposals and decision on the establishment of the "National High Performance Computing Association (NHR)". In this tender, supraregionally active and scientifically distinguished HPC centers were able to apply for 10-year funding as a national supercomputing center within the framework of a competition for excellence. PC2 was able to prevail in this scientific competition as one of initially 8 centers. In the period 2021-2030, up to 75 million euros will flow to Paderborn as part of the NHR funding, which will be used for investments, operations and personnel. In particular, scientific user support and the methodological advancement of supercomputing will be significantly strengthened by the further expansion of expert consulting at PC2. Within the NHR network, PC2 will contribute its expertise in applications and methods for atomistic simulations in chemistry, physics, and materials science, and its expertise in the use of heterogeneous computing architectures and hardware accelerators, in particular FPGAs and GPUs, for scientific computing. The establishment of an NHR center is not only a great success for PC2, but also an important milestone for the entire university location to further raise its profile in computational sciences.

Since all good things come in threes, the second expansion stage of the Noctua HPC system was pushed forward in a public tender in parallel with the construction of the computer center and the establishment of the NHR center. The procurement was timed so that the system could be installed there immediately after completion of the new data center. The contract for the delivery of the HPC system was awarded to Atos/Bull. The new HPC system, named "Noctua 2", was installed from November 2021 and handed over to the users in April 2022 during a ceremonial commissioning with representatives from science, industry and politics. With an investment volume of over 12 million euros, more than 1,000 servers, 140,000 CPU cores and a 6PB parallel memory system, Noctua 2 is by far the most powerful HPC system ever operated at PC2. Half of the funding for the computer came from the Noctua research build and half from the NHR grant.

In addition to these three highlights, our scientific users and staff were anything but idle. Over 250 peer-reviewed scientific articles were reported whose results were obtained using PC2 resources. During the reporting period, approximately 200 new computing time projects totaling 1,050 million CPU core hours were approved, with a total of 368 projects being allocated over 2 billion CPU core hours. Of these, over 120 projects were requested by individuals requesting computing time at PC2 for the first time. Special emphasis was placed on supporting young scientists: More than 40 applications were approved explicitly for thesis work, and applications were approved from 7 junior professors and 87 non-professorial project applicants.

I invite you to browse through the articles in this report, be inspired by the diverse topics, and follow the references for further interest. I wish you a stimulating read.

Christian Plessl

Prof. Dr. Christian Plessl
Managing Director and Chairman of the Board

HPC DATA CENTER IN NEW BUILDING X

During the reporting period, the new HPC data center in Building X was completed and handed over for its intended purpose. This marks a major milestone and a step forward for PC2 and Paderborn University as a whole.

In retrospect, this complex project was completed within the planned budget in a relatively short period from the application for funding in September 2016 to the start of construction in October 2019 to the handover of the building to the university in November 2021. It is truly remarkable that this was achieved under the adverse circumstances of the Corona pandemic and the scarce supply of building materials.

With Noctua 2, the first HPC system was installed in the new data center in December 2021 and declared operational in February 2022. Moving all the PC2 personnel from building O to building X was completed in February 2022. Some remaining work on the technical systems of the data center was completed in the following months.

CEREMONIAL COMPLETION OF CONSTRUCTION

The official handover of the Noctua 2 HPC system took place during the festive opening ceremony in April 2022 in the presence of the NRW Minister for Culture and Science Isabel Pfeiffer-Poensgen and the representative of the NRW Bau- und Liegenschaftbehörde BLB Dinah Heidemann (Fig. 1).

SUCCESSFUL CONSTRUCTION DESPITE ADVERSE CONDITIONS

Fig. 1: Inauguration of the HPC data center (front from left to right): Isabel Pfeiffer-Poensgen (NRW Minister of Culture and Science), Dinah Heidemann (BLB NRW), University President Prof. Dr. Birgitt Riegraf, (back from left to right) Udo Littke (Atos Germany), Prof. Dr. Christian Plessl (PC2), Prof. Dr. Christof Schütte (Zuse Institute Berlin) and Hans-Bernd Janzen (Deputy District Administrator of Paderborn).

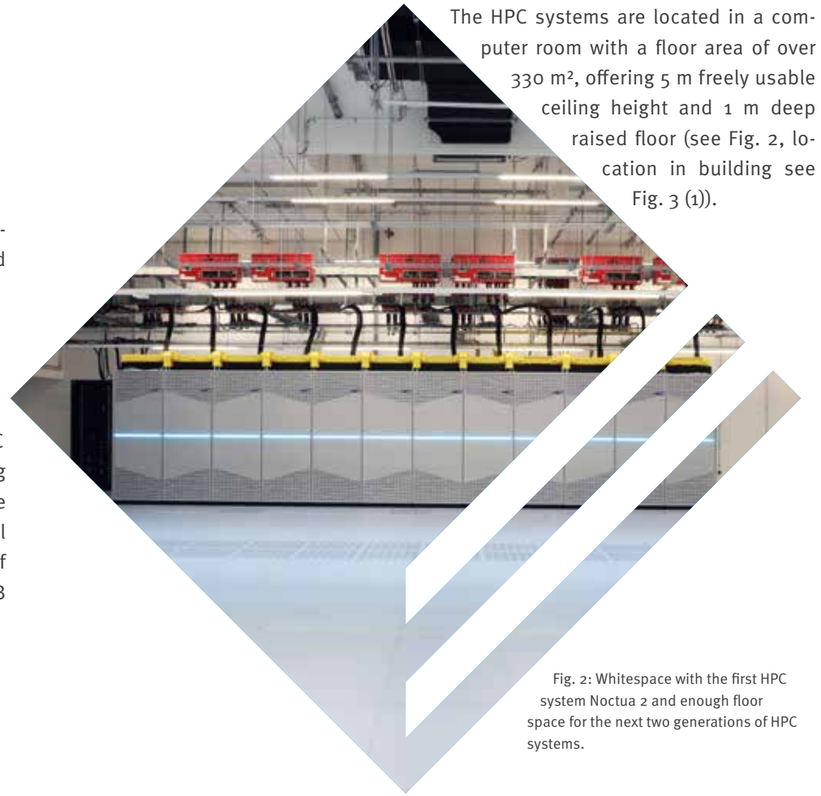


Fig. 2: Whitespace with the first HPC system Noctua 2 and enough floor space for the next two generations of HPC systems.

The HPC systems are located in a computer room with a floor area of over 330 m², offering 5 m freely usable ceiling height and 1 m deep raised floor (see Fig. 2, location in building see Fig. 3 (1)).

The computer room is divided into three segments. Each segment can accommodate one large HPC system with its specific requirements for electricity and cooling.
Power to the HPC systems is provided by busbar systems and ceiling-mounted outlet boxes, each with a maximum capacity of over 1 megawatt per HPC system. An electrical capacity of 2.6 megawatts is currently available for IT systems, and expansion to over 6 megawatts is being planned (location see Fig. 3 (6)).

COOLING IS IMPORTANT

The piping for the two cooling circuits, a cold-water circuit with an inlet temperature of 19 °C and a hot water circuit with an inlet temperature of ›32 °C are located in the raised floor. The hot water loop can discharge up to 1 megawatt per segment, depending on the inlet and outlet temperatures allowed by the HPC system. The chilled water loop has a maximum total capacity of up to 700 kW (Fig. 3 (3)) and also supplies the chillers for air cooling. An early fire detection system and fire detection sensors provide for alarming and, if necessary, extinguishing by introducing nitrogen (Fig. 3 (9)).
Another room with special fire protection is available for data backup and archiving.
The cooling systems of the computer center were designed in such a way that the waste heat of the computer systems can be dissipated and reused in a highly efficient manner. To this end, we consistently rely on hot water cooling, which can dissipate at least 85% of the waste heat. In order to be able to achieve a flow temperature of 32°C for the hot water circuit all year round, the heat exchangers on the roof can be moistened with water on particularly hot days. The humidification generates evaporative cooling and leads to a reduction of the temperature supplied by the heat exchanger, the so-called adiabatic cooling (Fig. 5 (4)).

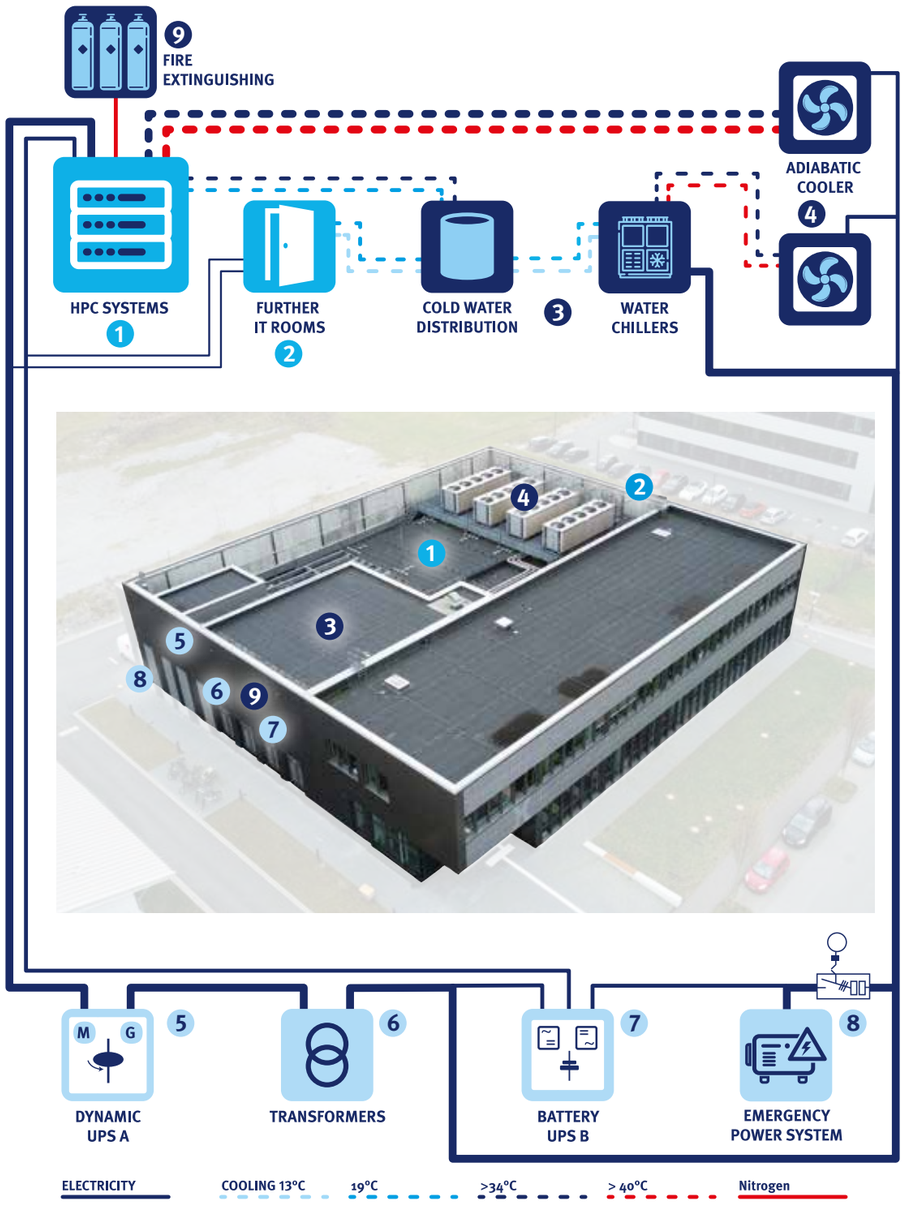


Fig. 3: Bird's eye view of the data center building X showing the technical infrastructure in a functional diagram.

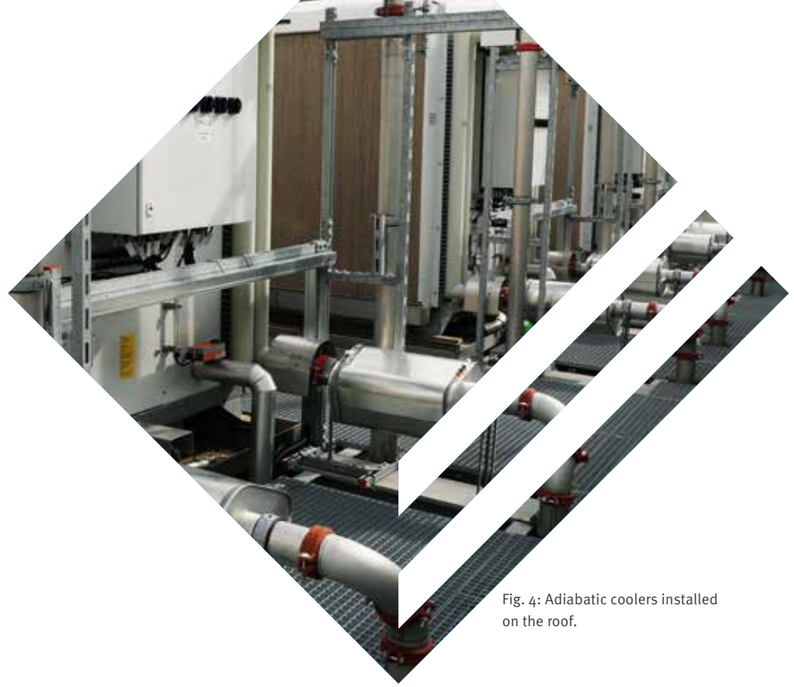


Fig. 4: Adiabatic coolers installed on the roof.

Due to the high temperature in the return of the hot water circuit, the waste heat can be used to heat buildings, for which a local heating network is being built on the university campus. The planned new campus buildings in the immediate vicinity of the computer center will be the first to benefit from this.

Only a maximum of 15% of the waste heat will be dissipated in the traditional way via air cooling, which is much more energy-intensive due to the generation of cold by compression chillers and distribution by fans.

SECURED ENERGY SUPPLY

Fail-safe operations require a specially designed power supply for the IT systems and the operation-critical technical systems. Therefore, we always use two separate power supply paths for the core components of the HPC system which include the data storage systems, server systems for administrative purposes and the core switches of the networks. In data center X, this concept is ensured by a power supply path A protected by a dynamic UPS system (line filter) (Fig. 5 and Fig. 3 (5)) and power supply path B protected by a battery-backed uninterruptible power supply (UPS (Fig. 3 (7)).

In the event of a prolonged failure of the mains supply, the battery UPS is supplied with power via an emergency power system with a diesel engine (Fig. 3 (8)).
This setup is technically complex and rather maintenance-intensive due to the batteries used and not ideal from the sustainability perspective because of the increased energy consumption.

To counteract this disadvantage, power supply path B is rated at 400 kW, the minimum size required for this function. Supply path A therefore does not only represent the second foot of supply for the most important IT components, but is thereby also the only central supply path for the large number of computing nodes.

Fig. 5: One dynamic uninterruptible power supply units (UPS) of the line filter system.

In the mains filter system, power is regenerated by a motor-generator combination, filtering out disturbances/fluctuations that may enter the building through the mains. A rotating flywheel in the system stores enough energy to bridge power outages for at least half a minute. Supply path A is designed for an output of over 2,000 kW (up to 6,000 kW is planned), so the high efficiency of the mains filter system benefits the entire data center.

Operation-critical technical systems such as pumps, fans of the air-circulation cooling units, chillers, etc. are only protected via the emergency power system, since this is available after a short downtime of just a few seconds and the systems can easily tolerate this brief interruption.

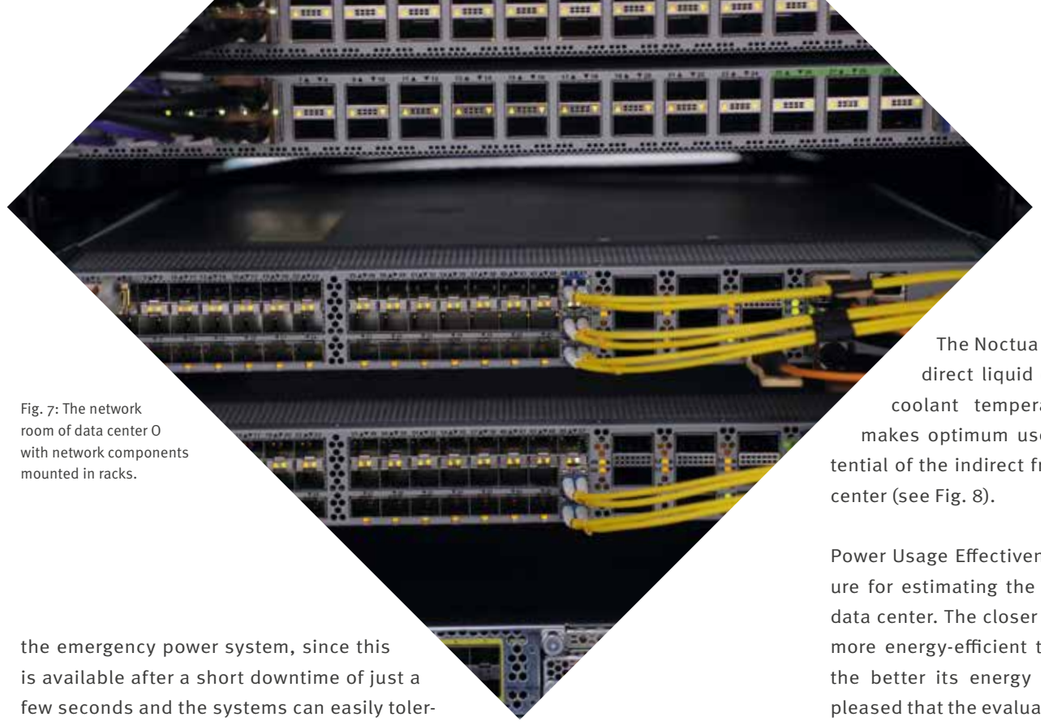


Fig. 7: The network room of data center O with network components mounted in racks.

CONNECTED TO THE WORLD

The existing computer rooms of PC2 in data center O together with data center X provide cross-site geo-redundancy. There are more than 1,000 communication lines between the network rooms of the two data centers, which were designed as fiber optic and copper cables and laid over two separate cable routes (see Fig. 6 and Fig. 7). The central storage system is distributed across both sites so that if one site fails, the unaffected site can continue to provide access to critical user data. This prevents service interruptions and data loss.
The efficient operation of HPC systems is an important criterion for us and is also required by the legislator in the current and future requirements for the sustainability of data centers.

Fig. 6: The network room of data center X with network components mounted in racks.

The Noctua 2 HPC system features direct liquid cooling (DLC) for high coolant temperatures and therefore makes optimum use of the efficiency potential of the indirect free cooling of the data center (see Fig. 8).

Power Usage Effectiveness (PUE) is a key figure for estimating the energy efficiency of a data center. The closer the value is to 1.0, the more energy-efficient the data center is and the better its energy balance. We are very pleased that the evaluation of the first months of operation confirm that the PUE value of 1.1 targeted in the planning could be achieved in data center X by using such HPC systems with DLC.

AN EXELLENT INFRASTRUCTURE

From the preceding considerations, it is already clear that sustainability aspects are of great importance in the planning and operation of the new data center. We are therefore striving to have our data center certified with the "Blue Angel" environmental label (DE-UZ 228), which distinguishes data centers that are operated in an energy-efficient and environmentally friendly manner. As part of a study sponsored by the German Federal Environmental Agency and consulting by a specialized consulting firm, we are examining whether the criteria for the eco-label can already be fulfilled or what deficits and potentials exist.

MOST IMPORTANT REQUIREMENTS FOR CERTIFICATION WITH BLUE ANGEL ECO LABEL FOR DATA CENTERS

- a particularly energy-efficient, climate-friendly and resource-saving operation of the technical building equipment.
- the development and implementation of a long-term strategy to increase energy and resource efficiency
- empowering users to implement their own measures to increase energy efficiency
- the implementation of operational monitoring and transparent reporting to ensure energy-efficient operation

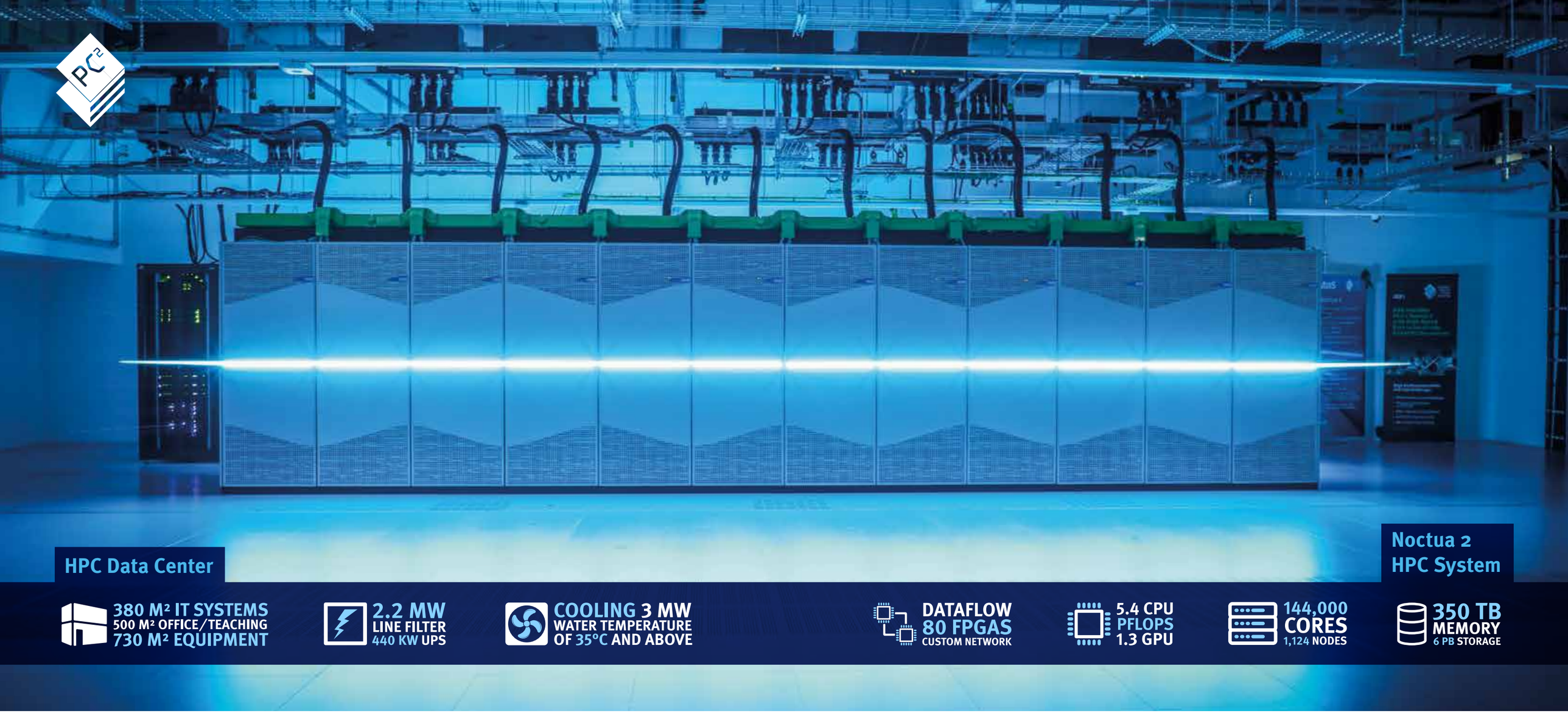


Fig. 8: HPC System Noctua 2.

Compliance with the minimum requirements will be verified by an independent auditor. The study is scheduled for completion in mid-2023, after which we will take the next steps to achieve certification by 2025.

VISIT US

In the first few months of operation, dozens of groups of visitors have already been guided through the data center.

In addition to interested staff and students from the University of Paderborn, numerous scientists, operators and planners of data centers from all over Germany learned about the underlying concepts and were able to visit the technical facilities.
Regular tours are offered, and individual tours can also be arranged upon request.

REPORT FROM THE RESOURCE ALLOCATION BOARD

Beginning in the Fall of 2021, we have fully adopted the NHR Association's rules for requesting compute time on our HPC systems. The previous project size classes of Small and Large have been expanded to three: Small, Normal, and Large. The Small project class enables local and regional users to apply for up to 4 million CPU core hours (currently) with little effort and a short turnaround time. The Normal and Large project classes are open to any member of a German university and follow the rules and procedures of the NHR Allocation Board. Proposals for the Normal class can be submitted at any time and are evaluated on an ongoing basis by external scientific reviewers. The allocation decision is made by the local Resource Allocation Board. In contrast, the NHR Large class, for allocations greater than 12 million CPU hours, has four calls per year with deadlines at the beginning of each quarter. Based on external scientific peer reviews, the local Resource Allocation Board makes a recommendation to the NHR-wide Allocation Board, which makes the final decision to ensure common evaluation standards, quality control, and load balancing across NHR centers.

Following the installation of the Noctua 2 system in late 2021 and the start of production operations in April 2022, the number of requests for computing time and the total amount of compute time requested increased dramatically.

From 2020 to 2022, we received 49 requests for Normal or Large projects and 293 requests for Small projects. The figure below shows the distribution of Principal Investigator affiliations weighted by the number of CPU core hours granted.
Compared to the two compute time proposals in 2019, 2019-1 and 2019-2, the ratio of compute time granted to projects from outside Paderborn University has increased from 27% to 45%. Similarly, the proportion of computing time granted to projects from outside the state of North Rhine-Westphalia (NRW) has increased from 14% to 24%. This shows the successful establishment of PC2 as an important computing center beyond the local or regional level.

We were very pleased to receive so many high-quality proposals from a wide range of scientific disciplines and institutions. The distribution by scientific field is shown in the figure below.

The funded projects are predominantly in the fields of condensed matter physics, physical chemistry, computer science, materials science and chemical engineering. However, PC2's outreach efforts have also resulted in projects in fields such as biology, medicine, humanities and social and behavioral sciences.

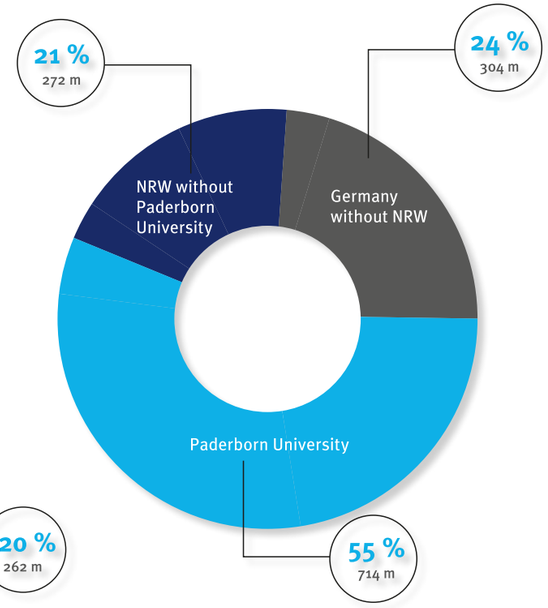


Fig. 1: Computing time projects awarded in CPU-core hours for proposals with start dates in 2020-2022, grouped by Principal Investigator affiliation.

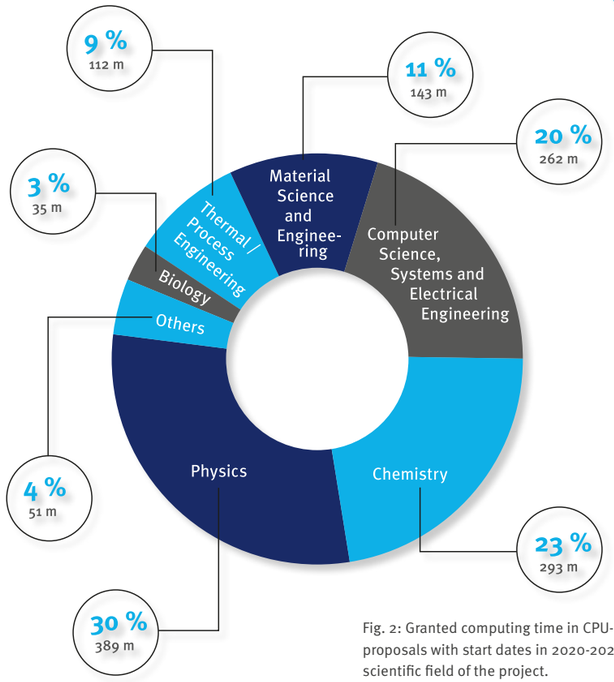


Fig. 2: Granted computing time in CPU-core hours for proposals with start dates in 2020-2022 according to the scientific field of the project.

HPC INFRASTRUCTURE PROVIDED BY PC2

The role of PC2 as a center for high-performance computing is to coordinate the procurement of central HPC systems and to make these systems available to scientists at Paderborn University, other research institutions in North Rhine-Westphalia and nationwide.

As a founding member of the Nation HPC Alliance (NHR), PC2 provides high-performance computing, services and consulting for academic users nationwide.
In the field of using FPGAs for high performance computing, PC2 possesses exceptional expertise, pioneering and a worldwide leading role. PC2 operates the HPC system Noctua 2, which is one of the world's largest and most advanced academic HPC production systems with FPGAs and is used by researchers from Germany, the UK, Switzerland, Sweden and the USA.

System administrators and technical advisors employed by PC2 support researchers for using the HPC systems effectively and provide guidance with porting and optimizing their scientific codes.

An overview of the main computing systems that have been in operation in the reporting period is shown in the table below. In Noctua 2, 48 Alveo U280 FPGA cards with High-Bandwidth Memory (HBM2) have been integrated and complemented with the 32 Stratix 10 FPGAs deployed originally in Noctua 1. For dedicated inter-FPGA networks, the network ports of all 80 FPGA cards are connected to a Calient S320 optical circuit switch (OCS) that also debuted in Noctua 1. This allows user-configurable direct point-to-point connections between FPGAs. For packet-switched communication between FPGAs, these links can also be forwarded to a newly added 100 Gbps Ethernet switch that is connected to the optical circuit switch.

TABLE 1: HPC SYSTEMS

NAME/ PURPOSE	SUPPLIER	INAUGURATION	ARCHITECTURE	NUMBER OF NODES/CORES	MEMORY PER NODE	INTERCONNECT
Noctua 2	Atos	2022	AMD Milan 7763 48x Xilinx Alveo U280 32x Intel Stratix 10GX 2800 136x NVIDIA A100 with NVLink	1,130/143,872	256 GB 512 GB 1024 GB up to 30 TB	InfiniBand 100/200 HDR, 1:2 blocking factor Direct FPGA interconnect 4x40 Gbps
Noctua 1	Cray	2018	Intel Xeon Gold 6148 32x Intel Stratix 10GX 2800 (until 2022) 18x NVIDIA A40 (since 7/2023)	274/10,960	192 GB	100 Gbps Omni-Path Direct FPGA interconnect 4x40 Gbps
OCuLUS	ClusterVision	2012 decomissioned 2022	Intel Xeon E5-2670 Intel Xeon E5-4670 NVIDIA GTX 1080Ti NVIDIA Tesla K20x	616/9,920	64 GB 256 GB 1024 GB	InfiniBand QDR

TABLE 2: STORAGE SYSTEMS

TYPE	MANUFACTURER	START OF OPERATION	CAPACITY	AVAILABLE ON
Parallel filesystem	DDN	2022	6 PB	Noctua 2 Noctua 1 (ro)
Parallel filesystem	Seagate/HPE	2018	720 TB	Noctua 1 Noctua 2 (ro)
UPB Storage	DELL/EMC PowerScale (Isilon)	2018	200 TB (PC2 pool)	All systems
PC2 central storage	DELL/EMC PowerScale (Isilon)	Q3 2023	9 PB raw (distributed to split on two systems and multiple tiers for redundancy, archive and recovery)	All systems

All storage systems are accessible on user's work computers from the university network or via VPN using SMB (CIFS) and NFS.

COMPUTING SYSTEM ACCESS

As a member of the NHR Association, any scientist at a German university can apply for a computing time allocation on our HPC systems. Proposals are scientifically evaluated in a peer review process. If approved, the access is granted free of charge. For more details, refer to the Report of the Resource Allocation board on page XX of this report.

There are different possibilities to access our clusters, among others, the systems can be accessed via JupyterHub web interface with the ability for users to build their own software environment and to start remote desktop environments. A list of services is shown below.

ADDITIONAL TECHNICAL INFORMATION AND APPLICATION FORMS

Additional technical information on our HPC infrastructure, installed software, access to the systems, computing time application forms and the current call for proposals can be found on our website.

TABLE 3: SERVICES

SERVICE	DESCRIPTION	FEATURE LIST	AVAILABLE ON
JupyterHub	JupyterHub JupyterHub is a multi-user capable web interface for spawning and managing Jupyter notebooks on our HPC systems.	Start Jupyter Notebooks on compute nodes Custom Singularity container with own software Graphical remote desktop environment	All users
ClusterCockpit	ClusterCockpit is a cluster-wide and job-specific system for monitoring and analyzing the execution of jobs.	Analyze performance issues of HPC jobs Graphical visualization	All users
PC2 Self-Service Portal	Introduction planned for Q3 2023.	HPC system status, maintenance notifications Accounting and resource usage overview Project membership management	All users

FURTHER TECHNICAL INFORMATION AND APPLICATION FORMS

Additional technical information on our HPC infrastructure, installed software, access to the systems, computing time application forms and the current call for proposals can be found on our website.

FACTS AND FIGURES

Dec 2022
Start of the installation of new central storage system from Dell/EMC Isilon

Apr 2022
Inauguration of new HPC center (building X)

Feb 2022
Move to the new office area in building X

Jun 2022
Shutdown of HPC system OCuLUS

Mar 2022
HPC system Noctua 2 ready for operation

Dec 2021
Start of installation of Noctua 2 from Atos/Bull

Nov 2020
Paderborn Center for Parallel Computing selected as National High-Performance Computing Center

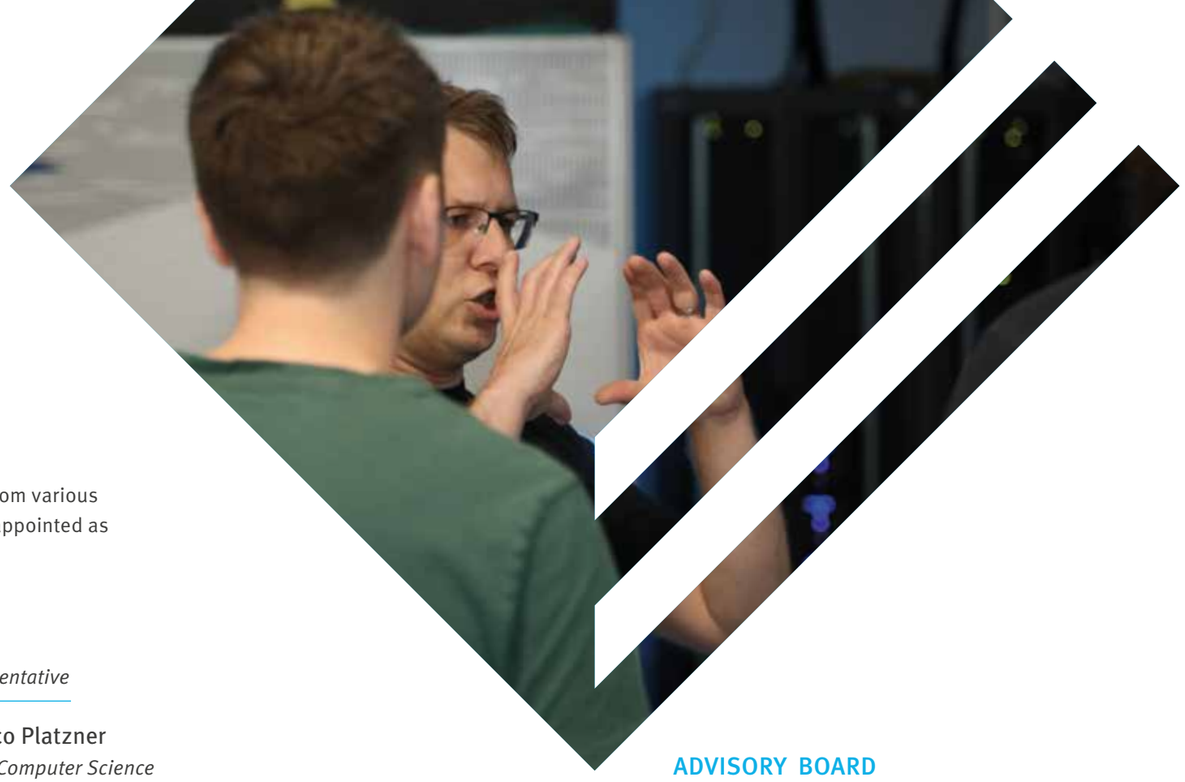
Oct 2019
Groundbreaking for construction of new HPC center

Sep 2018
HPC system Noctua 1 ready for operation

Jun 2017
Approval of research infrastructure proposal by Joint Science Conference (GWK)

Sep 2016
Submission of research infrastructure proposal to German Science and Humanities Council

BOARDS



MANAGEMENT BOARD

PC2 is headed by an interdisciplinary board comprising professors from various working groups of Paderborn University. The following people were appointed as Management Board members as of December 2022.

Prof. Dr. Michael Dellnitz
Department of Mathematics

Prof. Dr. Jens Förstner
Department of Electrical Engineering

Dr. Hendrik Rose
Department of Physics
Representative of Scientific Personnel

Prof. Dr. Thomas Kühne (Vice Chairman)
Department of Chemistry

Prof. Dr. Torsten Meier
Department of Physics

Prof. Dr. Burkhard Monien
Department of Computer Science (Emeritus)

Prof. Dr. Gudrun Oevel
Representative of the University's Central IT Services Unit (IMT)

Gerrit Pape
Student Representative

Prof. Dr. Marco Platzner
Department of Computer Science

Prof. Dr. Christian Plessl (Chairman)
Department of Computer Science

Dr. Robert Schade
Paderborn Center for Parallel Computing
Representative of Scientific Personnel

Prof. Dr. Wolf Gero Schmidt
Department of Physics

Marcel-Brian Wilkowsky
Paderborn Center for Parallel Computing
Representative of Technical and Administrative Personnel

ADVISORY BOARD

The management board of PC2 is supported by a scientific advisory board, which is composed of representatives from academia and industry. The advisory board provides expert input for strategic decisions and the continuous development of PC2 into a nationwide competence and service center for HPC and computational science.

Dr. Michaela Blott
Distinguished Engineer
AMD, Ireland

Prof. Dr. Dominik Marx
Institute for Technical Chemistry
Ruhr-University, Bochum, Germany

Dr. Franz-Josef Pfreundt
Chief Strategy Officer High Performance Computing
Fraunhofer Institute for Industrial Mathematics (ITWM), Kaiserslautern, Germany

Prof. Dr. Birgitt Riegraf
President Paderborn University
Paderborn, Germany

Prof. Dr. Roser Valenti
Institute for Theoretical Physics
Goethe-Universität Frankfurt am Main, Germany

Prof. Dr. Tilo Wettig
Institute for High-Energy Physics
University of Regensburg, Germany

PC2 STAFF

In the years 2020, 2021 and 2022, PC2 employed:

12 research associates

10 administrative and technical staff

2 trainees

4 students and graduate assistants

Dipl.-Inf. Bernard Bauer

Dr. Carsten Bauer

Markus Hegerkamp

Dipl.-Inf. Axel Keller

Michaela Kemper

Dr. Tobias Kenter

Dipl.-Ing. Andreas Krawinkel

Dr. Michael Laß

Dr. Lukas Mazur

Marius Meyer

Holger Nitsche

Prof. Dr. Christian Plessl

Dr. Heinrich Riebler

Stefan Rohde

Dr. Robert Schade

Alexander Schopf

Michael Schwarz

Dr. Jens Simon

Abdul Rehman Tareen

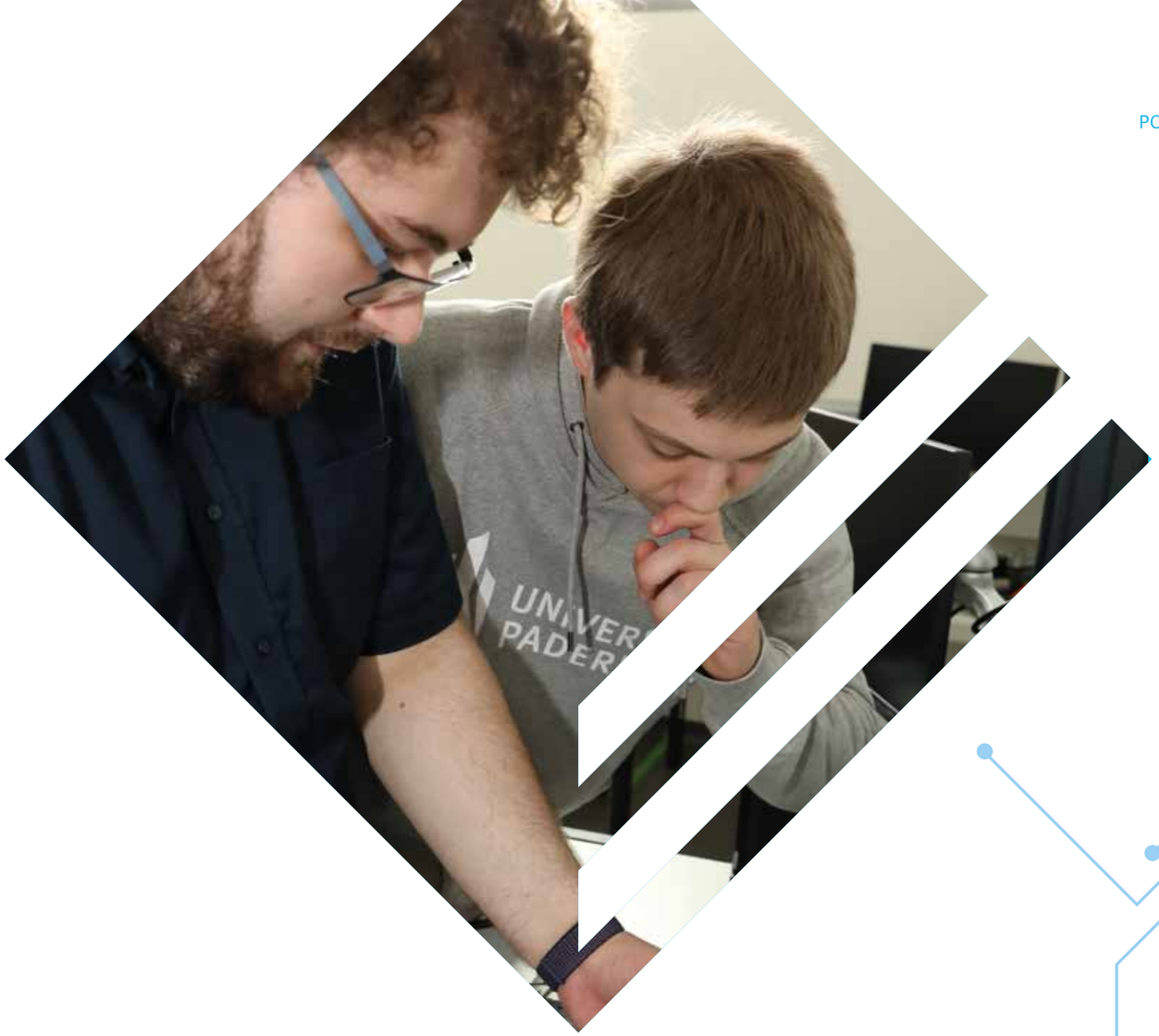
Alex Wiens

Marcel-Brian Wilkowsky

Nils Winnwa

Dr. Xin Wu

Mohamad Rami Zaranij



Additional support was provided by students and graduate assistants working in the fields of programming, user support or system administration.

René Lammert

Johannes Menzel

Jan-Oliver Opdenhövel

Gerrit Pape

SELECTED PC2 RESEARCH

Through their research and development activities, the scientific staff of PC2 contribute to advancing the state of the art in the thematic focus areas of PC2. Many of these research projects stem from requests from users or from problems that users experience in their research. However, there are also exploratory projects that seek to advance the state of the art or assess the feasibility of innovative ideas and technologies. Practically, these research projects are conducted by PC2 HPC advisors and domain experts in the form of intensive user support projects and in close collaboration with them. Some of the larger or longer running research projects during the reporting period and profile of our experts are featured below.

QUANTUM COMPUTING FOR QUANTUM CHEMISTRY

The computational problems that need to be solved in quantum chemistry and solid-state physics consume a major part of the computing resources at most HPC computing centers. The need for accurate descriptions of molecules, surfaces as well as solids arises in many of the challenges that we are facing, from material design for energy production like solar cells over energy-efficient and climate-friendly building materials to medical challenges like vaccines and cancer treatments.

PC2 is advancing the development of methods to solve these quantum chemical problems on classical computers, for example, by developing ab-initio methods that scale beyond 100 million atoms and beyond 1.1 ExaFLOP/s on thousands of GPUs [1-3]. Computations on classical computers are the workhorse to tackle the challenges mentioned above. While powerful approximation methods suitable for classical computers have been developed, the inherent quantum nature of the electronic structure problem implies an exponential scaling of the computational complexity for most interesting chemical systems if an accurate solution is desired.

However, the recent advances in quantum computers open the door to designing, implementing, and testing new algorithms for efficient quantum chemistry simulations on real quantum computers. Such algorithms have to be able to deal with challenges like the limited number of qubits, limited connection topologies, noise, limited coherence times, and imperfect gate/readout fidelities. Most of these aspects are expected to be challenges not only in the current age of noise intermediate-scale quantum (NISQ) computers but also once the technologies mature. It is expected that most future practical quantum computing algorithms will be hybrid quantum-classical algorithms, where the parts with polynomial complexity run on a traditional HPC system, which also prepares the inputs for the quantum computer and then post-processes the measurements to produce the actual solution.

We have recently proposed, implemented, and tested a novel algorithm for the quantum-chemical ground-state energy problem on gate-based quantum computers [4]. The algorithm is based on reduced density-matrix functional theory (RDMFT) and introduces a new parallelization layer, which enables the decomposition of a larger system, for example, a large molecule, into subsystems that can be treated with much smaller quantum computers than the original complete problem. The decomposition and the adaptive cluster approximation that is used to represent the environment of a subsystem can be converged to the exact solution. On the practical level, we present techniques that reduce the qubit count, the number of quantum programs, as well as their depth. Finally, we have demonstrated the viability of the algorithm for Hubbard-like systems on superconducting transmon qubits in IBM quantum computers.

References

[1] Michael Laß, Robert Schade, Thomas D. Kühne, Christian Plessl
A Submatrix-Based Method for Approximate Matrix Function Evaluation in the Quantum Chemistry Code CP2K
SC20: International Conference for High Performance Computing, Networking, Storage and Analysis
https://doi.org/10.1109/SC41405.2020.00084

[2] Robert Schade, Tobias Kenter, Hossam Elgabarty, Michael Laß, Ole Schütt, Alfio Lazzaro, Hans Pabst, Stephan mohr, Jürg Hutter, Thomas D. Kühne, Christian Plessl
Towards Electronic Structure-based ab-initio Molecular Dynamics simulations with Hundreds of Millions of Atoms
Parallel Computing, Volume 111, July 2022
https://doi.org/10.1016/j.parco.2022.102920

[3] Robert Schade, Tobias Kenter, Hossam Elgabarty, Michael Laß, Thomas D. Kühne, Christian Plessl
Breaking the Exascale Barrier for the Electronic Structure Problem in ab-initio Molecular Dynamics
The International Journal for High Performance Computing Applications
https://doi.org/10.1177/10943420231177631

[4] Robert Schade, Carsten Bauer, Konstantin Tamoev, Lukas Mazur, Christian Plessl, Thomas D. Kühne
Parallel Quantum Chemistry on Noisy Intermediate-scale Quantum Computers
Phys. Rev. Research 4, 033160
https://doi.org/10.1103/PhysRevResearch.4.033160

COMPUTATION AND COMPRESSION OF ELECTRON REPULSION INTEGRALS ON FPGAS

The computation of electron repulsion integrals (ERIs) over Gaussian-type orbitals is a challenging problem in *ab initio* molecular dynamics (AIMD) simulation based on the hybrid density functional theory (DFT). In practice, many trillions of ERIs may have to be computed for the energy calculation in each time step of the AIMD simulation. Therefore, it was dubbed as “the nightmare of the integrals” in the 1998 Nobel Lecture for Chemistry.

There are currently active development of CPU and GPU libraries for the ERI computation. However, the CPU and GPU architectures are all fixed at the time of fabrication. It is impossible to tailor the hardware to suit the varied requirements of the ERI computation for different quartet classes, ranging from the simplest [ss|ss] with a handful of floating-point operations (FLOPs) to [ff|ff], which is characterized by 2.5×10^5 FLOPs per quartet.

By contrast, the reconfigurability of FPGAs allows us to customize the on-chip memory to the desired data layout for parallel access to the intermediate buffers targeting individual quartet classes. In addition, the single work-item programming model on FPGAs enables the pipeline parallelism for the loop structures to achieve high throughput in the ERI computation. By adapting to the different computation characteristics of 256 quartet classes, from [ss|ss] to [ff|ff], distinctive FPGA designs are created with customized loop parallelization and appropriate local memory layout. Furthermore, a lossy compression algorithm utilizing arbitrary bitwidth integer is integrated in the FPGA kernels for the ERI computation to reduce the demanding memory usage. To the best of our knowledge, the integration of ERI computation and compression is a novelty that is not even covered by any CPU or GPU libraries so far.

The performance evaluation shows that the FPGA kernels parallelized on 2 Stratix 10 GX 2800 FPGAs outperform libint, an optimized library for the ERI computation, by factors up to 6.0× on two-socket server with 40 Intel Xeon Gold 6148 CPU cores and up to 1.9× on 128 AMD EPYC 7713 CPU cores. Meanwhile, up to 5× energy efficiency is achieved compared to the AMD CPUs (released in 2021 with 7 nm manufacturing technology). Numerical analysis has indicated that using 16-bit integer for the ERI compression leads to maximum absolute errors of around 10^{-7} – 10^{-5} Hartree.

The ERI computation is a key component in the hybrid-DFT-based AIMD simulations. This work paves the way for FPGA-accelerated quantum-mechanics-based atomistic simulations. Further development of a suitable libint-like library interface allowing the use of the FPGA kernels in many quantum chemistry codes is already on the way.

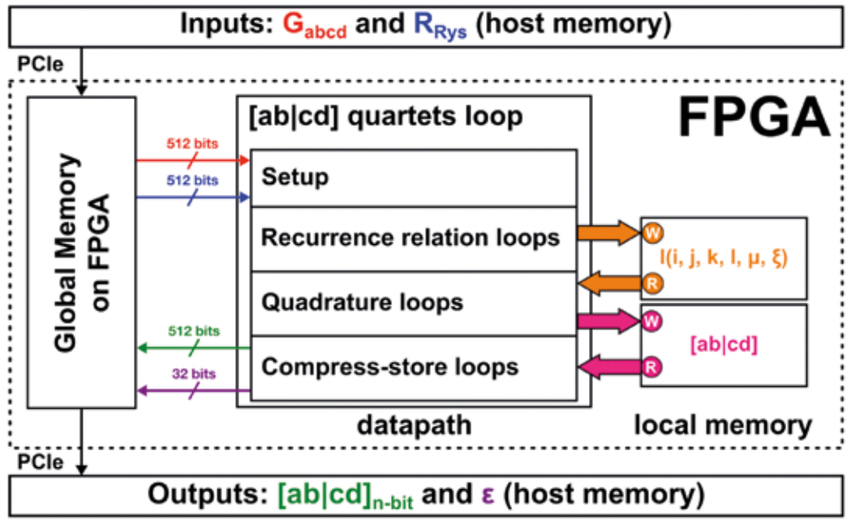


Figure 1. FPGA design for ERI computation and compression.

$$\int d\mathbf{r} \int d\mathbf{r}' \, g_{\mathrm{A},\mathbf{a},\alpha}(\mathbf{r}) \, g_{\mathrm{B},\mathbf{b},\beta}(\mathbf{r}) \, \frac{1}{|\mathbf{r}-\mathbf{r}'|} \, g_{\mathrm{C},\mathbf{c},\gamma}(\mathbf{r}') \, g_{\mathrm{D},\mathbf{d},\delta}(\mathbf{r}')$$

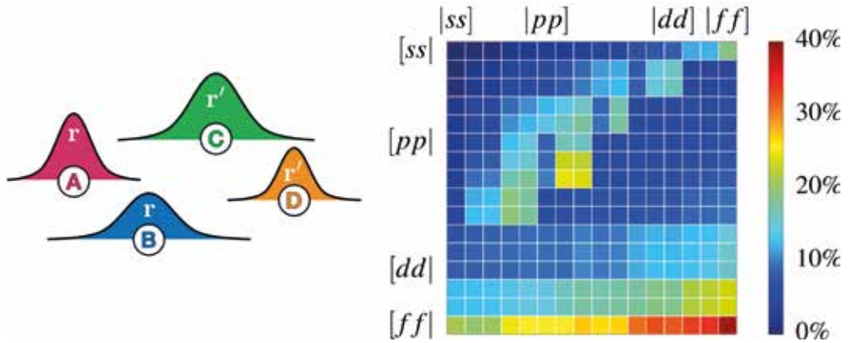


Figure 2. Mathematical and pictorial presentation of electron repulsion integrals and the DSP usage for 256 FPGA kernels for the ERI computation and compression on Intel Stratix 10 GX 2800.

STAFF PROFILE: DR. XIN WU

Xin Wu did his doctoral research on the topic of development of semiempirical quantum chemistry (SQC) at Max-Planck-Institut für Kohlenforschung (MPI KoFo) in Mülheim an der Ruhr and received his PhD degree from Heinrich Heine University Düsseldorf in 2014 [1]. Two essential issues of SQC methods were targeted in his PhD work: performance and accuracy in applications. To harness the computational power of Graphics Processing Unit (GPU) all hotspots (› 99% elapsed walltime) of the MNDO program were ported to the hybrid CPU-GPU architecture and the total computation times for static energy evaluation and geometry optimization of large molecules were reduced by one order of magnitude [2, 3]. Moreover, by taking advantage of parallelization with multiple CPUs, he implemented several numerical optimization algorithms, e.g., Nelder-Mead method, Gauss-Newton method, and Levenberg-Marquardt algorithm, in conjunction with the MNDO program for accurate simulation of complex chemical systems, e.g., enzymatic reaction [4] and proton transfer in water [5], by means of special-purpose parameterization.

He subsequently continued working as a postdoctoral researcher in an ERC Advanced Grant project at MPI KoFo. His major effort involved the development of new SQC methods with orthogonalization and dispersion corrections for accurate computation of both ground-state and excited-state molecular properties [6, 7, 8]. Furthermore, he performed a Big Data study for all kinds of *ab initio* molecular integrals in the non-orthogonal atomic basis as well as the symmetrically orthogonalized Löwdin basis. Based on the results of Big Data analytics, a novel semiempirical Hamiltonian was proposed to go beyond the classic neglect-of-diatomic-differential-overlap approximation [9].

At PC2 his primary research interest is the code optimization in quantum chemistry, especially focusing on the FPGA-accelerated kernels, e.g., the computation and compression of electron repulsion integrals for *ab initio* molecular dynamics simulation using the hybrid density functionals. Performance evaluation shows the optimized FPGA kernels deployed on two Stratix 10 GX 2800 FPGAs can achieve up to 1.9x – 6.0x speedup over the libint library on the compute nodes with 2x Xeon Gold 6148 CPUs (40 cores) or 2x EPYC 7713 CPUs (128 cores) and reach up to 5x energy efficiency [10]. In addition, he is actively involved in the regular HPC training courses at PC2, user support, particularly in the domain of quantum chemistry, as well as the North Rhine-Westphalian Competence Network for High Performance Computing (HPC.NRW).

References

[1] Wu, Xin (2014); **Semiempirical Quantum Chemistry on High-Performance Heterogeneous Computers;** PhD Thesis, Heinrich-Heine-Universität Düsseldorf https://docserv.uni-duesseldorf.de/servlets/DocumentServlet?id=28270

[2] Wu, Xin; Koslowski, Axel; Thiel, Walter (2012); **Semiempirical Quantum Chemical Calculations Accelerated on a Hybrid Multicore CPU–GPU Computing Platform;** Journal of Chemical Theory and Computation 8, 2272 - 2281

[3] Wu, Xin; Koslowski, Axel; Thiel, Walter (2016); **Semiempirical Quantum Chemistry;** In Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics; Walker, Ross C. and Götz, Andreas W. Eds. John Wiley & Sons, Inc.

[4] Doron, Dvir; Major, Dan Thomas; Kohen, Amnon; Thiel, Walter; Wu, Xin (2011); **Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface;** Journal of Chemical Theory and Computation 7, 3420 - 3437

[5] Wu, Xin and Thiel, Walter and Pezeshki, Soroosh and Lin, Hai (2013); **Specific Reaction Path Hamiltonian for Proton Transfer in Water: Reparameterized Semiempirical Models;** Journal of Chemical Theory and Computation 9, 2672 - 2686

[6] Dral, Pavlo O.; Wu, Xin; Spörkel, Lasse; Koslowski, Axel; Weber, Wolfgang; Steiger, Rainer; Scholten, Mirjam; Thiel, Walter (2016); **Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Theory, Implementation, and Parameters;** Journal of Chemical Theory and Computation 12, 1082 - 1096

[7] Dral, Pavlo O.; Wu, Xin; Spörkel, Lasse; Koslowski, Axel; Thiel, Walter (2016); **Semiempirical Quantum-Chemical Orthogonalization-Corrected Methods: Benchmarks for Ground-State Properties;** Journal of Chemical Theory and Computation 12, 1097 - 1120

[8] Dral, Pavlo O.; Wu, Xin; Thiel, Walter (2019); **Semiempirical Quantum-Chemical Methods with Orthogonalization and Dispersion Corrections;** Journal of Chemical Theory and Computation 15, 1743 - 1760

[9] Wu, Xin; Dral, Pavlo O.; Koslowski, Axel; Thiel, Walter (2019); **Big Data Analysis of ab initio Molecular Integrals in the Neglect of Diatomic Differential Overlap Approximation;** Journal of Computational Chemistry 40, 638 - 649

[10] Wu, Xin; Kenter, Tobias; Schade, Robert; Kühne, Thomas D.; Plessl, Christian (2023); **Computing and Compressing Electron Repulsion Integrals on FPGAs;** IEEE International Symposium on Field-Programmable Custom Computing Machines (FCCM), 31st Annual, 162 - 173

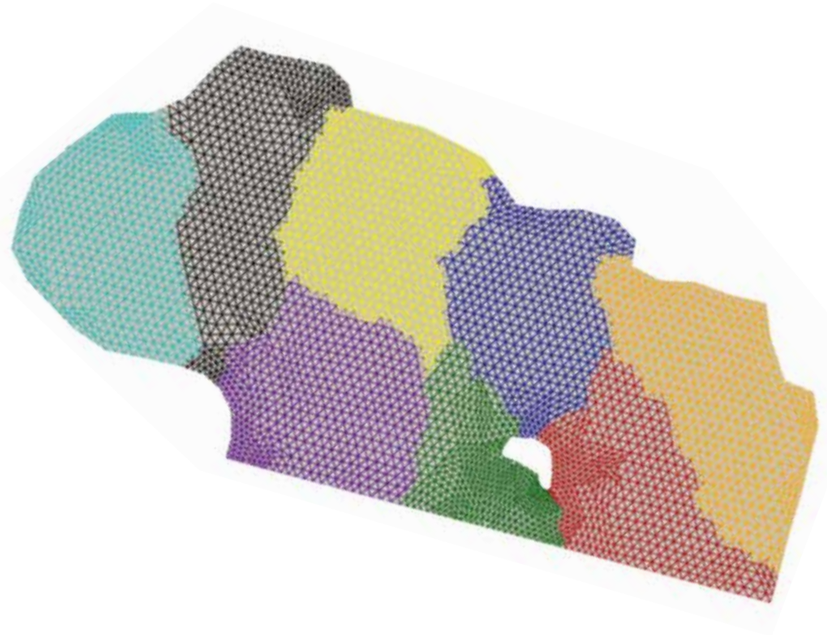
EXPLORING THE USE OF FPGAS FOR SOLVING THE SHALLOW WATER EQUATIONS

Modern flooding, weather, and climate prediction models critically rely on sophisticated numerical methods and ever increasing spatial and temporal resolution to deliver more accurate and physically comprehensive simulations. However, running high-resolution models on planet- or even region-sized domains sets a very high bar for the computational and energy efficiency of model codes on modern and future parallel and hybrid architectures. A particular challenge is the strong parallel scaling that is required to enable time-critical simulations or simulations over long time scales. In a collaboration with Bayreuth University and FAU Erlangen, PC2 is demonstrating and improving the use of FPGAs for simulations based on the Shallow Water Equations with a Discontiuous Galerkin discretization on unstructured meshes.

In a first work [1], published at PASC'21, we presented a design for Stratix 10 FPGAs that achieves a closed dataflow loop between all performance critical computation steps of the simulation. With a customized data layout distributed over the thousands of embedded memory blocks of the target FPGA, even the irregular data accesses along the mesh edges are deterministically scheduled to allow of a predictable high throughput. Thus, the FPGA outperforms a single-core CPU reference by up to 144x.

More recently [2], this architecture was extended with multi-FPGA support. This work leverages the unique inter-FPGA network infrastructure of the Noctua 2 system. The simulation mesh is spatially distributed to up to 10 FPGAs. For each compute job, up to four direct FPGA-to-FPGA links are configured that represent the topology of the partitioned mesh. These links are programmed as serial streaming interfaces that are directly integrated into the dataflow on each FPGA and forward the halo data at partition boundaries with a predictable and low latency. This multi-FPGA design allow to overcome mesh size limitations of the previous work that were caused by the reliance on local memory resources. At the same time, we observe strong scaling exactly in line with a performance model that shows perfect overlap of communication and computation from few hundred elements per FPGA upwards.

Further developments for Shallow Water Equations on FPGAs are ongoing, for example targeting AMD Alveo FPGAs using direct FPGA-to-FPGA communication with MPI, and also development of a SYCL codebase to investigate performance portability between FPGAs, CPUs and GPUs. Another recent work [3] complements the hand-optimized designs discussed in the previous paragraphs with a code generation approach that allows to automate large parts the acceleration process within the scope of a structured mesh that is mapped to a stencil-based FPGA design template.



References

[1] T. Kenter, A. Shambhu, S. Faghih-Naini, V. Aizinger
Algorithm-Hardware Co-Design of a Discontinuous Galerkin Shallow-Water Model for a Dataflow Architecture on FPGA
in: Proceedings of the Platform for Advanced Scientific Computing Conference, ACM, 2021.

[2] J. Faj, T. Kenter, S. Faghih-Naini, C. Plessl, V. Aizinger
Scalable Multi-FPGA Design of a Discontinuous Galerkin Shallow-Water Model on Unstructured Meshe
in: Proceedings of the Platform for Advanced Scientific Computing Conference, ACM, 2023.

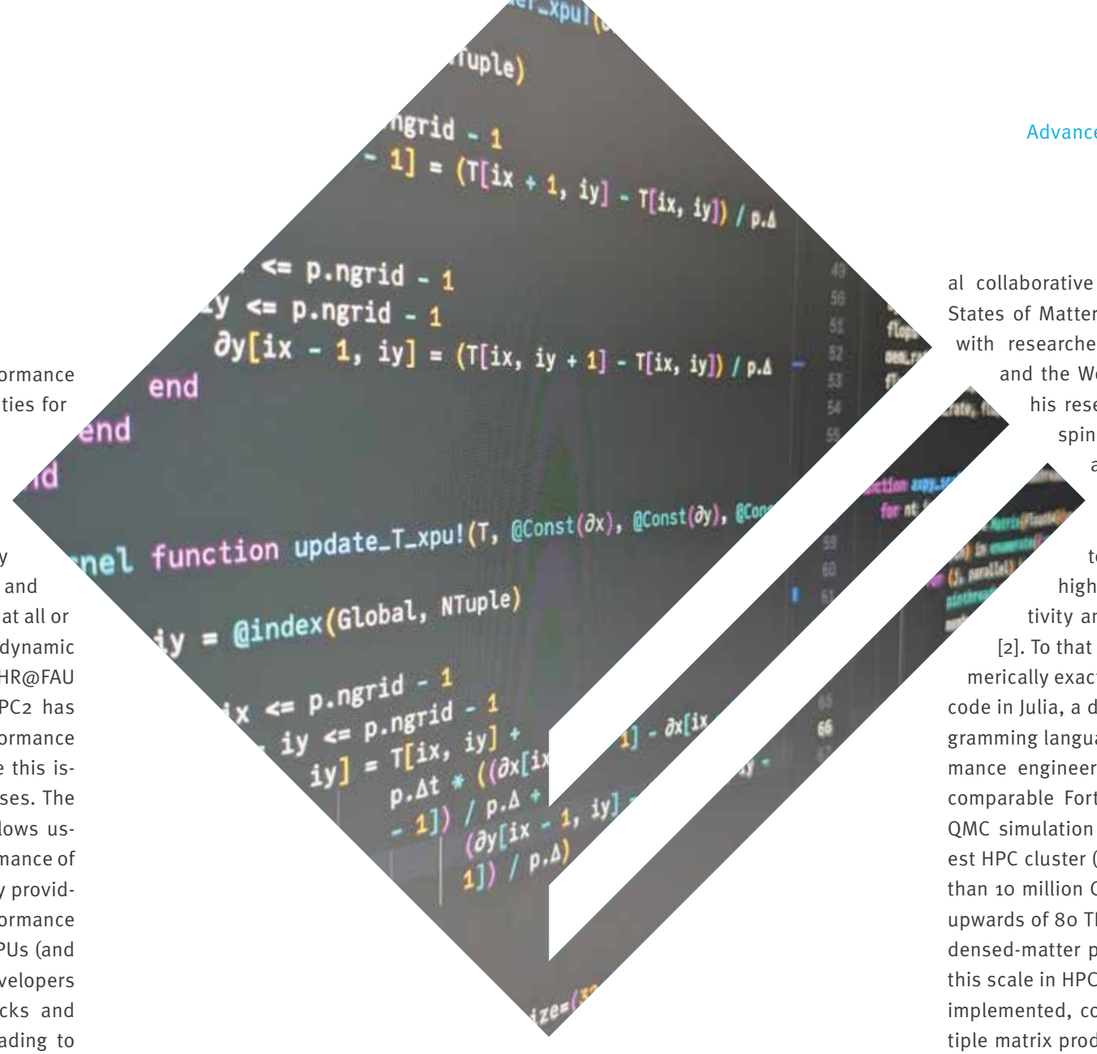
[3] C. Alt, T. Kenter, S. Faghih-Naini, J. Faj, J.-O. Opdenhövel, C. Plessl, V. Aizinger, J. Hönig, H. Köstler
Shallow Water DG Simulations on FPGAs: Design and Comparison of a Novel Code Generation Pipeline
in: Lecture Notes in Computer Science, Springer Nature Switzerland, Cham, 2023.

ADVANCING PRODUCTIVE HPC DEVELOPMENT WITH JULIA

PC2 is at the forefront of exploring and advancing modern approaches to high-performance computing with the Julia programming language. With its unique tradeoffs in language design, Julia enables interactive high-productivity scientific computing while still being competitive in terms of performance to established low-level languages (e.g., C or Fortran). Through its dedicated efforts in developing essential tools for Julia workflows on HPC clusters as well as fostering international community building, PC2 is in a distinguished position in Germany and one of the leading institutions in the Julia HPC landscape worldwide.

With a strong focus on parallel computing, PC² has made significant contributions to the Julia ecosystem by creating and maintaining several powerful packages tailored to satisfy the demands of modern parallel computing environments. One of PC2's flagship developments is ThreadPinning.jl, a Julia package that provides developers with a versatile and convenient set of tools to visualize and control the affinity of Julia threads in multithreaded applications. Systematic thread pinning is crucial for achieving the optimal performance on HPC cluster nodes, e.g., to avoid unnecessary non-uniform memory access (NUMA). ThreadPinning.jl enables users to readily specify the desired thread-core mapping at different levels of abstraction with several common configurations available as predefined options. One of the stand-out attributes is that all provided functionality can be dynamically employed at runtime. This enables interactive performance tuning and opens up novel opportunities for HPC teaching and training.

A tangential goal of PC2 is to establish Julia support for well-known HPC performance tools that originally target static programming languages and therefore either do not work with Julia at all or do not exploit the full potential of its dynamic nature. In close collaboration with NHR@FAU (Erlangen) within the NHR alliance, PC2 has created a Julia interface to the performance benchmarking suite LIKWID, to tackle this issue for intra-node performance analyses. The resulting Julia package, LIKWID.jl, allows users to interactively monitor the performance of their applications at hardware level by providing information from hardware performance counters that are built into modern CPUs (and GPUs). These valuable insights aid developers in identifying performance bottlenecks and optimizing their code, potentially leading to significant speed-ups. For MPI-parallel codes, PC2 has been working on seamless integration with the popular performance measurement and analysis infrastructure Score-P. This enables users to profile and trace their massively parallel Julia applications and make use of a rich set of visualization tools, such as Cube and Vampir.



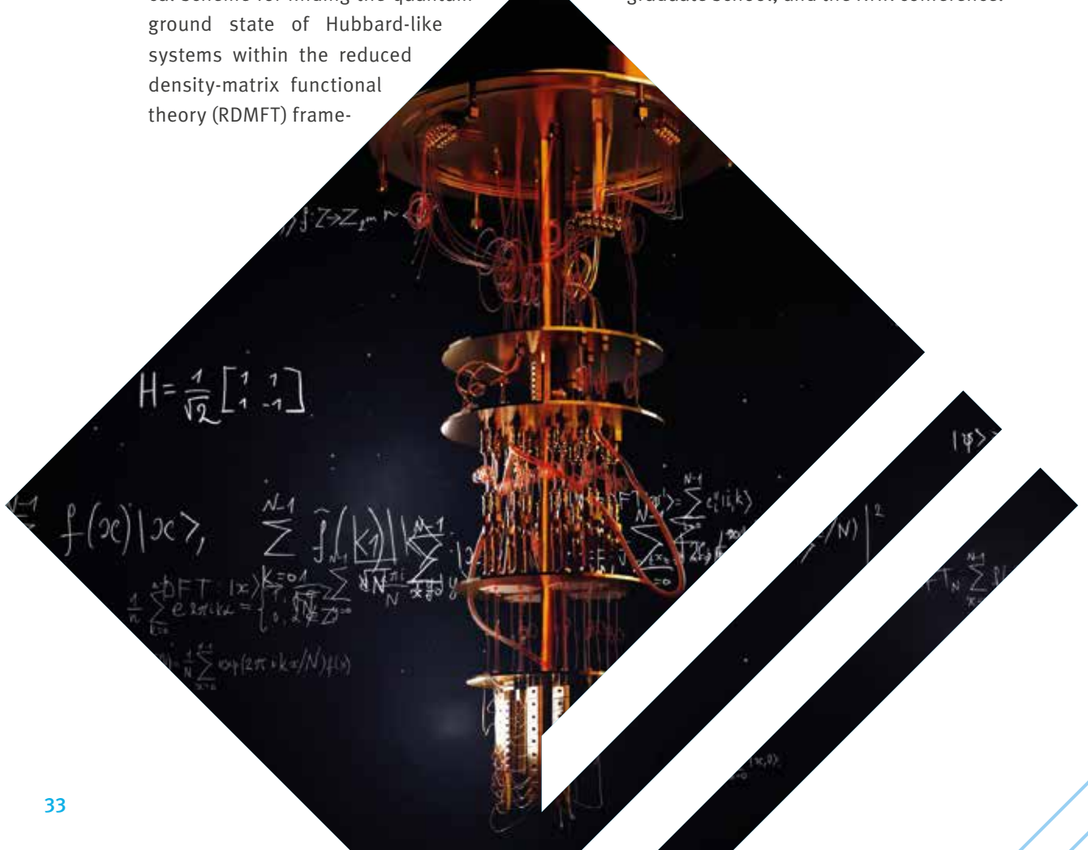
STAFF PROFILE: DR. CARSTEN BAUER

Carsten Bauer is a computational scientist who obtained his PhD in theoretical physics from the University of Cologne in 2020 [1]. During his PhD, Carsten investigated novel quantum phase transitions in two-dimensional itinerant electron systems within the international collaborative research center "Entangled States of Matter" (CRC 183). In collaboration with researchers from Stanford University and the Weizmann Institute of Science, his research focus was the onset of spin-density wave (SDW) order at metallic quantum critical points (QCP) – occurring at the absolute minimum of temperature – that give rise to high-temperature superconductivity and "strange metal" behaviour [2]. To that end, Carsten developed a numerically exact quantum Monte Carlo (QMC) code in Julia, a dynamic but yet compiled programming language, that, by thorough performance engineering, could often outperform comparable Fortran and C++ codes [3]. The QMC simulation code ran on Germanys fastest HPC cluster (JUWELS at the time) for more than 10 million CPU-core hours and produced upwards of 80 TB of data. It was the first condensed-matter physics application of Julia of this scale in HPC. As part of the code, Carsten implemented, compared, and optimized multiple matrix product stabilization methods [4] and, by studying the mathematics behind the QMC sign-problem, identified new sign-problem free model Hamiltonians for future studies [1].

Together with partners from Cornell University, Carsten invented a novel "quantum loop topography" approach to detect quantum critical points, phase transitions, and crossovers from QMC simulation data of itinerant electron systems [5, 6, 7]. The key features of the new method are that it is semi-automatic (super-

vised machine learning) and orders of magnitudes less computationally expensive than established numerical approaches. By applying the technique to the SDW QCP, they could demonstrate the functioning and robustness of the new method for a non-trivial complex quantum system [5].

At PC2, Carsten is investigating how quantum computers can be utilised in quantum physics and chemistry simulations. With collaborators from Paderborn University, he worked out a parallel hybrid quantum-classical scheme for finding the quantum ground state of Hubbard-like systems within the reduced density-matrix functional theory (RDMFT) framework [8]. A further line of Carsten's work at PC2 is to analyse and improve the capabilities of Julia for HPC in collaboration with international partners [9]. Here, the goal is to explore the HPC use cases for dynamic programming languages, in particular as a means for lower-barrier entry to HPC. Carsten is furthermore heading the training division at PC2 and, in his role as HPC advisor, is mentoring user compute projects from the condensed-matter physics domain. Carsten is engaged in the National High Performance Computing Alliance (NHR), especially in the NHR training group, the NHR graduate school, and the NHR conference.



References

[1] C. Bauer (2020), **Simulating and Machine Learning Quantum Criticality in a Nearly Antiferromagnetic Metal PhD Thesis**, Universität zu Köln http://kups.ub.uni-koeln.de/id/eprint/35405

[2] C. Bauer, Y. Schattner, S. Trebst, E.Berg (2020), **Hierarchy of Energy Scales in an O(3) Symmetric Antiferromagnetic Quantum Critical Metal: a Monte Carlo Study** Physical Review Research 2

[3] C. Bauer (2020), **julia-sdw-dqmc: Determinant Quantum Monte Carlo in Julia (1.0)** Zenodo, https://doi.org/10.5281/zenodo.3603345

[4] C. Bauer (2020), **Fast and stable determinant Quantum Monte Carlo** SciPost Physics Core 2, 2

[5] G. Driskell, S. Lederer, C. Bauer, S. Trebst, E.-A. Kim (2021), **Identification of Non-Fermi Liquid Physics in a Quantum Critical Metal via Quantum Loop Topography** Physical Review Letters 127, 046601

[6] Y. Zhang, C. Bauer, P. Broecker, S. Trebst, E.-A. Kim (2018), **Probing Transport in Quantum Many-Fermion Simulations Via Quantum Loop Topography** Physical Review B 99, 161120(R), Editors' Suggestion

[7] C. Bauer, S. Trebst (2018), **Machine Learning Transport Properties in Quantum Many-Fermion Simulations** In NIC Symposium 2020, Vol. 50, pp. 85–92, Forschungszentrum Jülich GmbH Zentralbibliothek, Verlag

[8] R. Schade, C. Bauer, K. Tamoev, L. Mazur, C. Plessl, T. D. Kühne (2022), **Parallel Quantum Chemistry on Noisy Intermediate-Scale Quantum Computers** Physical Review Research 4, 033160

[9] V. Churavy, W. F Godoy, C. Bauer, H. Ranocha, M. Schlottke-Lakemper, L. Räss, J. Blaschke, M. Giordano, E. Schnetter, S. Omlin, J. S. Vetter, A. Edelman (2022), **Bridging HPC Communities through the Julia Programming Language** arXiv:2211.02740

PROJECTS

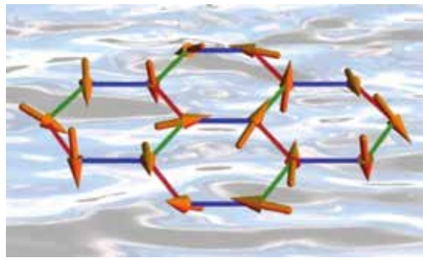
MULTILOOP MAJO-
RANA FUNCTIONAL
RENORMALIZATION
GROUP FOR FRUS-
TRATED QUANTUM

MULTILOOP MAJORANA FUNCTIONAL RENORMALIZATION GROUP FOR FRUSTRATED QUANTUM

In condensed matter physics, a recurring motif in a vast number of quantum materials is the formation of quantum magnetism from interactions between elementary electronic quantum spins. From a conceptual point of view, such interacting spin systems represent prime examples of quantum many-body problems in which the fundamental phenomenon of emergence manifests itself in a particularly impressive way. Emergence here means that the interaction of very many, but relatively simple constituents (in our case, quantum spins) gives rise to novel quantum effects or quantum phases that are not readily apparent from the properties of the individual constituents alone. The archetypal example of such an emergent state of matter, in the field of quantum magnetism, is a so-called quantum spin liquid. In these quantum liquids, the microscopic spins form a collective and coherent quantum state that is macroscopically entangled over large distances. The quantum spins in such a state remain strongly fluctuating, even at the lowest temperatures, and do not form any (magnetic) order — similar to the phenomenology of a conventional liquid. One of the most intriguing manifestations of the macroscopic entanglement of a quantum spin liquid is the emergence of topological non-trivial properties which come hand-in-hand with the formation of fractional quasiparticles, which expand the zoo of the elementary particles known from high-energy physics. Besides the conceptual beauty of the phenomena, quantum spin liquids promise technological applications, e.g., through the exploitation of topological protection in future quantum information applications.

Prof. Dr. Simon Trebst

Prof. Simon Trebst leads the Computational Condensed Matter Physics group at the Institute for Theoretical Physics at the University of Cologne. His group studies quantum many-body phenomena such as macroscopic entanglement, topological states of matter, and fractionalization in quantum materials and platforms for quantum computing. He is speaker of the pan-European CRC 183 “Entangled States of Matter” with nodes in Berlin, Copenhagen, Rehovot, and Cologne.



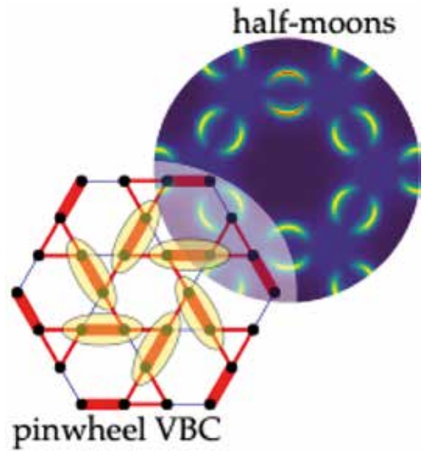
Schematic illustration of a quantum spin liquid. The elementary quantum spins interact via bond-directional exchanges (red, blue & green bonds) that cannot be simultaneously satisfied. As a result the spins seemingly form a state without any order, but closer inspection reveals macroscopic quantum mechanical entanglement.

The key underlying sources for such non-trivial magnetic behavior are strong quantum fluctuations usually induced by magnetic frustration effects, which arise from interaction energies between spins that cannot be simultaneously minimized. This keeps the spins fluctuating and liquid-like down to lowest temperatures. While many promising candidate materials have been identified for this to happen, unambiguous experimental evidence of a quantum spin liquid in a real material remains scarce.

Fascinating as the properties of such quantum phases may be, their theoretical investigation turns out to be extraordinarily difficult, since it generally requires a solution of the quantum mechanical many-body problem. Hence, progress can often only be achieved with the help of modern numerical methods that draw insights from statistical physics, quantum information theory and computational science as well as the use of powerful, large-scale computational resources. Although remarkable improvements have been made in recent years in the development of such methods, notably in the context of tensor network algorithms, there remains an urgent need for flexible numerical techniques that can handle the multitude of interaction scenarios between quantum spins as they exist in real materials. Precisely developing such tools is the goal of this research project.

Prof. Dr. Johannes Reuther

Prof. Johannes Reuther is a professor at the Physics Department of the Freie Universität Berlin and leads the department "Theory of Novel Quantum Materials" at the Helmholtz-Zentrum Berlin für Materialien und Energie. His research focuses on the study of quantum magnetic systems using numerical methods, particularly, the functional renormalization group. Before becoming a professor in Berlin, he was a postdoc at Caltech/USA.



In recent years, the pseudofermion functional renormalization group (pf-FRG) method has gained significant importance as a new numerical approach for the study of quantum spin systems. Initially pioneered by one of the principal investigators of this project some 15 years ago, the pf-FRG allows for a great numerical flexibility when applied to a large variety of quantum spin models. The methodological starting point is quite different from most other quantum many-body methods currently in use. In simple terms, pf-FRG simulates a kind of cooling process of a spin system, exploiting the fact that at high temperatures the system is initially in a simple (disordered) state already described by classical physics. As the temperature is slowly lowered (which here corresponds to a flow of renormalization group parameters), more and more quantum effects are taken into account until the system has reached the physically most interesting situation of absolute zero temperature. From a numerical point of view, this cooling process involves the solution of systems of tens to hundreds of millions of first-order coupled differential equations for the spin correlations. One advantage of this approach is that it enables the study of three-dimensional interacting spin systems, which are particularly relevant for applications for real materials, but remain difficult to treat for many other methods. The purpose of this compute time project is, on the one hand, to demonstrate the full potential of the pf-FRG approach by applying it to some of the most interesting frustrated quantum spin systems, and, on the other hand, to further improve its performance by further developments.

Particularly interesting applications in this compute time project were carried out for spin systems with flat magnetic band structures such as they occur, e.g., for spin models with phyrochlore lattice structures. The flat band structures ensure that quantum effects are particularly prominent, favoring the emergence of novel quantum phases such as the quantum spin liquid mentioned above. A first class of system studied were spin models on the 2agome lattice, where the effects of flat bands and the resulting spin phases were investigated under the simultaneous influence of quantum fluctuations and longer-range interactions [1]. The phase diagram which is obtained in this way enables deep insights into the magnetic structure of these strongly frustrated systems. In another model system, whose magnetic properties are also determined by the existence of flat bands, we investigated the appearance of particularly exotic quasiparticles, so-called fractons, which are being studied within a new emerging research field. These particles are characterized by the unusual property of being stationary in space, that is, completely immobile. This phenomenon is of great interest in quantum information theory but also in high energy physics. Our work [2] investigates the stability of these particles under realistic microscopic conditions, as they may occur in actual quantum materials. In another work [3], spin liquid behavior in a two-dimensional honeycomb structure is studied and interesting spin correlations are found that cannot be explained within classical physics.

Taken together, our results extend the understanding of interacting quantum spins and reveal new possibilities for realizing exotic quantum phases. Our methodological improvements, such as those demonstrated in [4], also pave the way for further investigations.

References

[1] D. Kiese, F. Ferrari, N. Astrakhantsev, N. Niggemann, P. Ghosh, T. Müller, R. Thomale, T. Neupert, J. Reuther, M. J. P. Gingras, S. Trebst, and Y. Iqbal, **Pinch-Points to Half-Moons and up in the Stars**, arXiv:2206.00264 (2022).

[2] N. Niggemann, Y. Iqbal, and J. Reuther, **Quantum Effects on Unconventional Pinch Point Singularities**, arXiv:2212.01318 (2022).

[3] Y. Watanabe, S. Trebst, and C. Hickey, **Frustrated Ferromagnetism of Honeycomb Cobaltates: Incommensurate Spirals, Quantum Disordered Phases, and Out-of-Plane Ising Order**, arXiv:2212.14053 (2022).

[4] B. Schneider, D. Kiese, and B. Sbierski, **Taming Pseudo-Fermion Functional Renormalization for Quantum Spins: Finite-Temperatures and the Popov-Fedotov Trick**, Phys. Rev. B 106, 235113 (2022).

PROJECTS

LARGE-SCALE ATOMISTIC SIMULATION OF DISLOCATION BEHAVIOUR IN W-MO-NB TERNARY REFRACTORY ALLOYS

LARGE-SCALE ATOMISTIC SIMULATION OF DISLOCATION BEHAVIOUR IN W-MO-NB TERNARY REFRACTORY ALLOYS

Alloys based on refractory metals play an important role in materials science and engineering, especially for high temperature applications. These metals can form homogenous complex alloys with bcc crystal lattice in a wide range of temperatures and compositions. Due to their high melting points and outstanding temperature strength, refractory alloys are heavily used as structural materials in aerospace and nuclear engineering (fission and fusion type), for metalworking tools and crucibles, and for chemical reaction vessels in corrosive environments. One of the most important characteristics of refractory alloys is their peculiar, strongly temperature-dependent plasticity. Plastic deformation of such alloys is a complicated phenomenon that links behavior of the crystal defects with macroscopic change in a sample shape. It is known that one of the basic mechanisms of plasticity is a motion of dislocations under applied stress. However, theoretical description of this phenomenon and, especially, the prediction of mechanical behavior beyond available experimental data still presents a very challenging task.

In this project, the plastic deformation in bcc refractory metals (pure metals and complex alloys) was studied with a large-scale atomistic modelling. The modelling was based on the interatomic potentials developed recently for refractory alloys with use of machine learning technique [1]. Using the computational resources of the Noctua 2 cluster at PC2, mobility and diffusion characteristics of single dislocations were investigated in detail. The temperature-dependent mobility functions of screw and edge dislocations were calculated from classical molecular dynamics simulation. The simulations of screw dislocation movement under applied shear stress revealed that the process can proceed in two different regimes: through thermally activated motion and athermal motion taking place at high temperature [2]. Hence, the dislocation velocity depends on the shear stress in a non-trivial way and such dependency can be calculated only with a large-scale atomistic simulation. As an example, Fig. 1 shows the calculated mobility function for pure Nb. The calculated data provided a way to evaluate basic macroscopic characteristics of plastic deformation (yield stress, activation volume and strain rate sensitivity) at various temperatures, alloy compositions and strain rates. The simulation results agree well with the existing experimental data and provide an opportunity to predict a plastic behavior in case where the measured data are absent. Fig. 2 illustrates the comparison between the calculated yield stress for pure Nb and measured one. In addition, this figure shows the calculated dependence of the yield stress on temperature for the Nb-30 at.%Zr alloy, for which experimental data is not available.

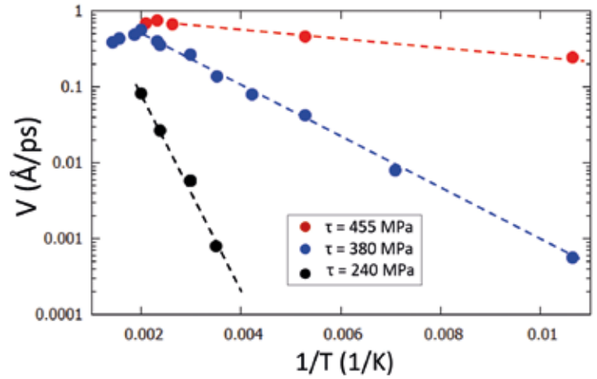


Fig.1 The dependency of screw dislocation velocity on temperature at three different shear stresses

Dr. Sergei Starikov

Dr. Sergei Starikov is a Project leader in the Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum. In 2011, he obtained a Ph.D. in Moscow Institute of Physics and Technology with specialization in Condensed matter physics. His primary research interest is computational materials science, focusing on development of interatomic potentials, atomic diffusion, and plastic deformation.

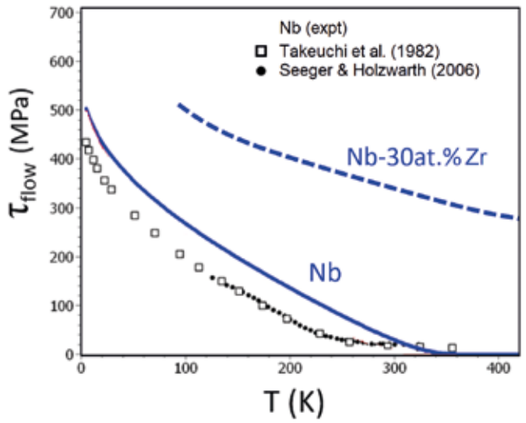


Fig. 2 The temperature dependency of yield shear stress: black symbols are experimental data for pure Nb; solid and dashed blue lines correspond to calculated yield stress for pure Nb and Nb-30 at.%Zr alloy, respectively.

The transition from a pure metal to a complex alloy leads to a significant strengthening effect due to strong decrease in the dislocation mobility. This effect was known from measurements, but the reasons for such strengthening are still being discussed. Our simulation revealed that the energy landscape of the moving dislocation in a complex alloy is significantly distorted compared to pure metal. Some local arrangements of atoms in alloy can be considered as a strong trap for the moving dislocation. Passage of a dislocation through such a trap state is often possible only with the emission of point defects (vacancy or self-interstitial atom), as shown in Fig. 3. Such trap configurations exist for both screw and edge dislocations. Therefore, mobility for screw and edge dislocations is equally suppressed, and the plastic deformation of complex refractory alloys can be controlled by both types of dislocations. The obtained data creates a basis for developing a general theory of strengthening which can be applied to any refractory alloys (for instance, Nb-Zr or W-Re or W-Mo-Nb).

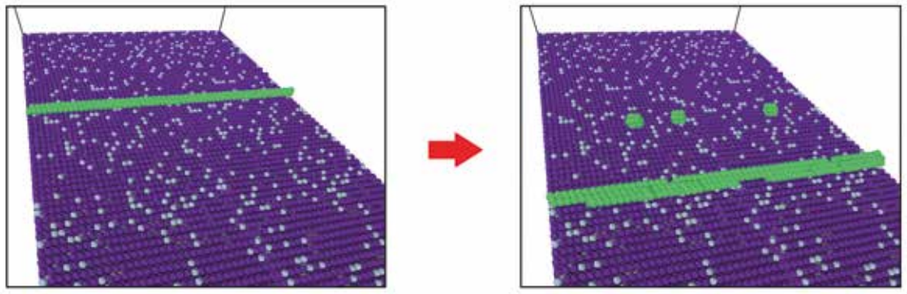
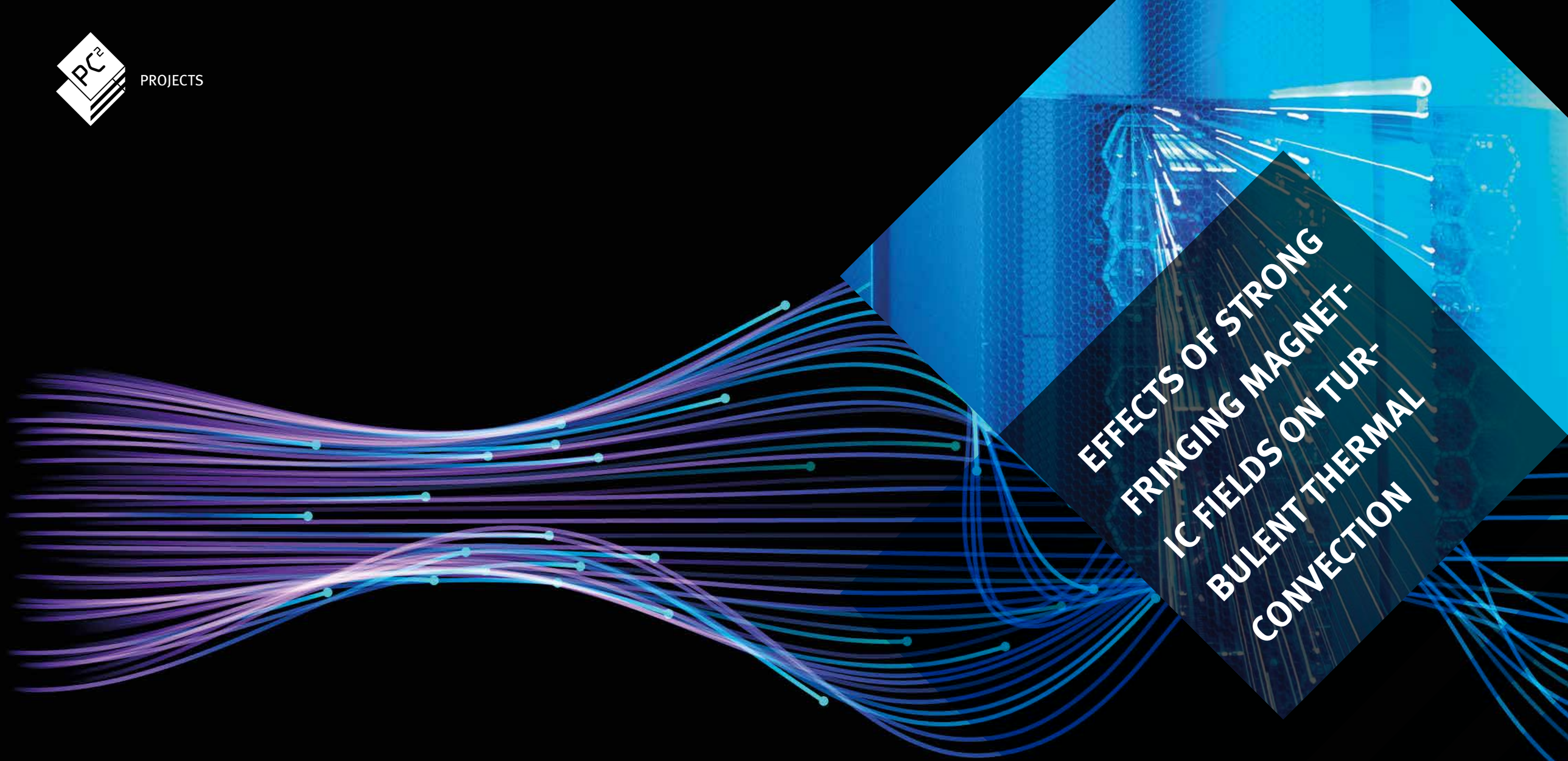


Fig. 3 Two snapshots of the simulation for the motion of screw dislocation in W-20 at.%Mo alloy under applied stress (only several atomic layers in the calculation cell are shown). Purple and grey atoms correspond to W and Mo atoms of the perfect lattice; green atoms represent crystal defects (dislocation and created vacancies). When the dislocation moves, the emission of point defects can occur while passing through the trapping states.

References

[1] S. Starikov and D. Smirnova, **Optimized Interatomic Potential for Atomistic Simulation of Zr-Nb alloy**, Computational Materials Science 197, 110581 (2021)

[2] S. Starikov and V. Tseplyaev, Two-scale simulation of plasticity in molybdenum: **Simulation of Plasticity in Molybdenum: Combination of Atomistic Simulation and Dislocation Dynamics with Non-Linear Mobility Function**, Computational Materials Science 179, 109585 (2020)



EFFECTS OF STRONG FRINGING MAGNET-IC FIELDS ON TUR-BULENT THERMAL CONVECTION

EFFECTS OF STRONG FRINGING MAGNETIC FIELDS ON TURBULENT THERMAL CONVECTION

At higher temperatures it occurs mainly through flowing liquids or gases. Energy generation and production of basic materials abound with such convective heat transfer processes, e.g., in boilers and engines, smelting of metals and in the production of basic chemicals in large reactors. In many circumstances, the flow is driven by buoyancy forces generated by temperature differences in the liquid. This is known as natural convection. Its counterpart is forced convection.

Natural convection is most familiar from the heating systems installed in our homes. It is also responsible for the motion of the Earth's atmosphere and of its liquid iron core. The Earth's magnetic field is created by the complex flow in the Earth's core through electromagnetic induction, i.e., by a fluid dynamo. The Sun also generates a magnetic field through a fluid dynamo, which is apparent through the Sun spots. These are the footprints of magnetic flux tubes protruding from the Sun's convective layer. Thermal convection in conducting fluids in the presence of magnetic fields is referred to as magnetoconvection. It is clearly of interest in geophysics and astrophysics but also for technological applications. However, the conditions for self-excitation of a magnetic field by the flow are usually not fulfilled in the latter cases. Induction of eddy currents in industrial or experimental liquid metal flows only takes place when an external magnetic field is present. Static magnetic fields are applied to control the natural convection in silicon crystal growth and other solidification processes. They are also present in the electrolysis cells for the production of aluminum and in the liquid-metal cooling blankets which are developed for fusion reactors. In the reduction cells, the field is generated by the electrical currents passing through the liquid oxide and aluminum layers. Fusion reactors have superconducting magnets to confine the fusion plasma.

A fundamental configuration of natural buoyancy-driven convection is a planar liquid layer confined between rigid walls, which is heated from below and cooled from above. It is known as Rayleigh-Bénard convection (RBC) and has been central to studies of spontaneous pattern formation in non-equilibrium thermodynamics. In RBC, a cellular flow pattern develops when a finite temperature difference is applied across the layer. The flow becomes increasingly complex as the temperature difference between the top and bottom walls is increased, i.e., the cellular flow patterns become more irregular and time-dependent. RBC eventually reaches the turbulent flow regime, where many small vortices are present and the fluid motions are chaotic in time and in space. The properties and mechanisms of heat transfer in turbulent RBC are currently extensively studied in experiments and simulations on supercomputers. A remarkable feature of turbulent RBC is that it retains a degree of spatial organization which is reminiscent of the cellular pattern found near the onset of RBC. These so-called superstructures become apparent when the flow is averaged over a time interval that allows a fluid element to traverse the liquid layer for a few times.

Our project is concerned with turbulent magnetoconvection in the RBC configuration with a spatially non-uniform field. Earlier works were exclusively concerned with homogeneous fields and considered relatively small aspect ratios, i.e., the horizontal dimensions of the layer were only a few times larger than the layer thickness [1]. We are particularly interested in the effect of the variable magnetic field on the superstructures, which requires large aspect ratios of the liquid layer.

Our investigations are therefore focused on a layer of mercury with height H and aspect ratio 16:32:1 with a magnetic field created in the gap between two semi-infinite planar magnetic poles. The convection layer is located near the edge of the gap (Fig 1). The magnetic field is almost absent in nearly half of the RBC cell, increases sharply around the midplane, and then becomes strong in the other half of the cell. The region where the gradient of the magnetic field is large is called the fringe zone.

PD Dr. Thomas Boeck

Dr. Boeck has been a lecturer (Akademischer Rat) in the Fluid Mechanics Group at TU Ilmenau since 2010. He studied physics at TU Dresden and obtained a PhD from TU Ilmenau. His work is concerned with fluid mechanics problems such as flow instabilities and transition to turbulence that can be investigated through mathematical models and numerical simulations. He is also interested in numerical methods for computational fluid dynamics.

Dr. Shashwat Bhattacharya

Dr. Bhattacharya is an Alexander von Humboldt Fellow in the Fluid Mechanics group of TU Ilmenau. He obtained his PhD in Mechanical Engineering from the Indian Institute of Technology in Kanpur, India. His work focuses on turbulent buoyancy-driven convection and its response to magnetic fields. He has experience in computational fluid dynamics and high performance computing.

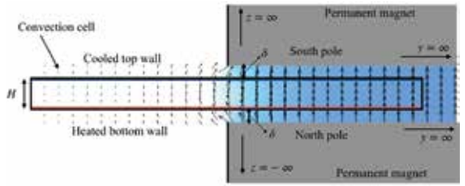


Fig. 1: Schematic of the magnetoconvection arrangement. The semi-infinite permanent magnets (colored in grey) generate the localized magnetic field represented by the vector plots drawn in the convection cell.

The steepness of this gradient and the fringe width depend on δ, which is the distance between the magnetic poles and the horizontal walls of the convection cell. Figs. 2(a,b) show the variations of the magnetic field with the horizontal direction y for different values of δ/H. For small values of δ, the fringe zone is narrow with a steep gradient of the vertical magnetic field. The fringe zone becomes wider as δ is increased. The magnitude of the horizontal component of the magnetic field in the fringe zone decreases with δ.

We performed direct numerical simulations of the above setup for H = 1 using an efficient parallel finite-difference solver [2]. The temperature difference between the horizontal plates and the maximum strength of the field are fixed. The magnetic field is strong enough to suppress the flow completely in the high magnetic flux region of the cell. The fringe zone is varied through changing δ.

The flow structures have horizontal dimensions which are typically a few times larger than H. As seen in Figs. 3(a,b), the superstructures outside the field have no preferred orientation, but become aligned perpendicular to the longitudinal sidewalls in the fringe zone. Furthermore, the vertical velocity fluctuations dominate the horizontal ones in the fringe zone. The characteristic length of the superstructures decreases with the increase of the local magnetic field strength.

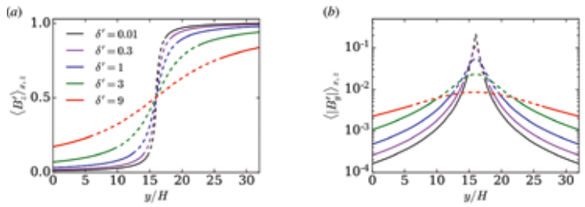


Fig. 2: Distribution of the profiles of (a) vertical magnetic field and (b) absolute value of the horizontal magnetic field, both averaged over x and z, along the lengthwise direction (normalized by the height H of the cell) for different values of the normalized gap (δ' = δ/H) between the magnetic poles and the thermal plates. The magnetic fields are normalized by the maximum value of the vertical magnetic field. The curves are represented as dashed lines in the fringe zone and as solid lines outside the fringe zone.

As the fringe width increases, the magnetic field becomes weaker in the strong magnetic flux region and stronger in the weak flux region. The increase of convection in the strong flux region is unable to compensate for the suppression of convection in the weak magnetic flux region, resulting in a decrease of the global heat transport with increasing fringe width. In the regions of strong flux, the convection in the bulk gets completely suppressed and the flow is confined near the sidewalls. The amplitudes of these wall modes away from the corners decrease when δ/H is decreased from 9 to 1, but begin to increase on further reduction of δ. The horizontal field components are expected to be important for the stability of the wall modes.

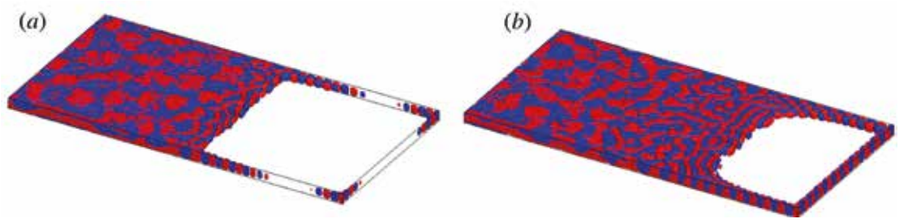


Figure 3: Isosurfaces of the vertical velocity uz = 0.01 (red) and uz=-0.01 (blue) for (a) δ = 1 and (b) δ = 9. In the regions with strong magnetic fields, convective motions are confined near the sidewalls.

In summary, the present work [3] provides important information about RBC with spatially varying magnetic fields. We expect that the same qualitative behavior holds for higher stronger thermal forcing. It may change for liquids with different values of the thermal diffusivity.

References

[1] R. Akhmedagaev, O. Zikanov, D. Krasnov and J. Schumacher, **"Turbulent Rayleigh-Bénard Convection in a Strong Vertical Magnetic Field"**, J. Fluid Mech. 894, R5 (2020).

[2] D. Krasnov, O. Zikanov and T. Boeck, **"Comparative Study of Finite Difference Approaches in Simulation of Magnetohydrodynamic Turbulence at Low Magnetic Reynolds Number"**, Comput. Fluids 50, 46-59 (2011).

[3] S. Bhattacharya, T. Boeck, D. Krasnov and J. Schumacher, **"Effects of Strong Fringing Magnetic Fields on Turbulent Thermal Convection"**, arXiv:2211.00559v2 (2022).

PROJECTS

QUANTUM PHASE DIAGRAM OF HYDROGEN AT EXTREME CONDITIONS

Dr. Sam Azadi

Dr. Sam Azadi began his academic career at the International School for Advanced Studies (SISSA) in Italy, where he received his Ph.D. in theoretical condensed matter physics. He then started his research on the problem of high pressure hydrogen and has held postdoctoral positions at the Johannes Gutenberg University Mainz, Imperial College London, the University of Cambridge and King's College London over the last few years. He is currently a Senior Researcher in the Department of Physics at the University of Oxford and a visiting scientist at Paderborn University.

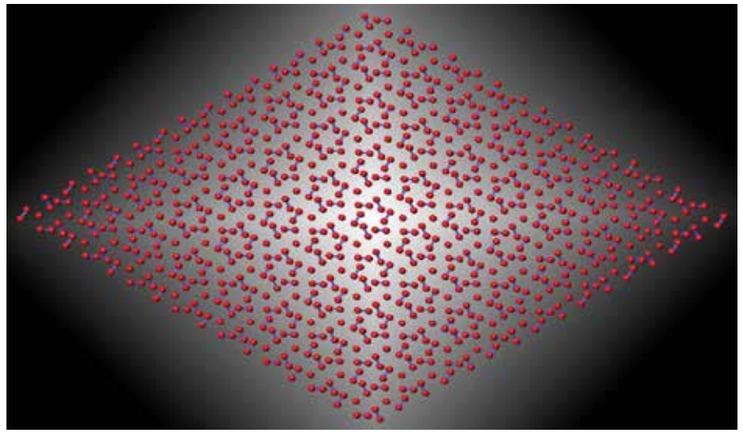


Fig 1: Solid hydrogen crystal structure

The phase diagram of high-pressure hydrogen is a challenging problem in condensed matter and high-pressure physics. It has been extensively studied since 1935 through experiment, theory, and, more recently, computational methods. The main interests are the relevance of solid metallic hydrogen to room-temperature superconductivity, the possible existence of a metallic liquid ground state, and astrophysics.

In this project, we used stochastic methods to solve the quantum mechanic equations governing the behaviour of hydrogen molecules and atoms under extreme conditions, which can be found in the centre of Jupiter. Calculating the thermodynamic parameters and quantum phase diagram predict the stability of a variety of molecular and atomic crystal structures within different pressure ranges.

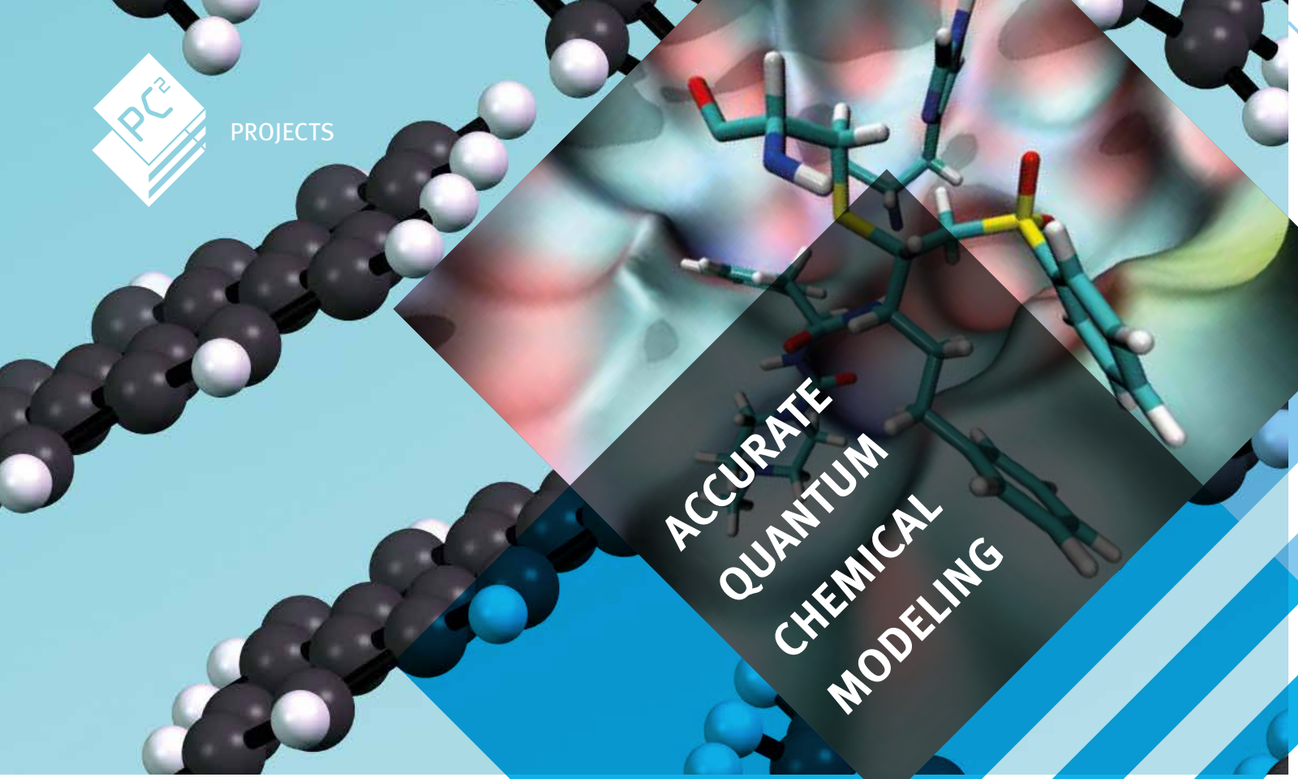
The complexity of the problem and the size of the quantum many-body wavefunction of the systems require a high-performance computing facility for solving the equations. We utilised the PC2 cluster to simulate the quantum-driven phenomena in high-pressure hydrogen [1,2].

References

[1] S. Azadi, and T.D. Kuehne, Phys. Rev. B 100, 155103 (2020)

[2] S. Azadi, G.H. Booth, and T.D. Kuehne, J. Chem. Phys. 153, 204107 (2020)

ACCURATE QUANTUM CHEMICAL MODELING



Prof. Dr. Bernd Engels

Bernd Engels is professor for theoretical chemistry (W2) at the Institute for Physical and Theoretical Chemistry at the University of Würzburg. He was the founder and coordinator of GRK 1221 Control of Electronic Properties of Aggregated π-conjugated Molecules (2006-2015) and GRK 690 Electron Density: Theory and Experiment (2001-2004). His research encompasses: UV-vis spectroscopy, organic semi-conductors, biradicals, reaction mechanisms and boron chemistry.

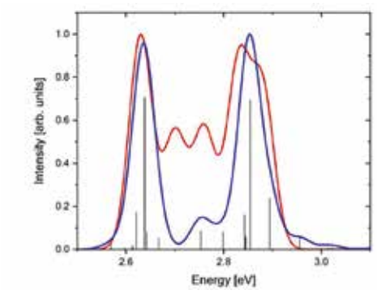


Fig. 1: TD-DFT absorption spectrum (blue) of a 14-membered 3D α-perylene cluster with CPCM-simulated crystal environment and 40 roots (stick spectrum) at the ωB97XD/def2-SVP level of theory as well as experimental absorption spectrum (red). The calculated spectrum has been redshifted by 0.2 eV to best fit the experimental data.

Theoretical modelling has become an indispensable part of chemistry and physics since many effects can only be understood and explained through cooperation between experiment and theory. In addition to the qualitative explanation of observed phenomena, our work focuses on the quantitative, i.e., very precise simulation of the chemical processes and properties. The investigations comprise computations for three different fields. To simulate photo-induced relaxation processes in organic semiconductors, i.e., in the solid state, we perform TD-DFT computations using optimally tuned functionals while employing our recently developed protocol (Figure 1). [1]. Within our investigations in medicinal chemistry, we use force field-based MD simulations which provide the starting structures for subsequent QM/MM or QM/QM/MM computations. The target of our work is to advance drug development by understanding and predicting the effect of medicinal products on enzymes. [2]. Our work in the field of inorganic chemistry is aimed at elucidating catalytic mechanisms of highly reactive main group element compounds by means of DFT calculations. Computations of the reaction mechanism involve large clusters which, beside catalyst and substrate, also include the counter ions and explicit solvent molecules. [3]. This approach ensures an accurate description of the molecule environment in solution which is crucial for negatively charged reactants. The PC2 HPC systems provide enough computational power to study large and complex systems like enzyme environments, as well as photophysical processes occurring in the solid state and reactions in solution.

References

[1] L. Craciunescu et al., J. Phys. Chem. Lett. 2022, 13, 16, 3726–3731.
[2] S. Jung et al., J. Med. Chem. 2021, 64, 16, 12322–12358.
[3] S. Prey et al., Chem. Sci. 2023, 14, 849–860.

EXPLORING AND EXPLOITING FUNCTIONAL ORGANIC MATERIALS IN SILICO

Ganna (Anya) Gryn'ova

Ganna (Anya) Gryn'ova is a head of the junior research group "Computational Carbon Chemistry" at the Heidelberg Institute for Theoretical Studies and Interdisciplinary Center for Scientific Computing at Heidelberg University. Using state-of-the-art computational chemistry, she investigates the role of topology in materials chemistry and develops interpretable predictive models for emergent properties in functional organic materials.

Functional, topologically complex organic molecules are rising stars in modern materials science due to their biocompatibility, structural variability, and wealth of physico-chemical properties. Their practical applications often involve interactions with small molecular targets (e.g., gases, small organic molecules, drugs, etc.) via relatively weak non-covalent forces. Key to these interactions are the topological features of host materials: arrangement of functional groups, pore size, and cavity volume.

In the ERC-StG-2021 project "PATTERNCHEM: Shape and Topology as Descriptors of Chemical and Physical Properties in Functional Organic Materials" graphenes, covalent-organic frameworks, and hyperbranched polymers provide a unique foundation for developing application-oriented fingerprints of their topological and non-covalent interaction features. Structural descriptors will be developed for these materials to reflect their unconventional topologies and facilitate machine-learning of their properties. Furthermore, a scheme for quantifying the propensity for non-covalent interactions and assessing host-guest complementarity at a quantum-chemical accuracy will be established. Chemical and physical performance indicators relevant to targeted applications (e.g., as sensors, filters, catalysts, and nanocarriers) will be computed in a high-throughput manner with multiscale approaches. Finally, structure-property relationships between computed performance indicators and developed descriptors will be established and implemented into predictive frameworks for functional organic materials.

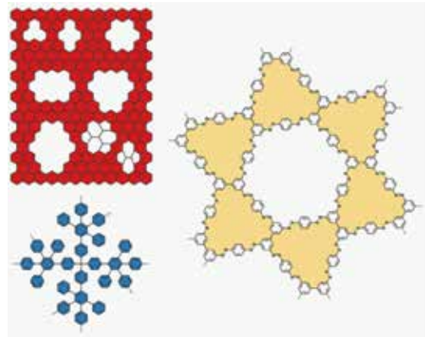
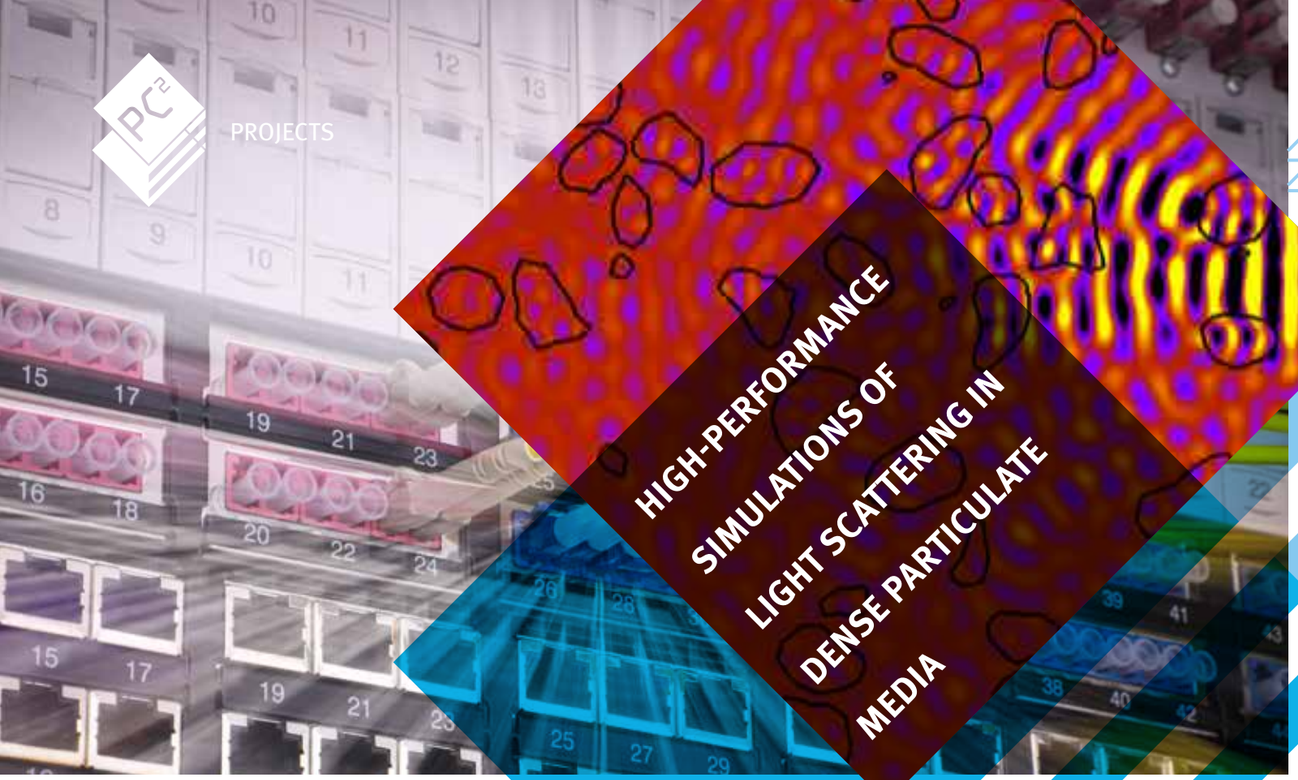


Figure. Example architectures of the topologically complex functional organic materials, investigated in PATTERNCHEM: graphene with defects and vacancies (red), hyperbranched polymer (blue), and dual-pore Kagome covalent organic framework (yellow).

Reference

[1] Citation: Ernst M., Poręba T., Gnägi L., Gryn'ova G. (2023)
Locating Guest Molecules inside Metal–Organic Framework Pores with a Multilevel Computational Approach
J. Phys. Chem. C 127(1):523-531. DOI: 10.1021/acs.jpcc.2c05561.



HIGH-PERFORMANCE SIMULATIONS OF LIGHT SCATTERING IN DENSE PARTICULATE MEDIA

Dr. Yevgen Grynko

Yevgen Grynko is Akademischer Oberrat at the Theoretical Electrical Engineering (TET) group at Paderborn University. He studied physics and astronomy at Kharkiv National University (Ukraine). During his PhD at Max Planck Institute for Solar System Research and Göttingen University he studied optical properties of cometary dust and particulate surfaces with numeric simulations. Currently, he works on computational photonics and electromagmetic scattering to better understand the mechanisms of light transport in dense disordered media and light backscattering phenomena in optical remote sensing applications.

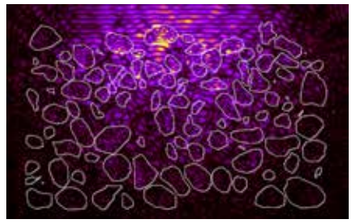


Fig. 1: Electromagnetic field intensity distribution inside a layer of densely packed dielectric particles illuminated by a focused beam from above.

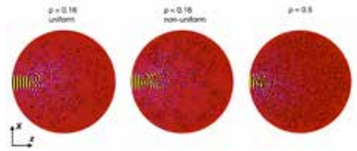


Fig. 2: Electric field amplitude distribution in spherical clusters of particles with different packing densities ρ and different topologies illuminated by a focused beam along Z axis. The figure shows different light transport regimes in sparse and dense structures.

Light scattering in discrete disordered media is a multidisciplinary problem that is solved in different fields from optics and photonics to remote sensing and planetary science. We are interested in the geophysical and planetary science optical remote sensing applications. In this field, a problem of data retrieval from photopolarimetric and spectroscopic measurements implemented for natural particulate surfaces like sands, soils, snow and planetary regolith is solved. Analysis of this data enables characterization of their physical properties and extracting information about the complex refractive index of the material, particles size and the medium topology. This requires numerical simulations of light backscattering from model structures that mimic real particulate surfaces which is challenging because of their multi-scale geometry. We apply a full wave solution and high-performance computing to solve the problem. Light propagation and interaction with the target structures is described by means of Maxwell's equations solved with the Discontinuous Galerkin Time Domain method. We show that high packing density of particles and a high degree of geometrical disorder causes light localization and near-field interactions result in a percolation-like light transport determined by the topology of the medium. This makes an impact on the backscattering phenomena: the intensity peak and negative linear polarization. Therefore, we can reveal the physical mechanisms behind both and establish a connection between the model topological parameters and its optical characteristics.

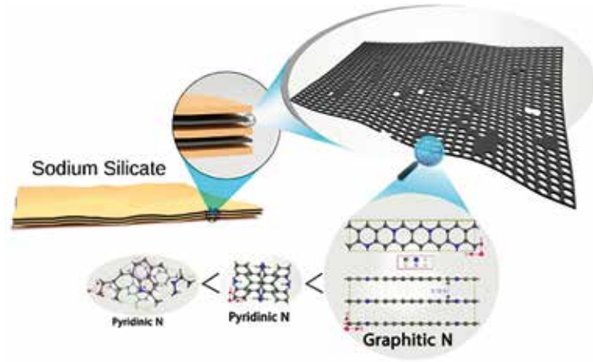
Reference

[1] Y. Grynko, Y. Shkuratov, S. Alhaddad, J. Förstner, **Light Scattering by Large Densely Packed Clusters of Particles**, in: A. Kokhanovsky (Ed.), Springer Series in Light Scattering: Volume 8: Light Polarization and Multiple Scattering in Turbid Media, Springer International Publishing, 125-155, 2022.

PHASE STABILITY IN MULTIFUNCTIONAL CATION-SUBSTITUTED PYROXENES BY HIGH THROUGHPUT DENSITY FUNCTIONAL SCREENING

Dr. Dorian Hanaor

Dr. Dorian Hanaor works as a Lecturer and Research Group Leader at the Chair of Advanced Ceramic Materials at TU Berlin. Working as a consultant, engineer, researcher and educator across 5 countries and 4 continents, Dorian has integrated practical and computational methods to create new insights and ideas in fields of materials science, civil engineering, energy systems and physics. Current research activities include mineral-inspired materials, sustainable technologies and processing of materials for biomedical implants.



Density functional theory, by calculating the electronic structures of materials, aids in predicting functional properties. When combined with novel predictive and analytical tools like high throughput calculations and machine learning, Density functional calculations offer a robust and cost-effective method for materials discovery. In this project, we initially wished to investigate a group of silicates, and similarly complex oxides, for their dielectric properties and bioactivity. However, our investigations led us to a set of new predictions in magnetism, thermoelectricity, and catalysis that we had not initially anticipated.

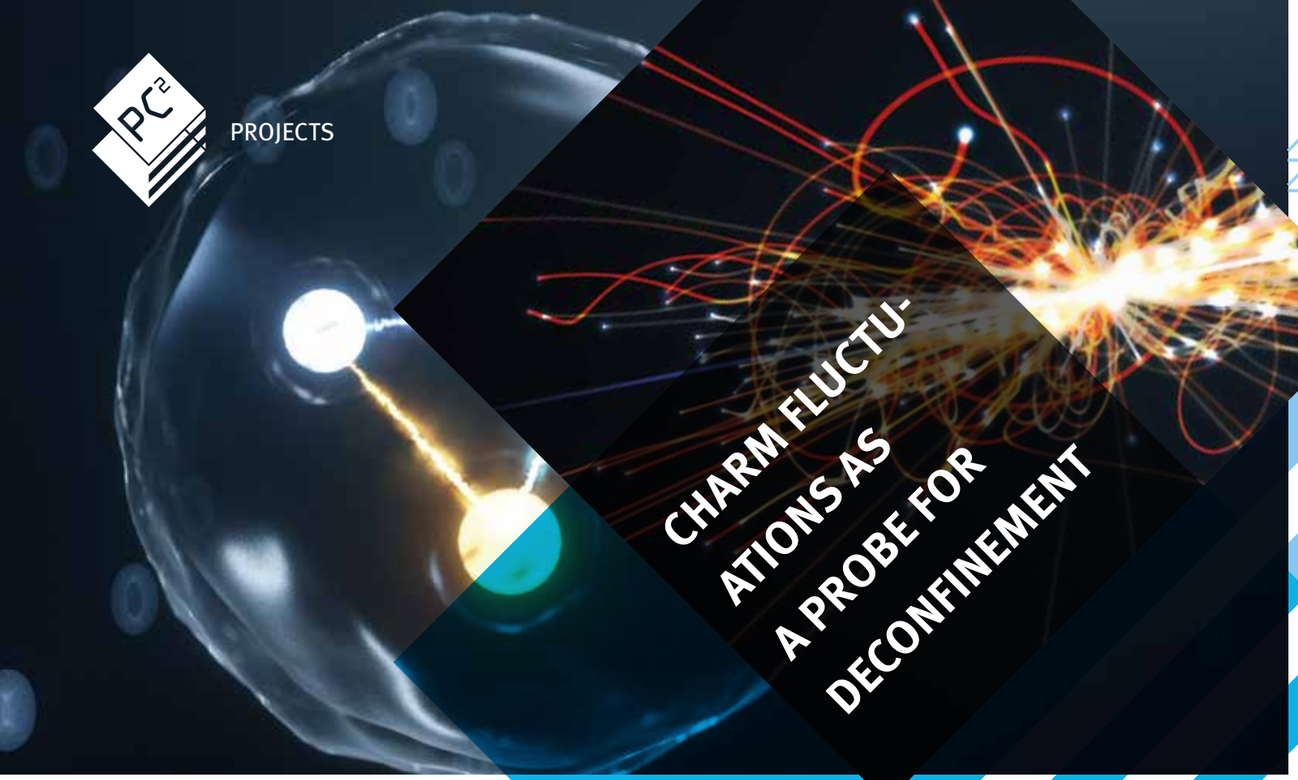
The use of sodium silicate as a sacrificial template for synthesizing novel nitrogen-doped carbon with excellent supercapacitance, which is attractive for energy storage applications. We also identified the detailed structure of bispropylurea bridged polysilsesquioxane, a silicate derivative, with applications in toxin removal and environmental remediation.

Additionally, we investigated the non-collinear magnetic interactions in a group of spinel materials in which the spin-orbit interaction plays a significant role. Here non-collinearity poses a particular computational challenge requiring substantially more computational resources than standard density functional calculations. In the same light, we also demonstrated how spin-orbit interaction can play a major role in Mg ion's diffusion in Mg-3Bi2, demonstrating its suitability for application as a Mg ion anode.

References

[1] Esmail Doustkhah, Mohamed Esmat, Naoki Fukata, Yusuke Ide, Dorian A.H. Hanaor, M. Hussein N. Assadi, **"MOF-derived nanocrystalline ZnO with controlled orientation and photocatalytic activity"** Chemosphere 303, 134932 (2022).

[2] M. Hussein N. Assadi1, Marco Fronzi, Dorian A. H. Hanaor, **"Unusual ferrimagnetic ground state in rhenium ferrite"** Eur. Phys. J. Plus 137, 21 (2022).



CHARM FLUCTUATIONS AS A PROBE FOR DECONFINEMENT

Dr. Sipaz Sharma

Sipaz Sharma is a postdoctoral fellow at the University of Bielefeld; she received her PhD from the Indian Institute of Science (IISc), Bengaluru, India in 2022. Her research area is based on using Lattice QCD techniques to study the properties of strongly interacting matter at high temperatures and densities. Her prime focus is on understanding the phase transitions occurring between different phases of the strongly interacting matter by exploiting symmetries of QCD.

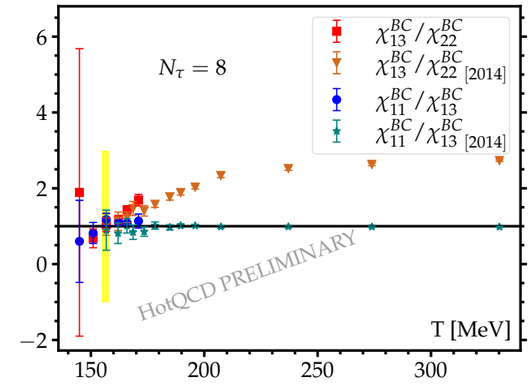


Fig. 1. Lattice results of specific cumulant ratios for different temperatures

Ten microseconds after the Big Bang, matter interacting via the strong force consisting of quarks and gluons underwent confinement to form nuclear matter and light hadrons with up, down and strange quarks as constituents. Experimentalists at the Large Hadron Collider (LHC) at CERN in Geneva are trying to answer whether the formation of hadrons containing the relatively heavier charm quark coincided with the light hadrons. One of the theoretical ways to approach this problem is by carrying out numerical calculations of Quantum Chromodynamics (QCD) - the theory of strong interactions - in the framework of Lattice QCD.

Processes mediated by strong interactions conserve various quantum numbers. We can probe the confinement/deconfinement transition of QCD by analyzing conserved charge distributions and their higher-order moments.

In particular, comparing various higher-order charm cumulants calculated on the lattice with the Hadron Resonance Gas (HRG) model predictions signal the melting of charm hadrons. In Fig. 1, lattice results of specific cumulant ratios for different temperatures are shown. These results provide evidence for the onset of confinement/deconfinement transitions of charm hadrons which coincides with that of light hadrons.

References

[1] S. Sharma, **Charm fluctuations in (2+1)-flavor QCD at high temperature**, PoS LATTICE2022 (2023) 191, https://doi.org/10.22323/1.430.0191.

[2] H.-T. Ding, O. Kaczmarek, A.L. Lorenz, H. Ohno, H. Sandmeyer and H.T. Shu, **Charm and beauty in the deconfined plasma from quenched lattice QCD**, Phys. Rev. D104 (2021) 114508, https://doi.org/10.1103/PhysRevD.104.114508

LARGE-SCALE LANGUAGE MODELS FOR LOW-RESOURCE LANGUAGES

Prof. Dr. Axel Ngonga

Axel Ngonga studied Computer Science in Leipzig. He completed his PhD and habilitation in the areas of knowledge acquisition and integration respectively. He is now a full professor at Paderborn University, where he leads the Data Science group. In his research, he develops full-stack solutions for knowledge graphs ranging from knowledge extraction to scalable machine learning, and makes them available as open-source software and open data.

Large Language Models (LLMs) require significant capital to be trained on a large number of datasets. Once pre-trained, these models have shown outstanding results for zero and few-shot learning on new tasks. Although the LLMs are changing the AI landscape, the needed resources for training these models are mainly monopolized by large tech companies such as Google, Meta and OpenAI.

Recently, the big tech companies have started releasing their models without the need of using private APIs such as OPT-175 from Meta. In addition, the BigScience project released BLOOM, which is a 176 Billion parameter LLM that covers 59 different languages. Here, 1,000 independent researchers aim to address the problem of inherited biases present in the current LLMs and claim that it is the first open multilingual model of its scale. The idea behind this new development is to reduce the carbon footprint, allow progress in the AI community and support transparency.

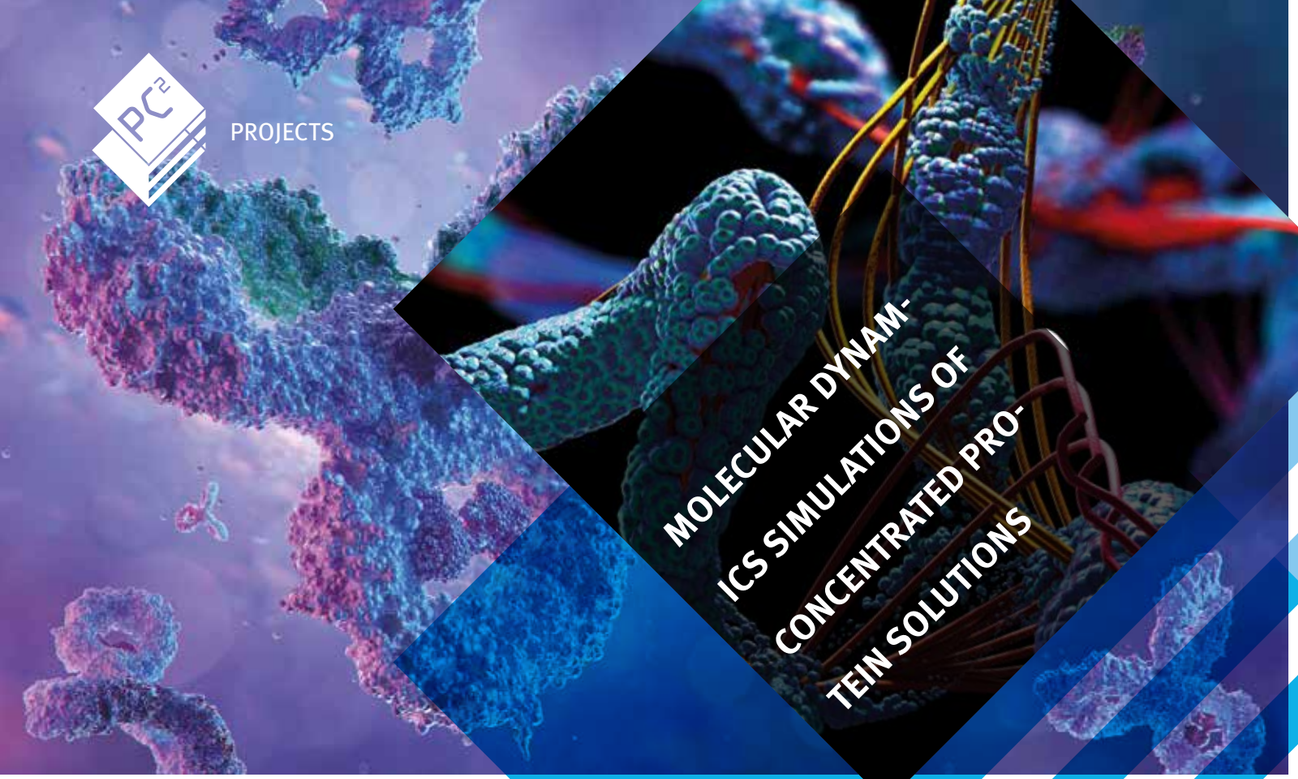
One important premise that none of the LLMs have taken into consideration is the importance of grouping languages together using language families and scripts. Previous works have demonstrated that the performance of a LM largely drops when trained along with languages from different language groups and utilizing different scripts. Currently, translation solutions between languages from different scripts such as Chinese to Irish are rarely available due to the lack of data and tools. To overcome this drawback, we aim to train LLM based on the language grouping to (1) enhance the multilingual performance of LLMs and (2) enable better transfer learning for low-resource languages, which are also rarely considered in existing LLMs.

References

[1] C. Demir, J. Lienen, and A.-C. Ngonga Ngomo, **Kronecker Decomposition for Knowledge Graph Embeddings**. arXiv preprint arXiv:2205.06560, 2022.

[2] D. Moussallem, A.-C. Ngonga Ngomo, P. Buitelaar, M. Arcan, **Utilizing Knowledge Graphs for Neural Machine Translation Augmentation.** In Proceedings of the 10th International Conference on Knowledge Capture, pages 139–146. ACM, 2019.

[3] D. Moussallem, D. Gnaneshwar, T. Castro Ferreira, A.-C. Ngonga Ngomo, **Nabu–Multilingual Graph-Based Neural rdf Verbalizer.** In International Semantic Web Conference, pages 420–437. Springer, 2020.



MOLECULAR DYNAMICS SIMULATIONS OF CONCENTRATED PROTEIN SOLUTIONS

Prof. Dr. Lars Schäfer

Lars Schäfer is the head of the Molecular Simulation group at the Center for Theoretical Chemistry at Ruhr University Bochum. After his chemistry studies at TU Braunschweig, he joined the Theoretical Biophysics department at the MPI for Biophysical Chemistry in Göttingen, where he received his PhD in 2007. After his postdoc at the University of Groningen, he lead an Emmy Noether research group at Goethe University Frankfurt in 2012. He has been a Professor at RUB since 2014.

High-concentration protein solutions play an important role in both biology and pharmaceutical applications. The cytoplasm of biological cells constitutes a densely packed environment, and the effects of molecular crowding on the structure, dynamics, and thermodynamic stability of the solvated biomolecules is actively researched. Likewise, for biopharmaceuticals, reaching the high protein concentrations in the liquid formulations while maintaining protein stability and efficacy is a challenge because of aggregation, low solubility and high viscosity. Such formulation aspects are particularly challenging for large and conformationally flexible molecules such as monoclonal antibodies (mAbs), which are one of the most important classes of biopharmaceuticals.

From the experimental perspective, characterizing high-concentration mAb solutions is time-consuming and material-consuming and thus difficult, especially in the early development phase where available material is limited. Hence, molecular dynamics (MD) simulations are an attractive alternative. However, the large system sizes and long time scales needed for dense protein solutions pose a tough computational challenge and require high-performance computing facilities, at least when an accurate fully atomistic simulation model is desired.

We performed multi-microsecond time scale all-atom MD simulations with explicit solvation of dense solutions of a humanized monoclonal IgG1 antibody at concentrations up to 250 mg/ml. The extensive MD simulations enabled the computation of the shear viscosity of these systems from the pressure fluctuations via a Green-Kubo approach with reasonable statistical precision. The computed shear viscosities are well above 10 cP and correspond to with experimental values representative for the high-viscosity regime of mAb solutions. These findings encourage the use of MD simulations to predict the viscosities of such dense protein solutions and their targeted modulation, e.g., by mAb mutations or by excipients.

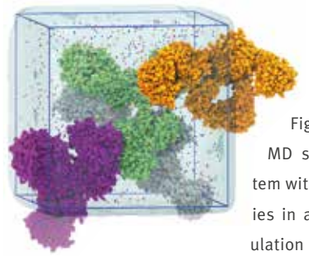


Fig. 1: Atomistic MD simulation system with four antibodies in a periodic simulation box, solvated by water and 150 mM ions. The total system comprises over 500.000 atoms.

References

[1] P. Garidel, A. B. Kuhn, L. Schäfer, A. R. Karow-Zwick, M. Blech. **High-Concentration Protein Formulations: How High is High?** Eur. J. Pharm. Biopharm. 119, 353-360 (2017).

[2] A. B. Kuhn, S. Kube, A. R. Karow-Zwick, D. Seeliger, P. Garidel, M. Blech, L. Schäfer. **Improved Solution-State Properties of Monoclonal Antibodies by Targeted Mutations.** J. Phys. Chem. B 121, 10818-10827 (2017).

FINDING REALISTIC SEA ROUTES CONSIDERING THE WEATHER USING GENETIC ALGORITHMS

Prof. Dr. Kevin Tierney

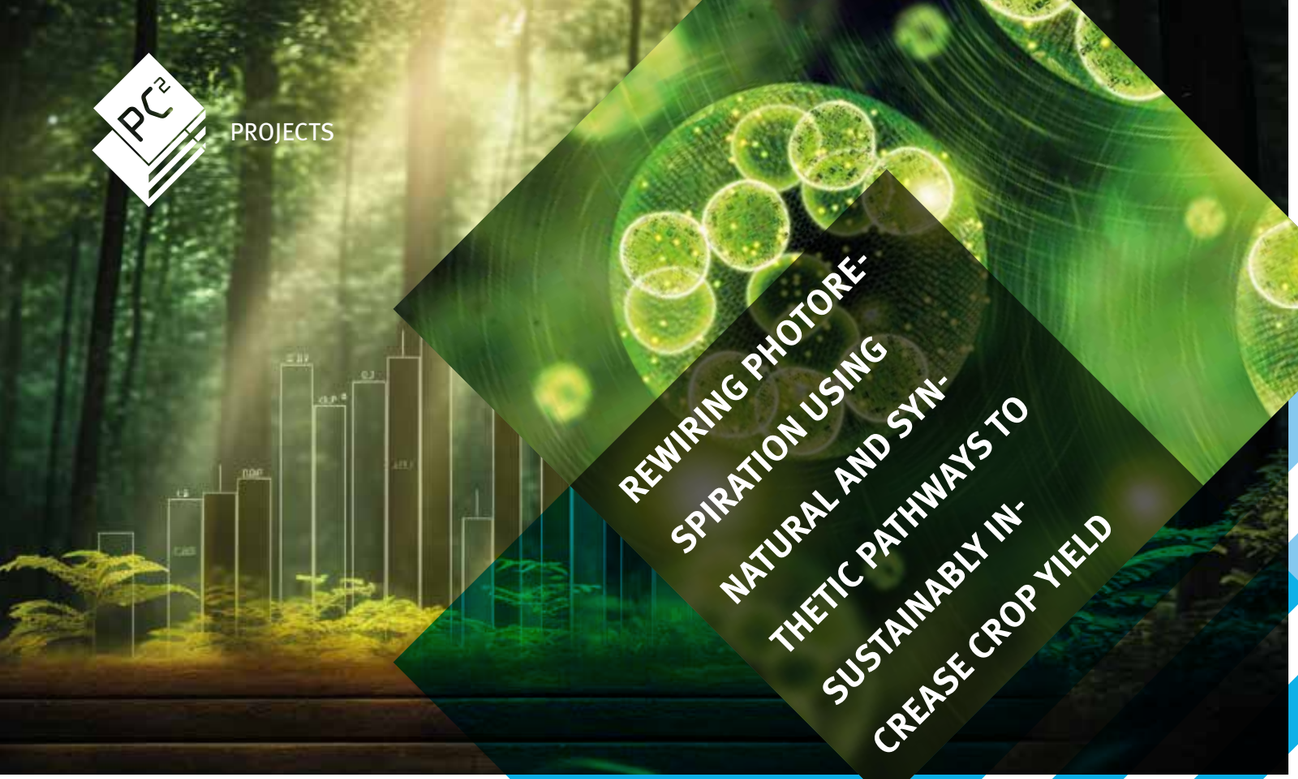
Prof. Dr. Kevin Tierney is a full professor for Decision and Operation Technologies at Bielefeld University in Germany. He holds a B.Sc. in Computer Science from Rochester Institute of Technology, an Sc.M. in Computer Science from Brown University, and a PhD from the IT University of Copenhagen in Denmark. He was previously an assistant professor at Paderborn University. His research interests include algorithm configuration, learning to solve optimization problems, and solving logistics problems. His work on Neural Large Neighborhood Search won the distinguished paper award at ECAI 2020.

The weather has a major impact on the profitability, safety, and environmental sustainability of the routes sailed by seagoing vessels. The prevailing weather strongly influences the course of routes, affecting not only the safety of the crew, but also the fuel consumption and therefore the emissions of the vessel. Effective decision support is required to plan the route and the speed of the vessel considering the forecasted weather. We implement a genetic algorithm to minimize the fuel consumption of a vessel taking into account the two most important influences of weather on a ship: the wind and the waves. Our approach assists route planners in finding cost minimal routes that consider the weather, avoid specified areas, and comply with arrival time constraints. Furthermore, it supports ship speed control to avoid areas with weather conditions that would result in high fuel costs or risk the safety of the vessel. The algorithm is evaluated for a variety of instances to show the impact of weather routing on the routes and the fuel and travel time savings that can be achieved with our approach. Including weather into the routing leads to a savings potential of over 10% of the fuel consumption. The application of this work in industry therefore has the potential to eliminate thousands of tons of unnecessary CO_2 emissions. Furthermore, we show that ignoring the weather when creating routes can lead to routes that cannot be sailed in practice. Finally, we evaluate our algorithm with stochastic weather data to show that it can provide high-quality routes under real conditions even with uncertain weather forecasts. (Joint work with Dr. Stefan Kuhlemann)

Figure: Our algorithm chooses the southern route (black line) to avoid bad weather, shown in shades of red, along a ship's path from Hamburg to New York City. Even though this route is 4% longer than the northern route (gray line), it uses 3.2% less fuel (credits: Kuhlemann/Thierney CC BY-SA 4.0).

Reference

[1] Kuhlemann, S., Tierney, K., **A Genetic Algorithm for Finding Realistic Sea Routes Considering the Weather.** J Heuristics 26, 801–825 (2020). https://doi.org/10.1007/s10732-020-09449-7



Prof. Dr. Benjamin Stich

From 2000 to 2004, he studied agricultural biology at the University of Hohenheim. After completing his doctorate in 2007 at the Institute of Plant Breeding, Seed Research and Population Genetics at the University of Hohenheim and his habilitation in 2010, he became an adjunct professor at the University of Hohenheim in 2015. He is Director of the Julius Kühn Institute (JKI) and Head of the Institute for Breeding Research on Agricultural Crops at the JKI and holds the professorship for "Breeding Utilisation of Plant Genetic Resources" at the Faculty of Agricultural and Environmental Sciences in Rostock.

GAIN4CROPS aims to boost plant productivity using novel strategies to minimize the inefficiencies of photorespiration. This process reduces CO_2 assimilation efficiency and, thus, biomass yield and agricultural productivity. The project aims to improve the efficiency of the most common photosynthetic metabolism in plants, the C_3 metabolism, by following a stepwise approach. To achieve the goals of this project, we will develop high-quality draft genome assemblies and annotations for tens of Asteraceae species which contain different photosynthetic traits such as C_3, C_3-C_4 and C_4. Genomes will be sequenced using a combination of short- and long-read technologies. We will use various state-of-the-art computation tools to assemble the genomes, followed by their functional annotation. The computational tools require highly sophisticated high-end servers, for example, genome assembling tools like Supernova, Canu, and Helixer. We will analyze these datasets in conjunction with phenotypic information by employing across-species association mapping to unravel the genetic architecture, including regulatory elements, underpinning C_3-C_4 intermediacy by quantitative and statistical genetics approaches. Finally, we will integrate these genomic and phenotypic datasets to generate a prioritized catalogue of candidate alleles to be introduced into C_3 backgrounds by genome editing and transgenesis. So far, we have completed most species' genome assembling and annotation, and the planned downstream analyses are ongoing. For more details, please log on to http://gain4crops.eu/.

Reference

[1] E. N. Smith, M. van Aalst, T. Tosens, Ü. Niinemets, B. Stich, T. Morosinotto, A. Alboresi, T. J.Erb, P. A. Gómez-Coronado, D. Tolleter, G. Finazzi, G. Curien, M. Heinemann, O. Ebenhöh, J. M. Hibberd, U. Schlüter, T. Sun, A. P. M. Weber.
Improving Photosynthetic Efficiency Toward Food Security: Strategies, Advances, and Perspectives.
Mol Plant. 2023 Oct 2;16(10):1547-1563. doi: 10.1016/j.molp.2023.08.017. Epub 2023 Sep 1.
PMID: 37660255

As HPC systems are complex and require specialized knowledge and skills to operate efficiently, we offer targeted training programs to satisfy the diverse needs of our users. Our aim is to enable researchers to fully utilize the capabilities of the system, develop best practices for software optimization and performance tuning, and ultimately drive scientific discovery and innovation. Embedded in the educational efforts by the national high-performance computing alliance NHR (https://www.nhr-verein.de/kurse-und-workshops), our training events and workshops are generally open to all members of German research institutions.

Our course program has offerings for all skill levels and includes basic HPC qualification courses, mini-tutorials, as well as focused, in-depth training. To provide forums for scientific exchange between our users, we regularly organize domain-specific or computing technology-specific workshops and courses. Finally, for students at Paderborn University, HPC-related subjects are taught as part of the curriculum of the Computer Science and Computer Engineering tracks by members of the Paderborn Center for Parallel Computing.

HPC QUALIFICATION PROGRAM

Empowering more researchers to use high-performance computing resources is one of the main missions of PC2. Our HPC qualification program for researchers and students (http://pc2.de/go/training) is tailored to this goal with courses composed of lectures and hands-on sections. The program is offered on a rolling basis and has a “ladder” structure where courses build on top of each other. This allows participants to join at any time and enter at a level that suits their prior HPC knowledge. Each course is accompanied by a self-assessment test that helps potential participants to judge their level of experience.

Our “HPC course ladder” currently consists of four training modules. The first course is a basic, one afternoon Linux introduction course for users who are new to UNIX-like operating systems and using a shell. The second element is titled "HPC Introduction Course" and informs participants about the available computing resources and compute time proposals, the SLURM workload manager and job scripts, as well as the basics of running parallelized programs on the cluster systems at PC2. The third module is a full-day course and covers more advanced topics of HPC. Specifically, it explains the various levels of hierarchy in modern HPC systems and touches on topics such as profiling, scaling analysis, pinning, software containers and accelerators. Finally, the fourth course focuses on "Performance Engineering" and is aimed at research software developers. It discusses common bottlenecks and performance patterns at a source code (and sometimes even assembler instruction) level and introduces low-level tools for effectively monitoring the performance of code on our hardware.

SELECTED LECTURES AND COURSES ON HPC TOPICS TAUGHT BY PC2 STAFF

Lecture: High-Performance Computing (Master CS, CE)	Prof. Dr. Christian Plessl	Winter term 2020/2021 and Summer terms 2021 and 2022
Lecture: Advanced Computer Architecture (Master CS, CE)	Prof. Dr. Christian Plessl	Winter term 2020/2021 and Winter term 2021/2022
Lecture: Architektur Paralleler Rechnersystem (Master CS, CE)	Dr. Jens Simon	Summer term 2020
Project group: HPC Performance Almanac (Master CS)	Stefan Rohde, Prof. Dr. Christian Plessl	Winter term 2021/2022 and Summer term 2022
System design team project: Performance-Monitoring for Supercomputers (Bachelor CE)	Dr. Robert Schade	Winter term 2020/2021

SELECTED WORKSHOPS AND EVENTS ORGANIZED BY PC2

PC2 User Day	Annual meeting to provide a platform for scientific exchange and networking between users of the PC² infrastructure. The event consisted of three sessions: general updates from the compute center, user-provided talks from various domains, and upcoming developments at the PC². These events also include a poster session and a coffee break for networking and questions. Updates by PC² staff regarding upgrades to the HPC infrastructure.	November 3, 2022, November 10, 2021, and November 26, 2020
Julia for High-Performance Computing	Four-day course on the Julia programming language as a modern approach to high-performance numerical computing. Co-organized by HLRS. Participants learned the foundations and features of Julia, such as multiple dispatch, type inference, and parallelism. They also practiced how to write efficient and expressive code in Julia, and how to use NVIDIA GPUs for offloading computations.	September 20-23, 2022
Hands-on Course on Density-Functional Calculations - International CP-PAW Autumn School	This block course introduced first-principles electronic-structure calculations for physicists and chemists. The participants learned the theoretical and practical aspects of methods and materials using the CP-PAW code. The course also offered an optional second week for a self-study project and a seminar presentation. The course was offered simultaneously at Göttingen and Paderborn.	September 12-23, 2022
Introduction to Noctua 1/2 for New PC2 Users + Migration Courses	Two migration courses for users who were switching from one cluster system to another. The first course was for users who were moving from Noctua 1 to Noctua 2, and the second course was for users who were moving from OCuLUS to Noctua 1. Both courses covered the basics of the new system, such as hardware, file systems, software and job management. Both courses also had a hands-on session.	May 5 and May 25, 2022
Advanced Research in Quantum Chemistry and Solid State Physics with ORCA, CP2K, TRAVIS, and CP-PAW	Workshop on computational spectroscopy using the quantum chemistry program CP2K with scientific talks by Jürg Hutter, Thomas D. Kühne, Marcella Iannuzzi, Matthias Krack and others as well as hands-on sessions organized in collaboration with the Dynamics of Condensed Matter Research Group of Thomas D. Kühne.	April 7–8, 2022
oneAPI for CPUs, GPUs and FPGAs: Overview and Hands-On	Workshop that introduced the participants to oneAPI, a cross-industry, open, standards-based unified programming model that delivers a common developer experience across multiple accelerator architectures. The workshop introduced the new development environment and taught the participants how to program GPU and FPGA code with oneAPI and how to migrate GPU code from other programming models like CUDA. The workshop also included hands-on sessions to apply the concepts with exercises using Intel’s oneAPI product.	December 2, 2021
International Winter School on Electronic Structure Calculations	Winter school on how to perform efficient electronic structure calculations as well as ab-initio molecular dynamics calculations for molecules and solids. The school included lectures from experts in the corresponding methods and codes as well as hands-on tutorials. The participants learned how to use various software packages and tools for performing and analyzing DFT and QMC simulations on high-performance computing systems.	February 10-14, 2020

PUBLICATION LIST

The following publications were published in the reporting period, the results of which were achieved through computing time projects on PC2 computer systems.

2022

- **Optimization of Optical Waveguide Antennas for Directive Emission of Light**
  H. Farheen, T. Leuteritz, S. Linden, V. Myroshnychenko, J. Förstner, Journal of the Optical Society of America B 39 (2022) 83.

- **Numerical Analysis of the Coherent Mechanism Producing Negative Polarization at Backscattering From Systems of Absorbing Particles**
  S. Alhaddad, Y. Grynko, H. Farheen, J. Förstner, Optics Letters 47 (2022) 58.

- **In-depth FPGA Accelerator Performance Evaluation with Single Node Benchmarks from the HPC Challenge Benchmark Suite for Intel and Xilinx FPGAs using OpenCL**
  M. Meyer, T. Kenter, C. Plessl, Journal of Parallel and Distributed Computing (2022).

- **MUSCAT: MUS-based Circuit Approximation Technique**
  L.M. Witschen, T. Wiersema, M. Artmann, M. Platzner, in: Proc. Design, Automation and Test in Europe (DATE), (2022).

- **Modelling Film and Rivulet Flows on Microstructured Surfaces using CFD Methods**
  R. Bertling, M. Hack, I. Ausner, B. Horschitz, S.A. Bernemann, E. Kenig, Chemical Engineering Science 251 (2022).

- **Early Time Behavior of Spatial and Momentum Anisotropies in Kinetic Theory Across Different Knudsen Numbers**
  N. Borghini, M. Borrell, H. Roch, ArXiv:2201.13294 (2022).

- **Even Anisotropic-Flow Harmonics Are From Venus, Odd Ones Are From Mars**
  B. Bachmann, N. Borghini, N. Feld, H. Roch, ArXiv:2203.13306 (2022).

- **Linearly Shifting Ferromagnetic Resonance Response of Lao.7Sro.3MnO3 Thin Film for Body Temperature Sensors**
  W. Hou, Y. Yao, Y. Li, B. Peng, K. Shi, Z. Zhou, J. Pan, M. Liu, J. Hu, Frontiers of Materials Science 16 (2022).

- **Dataset for Random Uniform Distributions of 2D Circles and 3D Spheres**
  M. Wojciechowski, Data Brief 43, (2022) 108318.

- **Inverses Verfahren zur Bestimmung viskoelastischer Materialparameter**
  S. Johannesmann, Proc. Workshop Messtechnische Anwendungen von Ultraschall, Drübeck, 2022.

- **Light Backscattering From Numerical Analog of Planetary Regoliths**
  Y. Grynko, Y. Shkuratov, S. Alhaddad, J. Förstner, in: Proc. 16th Europlanet Science Congress, 2022.

- **AI Assisted Interference Classification to Improve EMC Troubleshooting in Electronic System Development**
  J. Maalouly, D. Hemker, C. Hedayat, C. Rückert, I. Kaufmann, M. Olbrich, S. Lange, H. Mathis, in: Proc. 2022 Kleinheubach Conference, IEEE, 2022.

- **Entwicklung eines innovativen Trennapparates zur Stickstoffrückgewinnung aus landwirtschaftlichen Abfällen**
  S.A. Bernemann, J. Makowiak, J. Makowiak, R. Bertling, N. Lutters, E. Kenig, in: Proc. Jahrestreffen Fluidverfahrenstechnik und Hochdruckverfahrenstechnik, 2022.

- **Untersuchung von kleinskaligen Flüssigkeitselementen auf mikrostrukturierten Packungsoberflächen**
  C. Dechert, E. Kenig, in: Proc. Jahrestreffen der ProcessNet Fachgruppen Fluidverfahrenstechnik und Hochdruckverfahrenstechnik, 2022.

- **Broadband Optical TO5 Antennas for Directional Emission of Light**
  H. Farheen, L.-Y. Yan, V. Quiring, C. Eigner, T. Zentgraf, S. Linden, J. Förstner, V. Myroshnychenko, Optics Express 30 (2022) 19288.

- **Negative Polarization of Light at Backscattering From a Numerical Analog of Planetary Regoliths**
  Y. Grynko, Y. Shkuratov, S. Alhaddad, J. Förstner, Icarus 384 (2022) 115099.

- **Parallel Quantum Chemistry on Noisy Intermediate-Scale Quantum Computers**
  R. Schade, C. Bauer, K. Tamoev, L. Mazur, C. Plessl, T. Kühne, Phys. Rev. Research 4 (2022) 033160.

- **Lamb Wave Based Approach to the Determination of Acoustic Material Parameters**
  S. Johannesmann, L. Claes, N. Feldmann, H. Zeipert, B. Henning, Tm - Technisches Messen 89 (2022) 493–506.

- **Breaking the Exascale Barrier for the Electronic Structure Problem in Ab-Initio Molecular Dynamics**
  R. Schade, T. Kenter, H. Elgabarty, M. Lass, T. Kühne, C. Plessl, ArXiv:2205.12182 (2022).

- **CP2K on the Road to Exascale**
  T. Kühne, C. Plessl, R. Schade, O. Schütt, ArXiv:2205.14741 (2022).

- **Learning Bilinear Models of Actuated Koopman Generators From Partially-Observed Trajectories**
  S.E. Otto, S. Peitz, C.W. Rowley, ArXiv:2209.09977 (2022).

- **Neural Network Based Carrier Frequency Offset Estimation From Speech Transmitted Over High Frequency Channels**
  J. Heitkämper, J. Schmalenstroeer, R. Haeb-Umbach, in: Proc. European Signal Processing Conference (EUSIPCO), 2022.

- **Roadmap on Electronic Structure Codes in the Exascale Era**
  V. Gavini, S. Baroni, V. Blum, D.R. Bowler, A. Buccheri, J.R. Chelikowsky, S. Das, W. Dawson, P. Delugas, M. Dogan, C. Draxl, G. Galli, L. Genovese, P. Giannozzi, M. Giantomassi, X. Gonze, M. Govoni, A. Gulans, F. Gygi, J.M. Herbert, S. Kokott, T. Kühne, K.-H. Liou, T. Miyazaki, P. Motamarri, A. Nakata, J.E. Pask, C. Plessl, L.E. Ratcliff, R.M. Richard, M. Rossi, R. Schade, M. Scheffler, O. Schütt, P. Suryanarayana, M. Torrent, L. Truflandier, T.L. Windus, Q. Xu, V.W.-Z. Yu, D. Perez, ArXiv:2209.12747 (2022).

- **Detection of Defects on Irregularly Structured Surfaces using Supervised and Semi-Supervised Learning Methods**
  T. Sander, S. Lange, U. Hilleringmann, V. Geneiß, C. Hedayat, H. Kuhn, in: Proc. Smart Systems Integration (SSI), IEEE, 2022.

- **Development of an Innovative Separation Unit for Nitrogen Recovery From Agricultural Waste**
  S.A. Bernemann, J. Makowiak, J. Makowiak, R. Bertling, N. Lutters, E. Kenig, in: Proc. ACHEMA Congress, 2022.

- **CFD-Based Investigation of the Packing Microstructure Influence on Droplet Behavior and Film Flow**
  C. Dechert, E. Kenig, in: Proc. Int. Conf. Distillation & Absorption, 2022.

- **An Initialization Scheme for Meeting Separation with Spatial Mixture Models**
  C. Boeddeker, T. Cord-Landwehr, T. von Neumann, R. Haeb-Umbach, in: Proc. Interspeech, ISCA, 2022.

- **MMS-MSG: A Multi-purpose Multi-Speaker Mixture Signal Generator**
  T. Cord-Landwehr, T. von Neumann, C. Boeddeker, R. Haeb-Umbach, in: Proc. Int. Work. on Acoustic Signal Enhancement (IWAENC), 2022.

- **SA-SDR: A Novel Loss Function for Separation of Meeting Style Data**
  T. von Neumann, K. Kinoshita, C. Boeddeker, M. Delcroix, R. Haeb-Umbach, in: Proc. IEEE Int. Conf. on Acoustics, Speech and Signal Processing (ICASSP), IEEE, 2022.

- **Monaural source separation: From anechoic to reverberant environments**
  T. Cord-Landwehr, C. Boeddeker, T. von Neumann, C. Zorila, R. Doddipatla, R. Haeb-Umbach, in: Proc. Int. Work. on Acoustic Signal Enhancement (IWAENC), IEEE, 2022.

- **Informed vs. Blind Beamforming in Ad-Hoc Acoustic Sensor Networks for Meeting Transcription**
  T. Gburrek, J. Schmalenstroeer, J. Heitkaemper, R. Haeb-Umbach, in: Proc. Int. Work. on Acoustic Signal Enhancement (IWAENC), IEEE, 2022.

- **A Meeting Transcription System for an Ad-Hoc Acoustic Sensor Network**
  T. Gburrek, C. Boeddeker, T. von Neumann, T. Cord-Landwehr, J. Schmalenstroeer, R. Haeb-Umbach, A Meeting Transcription System for an Ad-Hoc Acoustic Sensor Network, arXiv, 2022.

- **Light Scattering by Large Densely Packed Clusters of Particles**
  Y. Grynko, Y. Shkuratov, S. Alhaddad, J. Förstner, in: A. Kokhanovsky (Ed.), Springer Series in Light Scattering - Volume 8: Light Polarization and Multiple Scattering in Turbid Media, Springer International Publishing, Cham, 2022.

- **Far-field Calculation from magnetic Huygens Box Data using the Boundary Element Method**
  C. Marschalt, D. Schroder, S. Lange, U. Hilleringmann, C. Hedayat, H. Kuhn, D. Sievers, J. Förstner, in: Proc. Smart Systems Integration (SSI), IEEE, 2022.

- **CausalQA: A Benchmark for Causal Question Answering**
  A. Bondarenko, M. Wolska, S. Heindorf, L. Blübaum, A.-C. Ngonga Ngomo, B. Stein, P. Braslavski, M. Hagen, M. Potthast, in: Proc. Int. Conf. on Computational Linguistics, International Committee on Computational Linguistics, 2022, pp. 3296–3308.

- **Multiple Rabi rotations of trions in InGaAs quantum dots observed by photon echo spectroscopy with spatially shaped laser pulses**
  S. Grisard, H. Rose, A.V. Trifonov, R. Reichhardt, D.E. Reiter, M. Reichelt, C. Schneider, M. Kamp, S. Höfling, M. Bayer, T. Meier, I.A. Akimov, Physical Review B 106 (2022).

- **Coherent Contributions to Population Dynamics in a Semiconductor Microcavity**
  J. Paul, H. Rose, E. Swagel, T. Meier, J.K. Wahlstrand, A.D. Bristow, Physical Review B 105 (2022).

- **Clean and HydrogenAdsorbed AlInP(001) Surfaces: Structures and Electronic Properties**
  L.J. Glahn, I.A. Ruiz Alvarado, S. Neufeld, M.A. Zare Pour, A. Paszuk, D. Ostheimer, S. Shekarabi, O. Romanyuk, D.C. Moritz, J.P. Hofmann, W. Jaegermann, T. Hannappel, W.G. Schmidt, Physica Status Solidi (b) 259 (2022).

- **Super-Bloch Oscillations With Parametric Modulation of a Parabolic Trap**
  T. Meier, U. Ali, Condensed Matter (2022).

- **P-Terminated InP(001) Surfaces: Surface Band Bending and Reactivity to Water**
  D.C. Moritz, I.A. Ruiz Alvarado, M.A. Zare Pour, A. Paszuk, T. Frieß, E. Runge, J.P. Hofmann, T. Hannappel, W.G. Schmidt, W. Jaegermann, ACS Applied Materials & Interfaces 14 (2022) 47255–47261.

- **Electrochemical Performance of $KTiOAsO_4$ (KTA) in Potassium-Ion Batteries From Density-Functional Theory**
  A. Bocchini, U. Gerstmann, T. Bartley, H.-G. Steinrück, G. Henkel, W.G. Schmidt, Phys. Rev. Materials 6 (2022) 105401.

- **DC Ionic Conductivity in KTP and Its Isomorphs: Properties, Methods for Suppression, and Its Connection to Gray Tracking**
  L. Padberg, V. Quiring, A. Bocchini, M. Santandrea, U. Gerstmann, W.G. Schmidt, C. Silberhorn, C. Eigner, Crystals 12 (2022).

- **Oxygen Vacancies in KTiOPO: Optical Absorption From Hybrid DFT**
  A. Bocchini, U. Gerstmann, W.G. Schmidt, Phys. Rev. B 105 (2022) 205118.

- **Bound Polaron Formation in Lithium Niobate From Ab Initio Molecular Dynamics**
  M. Krenz, U. Gerstmann, W.G. Schmidt, Applied Physics A 128 (2022).

- **Water/InP(001) from Density Functional Theory**
  I.A. Ruiz Alvarado, W.G. Schmidt, ACS Omega 7 (2022) 19355–19364.

- **Steady States of 9b-Type Three-Level Systems Excited by Quantum Light With Various Photon Statistics in Lossy Cavities**
  H. Rose, O.V. Tikhonova, T. Meier, P. Sharapova, New Journal of Physics 24 (2022).

- **Microscopic Simulations of High Harmonic Generation From Semiconductors**
  A. Trautmann, R. Zuo, G. Wang, W.-R. Hannes, S. Yang, L.H. Thong, C. Ngo, J. Steiner, M. Ciappina, M. Reichelt, H.T. Duc, X. Song, W. Yang, T. Meier, in: Proc. Ultrafast Phenomena and Nanophotonics XXVI, SPIE, 2022.

- **Theoretical Analysis of Correlations Between Two Quantum Fields Exciting a Three-Level System Using the Cluster-Expansion Approach**
  H. Rose, O.V. Tikhonova, T. Meier, P. Sharapova, in: Proc. Ultrafast Phenomena and Nanophotonics XXVI, SPIE, 2022.

- **Protonation-Induced Charge Transfer and Polaron Formation in Organic Semiconductors Doped by Lewis Acids**
  F. Bauch, C.-D. Dong, S. Schumacher, RSC Advances 12 (2022) 13999–14006.

- **Microscopic Study of Molecular Double Doping**
  T. Bathe, C.-D. Dong, S. Schumacher, The Journal of Physical Chemistry A 126 (2022) 2075–2081.

- **Switching Off a Microcavity Polariton Condensate Near the Exceptional Point**
  Y. Li, X. Ma, Z. Hatzopoulos, P.G. Savvidis, S. Schumacher, T. Gao, ACS Photonics 9 (2022) 2079–2086.

- **Quasiparticle energies and optical response of $RbTiOPO_4$ and $KTiOAsO_4$**
  S. Neufeld, A. Schindlmayr, W.G. Schmidt, Journal of Physics: Materials 5 (2022).

- **Pulse Shaping for On-Demand Emission of Single Raman Photons From a Quantum-Dot Biexciton**
  T. Praschan, D. Heinze, D. Breddermann, A. Zrenner, A. Walther, S. Schumacher, Physical Review B 105 (2022).

- **Dynamics of Phase Defects Trapped in Optically Imprinted Orbits in Dissipative Binary Polariton Condensates**
  J. Wingenbach, M. Pukrop, S. Schumacher, X. Ma, Physical Review B 105 (2022).

- **Two-Colour Spectrally Multimode Integrated SU(1,1) Interferometer**
  A. Ferreri, P. Sharapova, Symmetry 14 (2022).

- **A Density-Functional Theory Study of Hole and Defect-Bound Exciton Polarons in Lithium Niobate**
  F. Schmidt, A.L. Kozub, U. Gerstmann, W.G. Schmidt, A. Schindlmayr, Crystals 12 (2022).

2021

- **Electron Polarons in Lithium Niobate: Charge Localization, Lattice Deformation, and Optical Response**
  F. Schmidt, A.L. Kozub, U. Gerstmann, W.G. Schmidt, A. Schindlmayr, in: New Trends in Lithium Niobate: From Bulk to Nanocrystals, MDPI, 2022, pp. 231–248.

- **Towards Performance Characterization of FPGAs in Context of HPC using OpenCL Benchmarks**
  M. Meyer, in: Proc. Int. Symp. on Highly Efficient Accelerators and Reconfigurable Technologies, 2021.

- **AutoML for Multi-Label Classification: Overview and Empirical Evaluation**
  M.D. Wever, A. Tornede, F. Mohr, E. Hüllermeier, IEEE Transactions on Pattern Analysis and Machine Intelligence (2021) 1–1.

- **Far-Field Automatic Speech Recognition**
  R. Haeb-Umbach, J. Heymann, L. Drude, S. Watanabe, M. Delcroix, T. Nakatani, Proceedings of the IEEE 109 (2021) 124–148.

- **Predicting Machine Learning Pipeline Runtimes in the Context of Automated Machine Learning**
  F. Mohr, M.D. Wever, A. Tornede, E. Hüllermeier, IEEE Transactions on Pattern Analysis and Machine Intelligence, 2021.

- **Guanine Condensates as Covalent Materials and the Concept of Cryptopores**
  J. Kossmann, D. Piankova, N. V. Tarakina, J.J. Heske, T. Kühne, J. Schmidt, M. Antonietti, N. López-Salas, Carbon 172 (2021) 497–505.

- **Development of a Submodel Technique for FFT-Based Solvers in Micromechanical Analysis**
  S.R. Tinkloh, T. Wu, T. Tröster, T. Niendorf, in: Proc. Int. Conf. on Theoretical, Analytical and Computational Methods for Composite Materials and Composite Structures, 2021.

- **Coevolution of Remaining Useful Lifetime Estimation Pipelines for Automated Predictive Maintenance**
  T. Tornede, A. Tornede, M.D. Wever, E. Hüllermeier, in: Proc. Genetic and Evolutionary Computation Conference, 2021.

- **Stofftransportmessung und -visualisierung am ruhenden und bewegten Einzeltropfen**
  J. Heine, C. Wecker, E. Kenig, H.-J. Bart, in: Proc. Jahrestreffen der ProcessNet-Fachgruppe Extraktion, 2021.

- **Numerische Untersuchung der Marangonikonvektion in Flüssig-Flüssig-Systemen: Von der Tropfenbildung bis zur Tropfeninteraktion**
  C. Wecker, A. Schulz, J. Heine, H.-J. Bart, E. Kenig, in: Proc. Jahrestreffen der ProcessNet-Fachgruppe Extraktion, 2021.

- **Numerische Untersuchungen zu Fluiddynamik und Stofftransport binärer Tropfeninteraktion unter Berücksichtigung von Marangonikonvektion**
  C. Wecker, A. Hoppe, A. Schulz, J. Heine, H.-J. Bart, E. Kenig, in: Proc. Jahrestreffen der ProcessNet-Fachgruppe Wärme- und Stofftransport, 2021.

- **Mehrkomponenten-Stofftransport an bewegten Phasengrenzflächen unter Berücksichtigung von Diffusionskreuzeffekten**
  A. Schulz, C. Wecker, E. Kenig, in: Proc. Jahrestreffen der ProcessNet-Fachgruppe Mehrphasenströmung, 2021.

- **HighPerMeshes – A Domain-Specific Language for Numerical Algorithms on Unstructured Grids**
  S. Alhaddad, J. Förstner, S. Groth, D. Grünewald, Y. Grynko, F. Hannig, T. Kenter, F.-J. Pfreundt, C. Plessl, M. Schotte, T. Steinke, J. Teich, M. Weiser, F. Wende, in: Proc. Euro-Par 2020: Parallel Processing Workshops, Cham, 2021.

- **CFD-basierte Untersuchung von Zweiphasenströmungen in strukturierten Packungen**
  R. Bertling, M. Hack, I. Ausner, B. Horschitz, E. Kenig, in: Proc. Jahrestreffen der ProcessNet-Fachgruppen Fluidverfahrenstechnik und Wärme- und Stoffübertragung, 2021.

- **Development of a Hybrid Crash-Relevant Car Body Component With Load-Adapted Thickness Properties: Design, Manufacturing and Testing**
  A.A. Camberg, T. Tröster, C. Latuske, in: Proc. Conf. Future Production of Hybrid Structures (FPHS 2020) Springer, 2021.

- **Development of Methods for Coil-Based Localization by Magnetic Fields of Miniaturized Sensor Platforms in Bioprocesses**
  S. Lange, D. Schröder, C. Hedayat, H. Kuhn, U. Hilleringmann, in: Proc. Int. Conf. on Industrial Technology (ICIT), IEEE, 2021.

- **Impact of Screening and Relaxation on Weakly Coupled Two-Dimensional Heterostructures**
  T.T.N. Nguyen, T. Sollfrank, C. Tegenkamp, E. Rauls, U. Gerstmann, Physical Review B (2021).

- **Timing Optimization for Virtual FPGA Configurations**
  L.M. Witschen, T. Wiersema, M. Raeisi Nafchi, A. Bockhorn, M. Platzner, in: Proc. Int. Symp. on Applied Reconfigurable Computing (ARC), Springer Lecture Notes in Computer Science, 2021.

- **The Effect of Fiber Waviness on the Residual Stress State and Its Prediction by the Hole Drilling Method in Fiber Metal Laminates: A Global-Local Finite Element Analysis**
  S.R. Tinkloh, T. Wu, T. Tröster, T. Niendorf, Metals (2021).

- **On the Reliability of Residual Stress Measurements in Unidirectional Carbon Fibre Reinforced Epoxy Composites**
  A. Magnier, T. Wu, S.R. Tinkloh, T. Tröster, B. Scholtes, T. Niendorf, Polymer Testing (2021).

- **Measurement Procedure for Acoustic Absorption and Bulk Viscosity of Liquids**
  L. Claes, R.S. Chatwell, E. Baumhögger, T. Hetkämper, H. Zeipert, J. Vrabec, B. Henning, Measurement (2021).

- **Steady States of 9b-Type Three-Level Systems Excited by Quantum Light in Lossy Cavities**
  H. Rose, O.V. Tikhonova, T. Meier, P.R. Sharapova, ArXiv:2109.00842 (2021).

- **How Irreversible Are Steady-State Trajectories of a Trapped Active Particle?**
  L. Dabelow, S. Bo, R. Eichhorn, Journal of Statistical Mechanics: Theory and Experiment (2021).

- **Towards Electronic Structure-Based Ab-Initio Molecular Dynamics Simulations with Hundreds of Millions of Atoms**
  R. Schade, T. Kenter, H. Elgabarty, M. Lass, O. Schütt, A. Lazzaro, H. Pabst, S. Mohr, J. Hutter, T.D. Kühne, C. Plessl, ArXiv:2104.08245 (2021).

- **Optimization of Optical Waveguide Antennas for Directive Emission of Light**
  H. Farheen, T. Leuteritz, S. Linden, V. Myroshnychenko, J. Förstner, ArXiv:2106.02468 (2021).

- **Interfacial Covalent Bonds Regulated Electron-Deficient 2D Black Phosphorus for Electrocatalytic Oxygen Reactions**
  X. Wang, R. Kormath Madam Raghupathy, C.J. Querebillo, Z. Liao, D. Li, K. Lin, M. Hantusch, Z. Sofer, B. Li, E. Zschech, I.M. Weidinger, T. Kühne, H. Mirhosseini, M. Yu, X. Feng, Advanced Materials 33 (2021) 2008752.

- **Thermodynamically Stable Polymorphs of Nitrogen-Rich Carbon Nitrides: A N_5 Study**
  A. Ghasemi, H. Mirhosseini, T. Kühne, Phys. Chem. Chem. Phys. 23 (2021) 6422–6432.

- **Convolutive Transfer Function Invariant SDR Training Criteria for Multi-Channel Reverberant Speech Separation**
  C. Boeddeker, W. Zhang, T. Nakatani, K. Kinoshita, T. Ochiai, M. Delcroix, N. Kamo, Y. Qian, R. Haeb-Umbach, in: Proc. Int. Conf. Acoustics, Speech and Signal Processing (ICASSP), 2021.

- **Explicit Multiobjective Model Predictive Control for Nonlinear Systems With Symmetries**
  S. Ober-Blöbaum, S. Peitz, International Journal of Robust and Nonlinear Control 31(2) (2021) 380–403.

- **Artificial Neural Networks for the Kinetic Energy Functional of Non-Interacting Fermions**
  S.A. Ghasemi, T.D. Kühne, The Journal of Chemical Physics 154 (2021) 074107.

- **Adsorption and Reaction of PbPc on Hydrogenated Epitaxial Graphene**
  D. Slawig, M. Gruschwitz, U. Gerstmann, E. Rauls, C. Tegenkamp, The Journal of Physical Chemistry C 125 (2021) 20087–20093.

- **Hyperfine and Nuclear Quadrupole Splitting of the NV Ground State in 4H-SiC**
  F.F. Murzakhanov, B.V. Yavkin, G.V. Mamin, S.B. Orlinskii, H.J. von Bardeleben, T. Biktagirov, U. Gerstmann, V.A. Soltamov, Physical Review B 103 (2021).

- **Impact of Screening and Relaxation on Weakly Coupled Two-Dimensional Heterostructures**
  T.T.N. Nguyen, T. Sollfrank, C. Tegenkamp, E. Rauls, U. Gerstmann, Physical Review B 103 (2021).

- **Nondegenerate Two-Photon Absorption in ZnSe: Experiment and Theory**
  L. Krauss-Kodytek, W.-R. Hannes, T. Meier, C. Ruppert, M. Betz, Physical Review B (2021).

- **Assessing the Sufficiency of Arguments through Conclusion Generation**
  T. Gurcke, M. Alshomary, H. Wachsmuth, in: Proc. Work. Argument Mining, 2021, pp. 67–77.

- **Algorithm Selection as Superset Learning: Constructing Algorithm Selectors from Imprecise Performance Data**
  J.M. Hanselle, A. Tornede, M.D. Wever, E. Hüllermeier, (2021).

- **Messverfahren für die akustische Absorption in reinen Fluiden zur Bestimmung der Volumenviskosität**
  L. Claes, Dissertation, Universität Paderborn, 2021.

- **The HighPerMeshes Framework for Numerical Algorithms on Unstructured Grids**
  S. Alhaddad, J. Förstner, S. Groth, D. Grünewald, Y. Grynko, F. Hannig, T. Kenter, F. Pfreundt, C. Plessl, M. Schotte, T. Steinke, J. Teich, M. Weiser, F. Wende, Concurrency and Computation: Practice and Experience (2021) e6616.

- **Generating Physically Sound Training Data for Image Recognition of Additively Manufactured Parts**
  T. Nickchen, S. Heindorf, G. Engels, in: 2021 Proc. IEEE Winter Conf. Applications of Computer Vision (WACV), IEEE, 2021.

- **Contrastive Predictive Coding Supported Factorized Variational Autoencoder for Unsupervised Learning of Disentangled Speech Representations**
  J. Ebbers, M. Kuhlmann, T. Cord-Landwehr, R. Haeb-Umbach, in: Proc. Int. Conf. Acoustics, Speech and Signal Processing (ICASSP), 2021, pp. 3860–3864.

- **Speeding Up Permutation Invariant Training for Source Separation**
  T. von Neumann, C. Boeddeker, K. Kinoshita, M. Delcroix, R. Haeb-Umbach, in: Proc. Speech Communication, ITG Conference, 2021.

- **Self-Trained Audio Tagging and Sound Event Detection in Domestic Environments**
  J. Ebbers, R. Haeb-Umbach, in: Proc. Detection and Classification of Acoustic Scenes and Events 2021 Workshop (DCA), 2021, pp. 226–230.

- **Adapting Sound Recognition to A New Environment Via Self-Training**
  J. Ebbers, M.C. Keyser, R. Haeb-Umbach, in: Proc. European Signal Processing Conference (EUSIPCO), 2021, pp. 1135–1139.

- **A Database for Research on Detection and Enhancement of Speech Transmitted over HF links**
  J. Heitkaemper, J. Schmalenstroeer, V. Ion, R. Haeb-Umbach, in: Proc. Speech Communication, 14th ITG-Symposium, 2021, pp. 1–5.

- **Graph-PIT: Generalized Permutation Invariant Training for Continuous Separation of Arbitrary Numbers of Speakers**
  T. von Neumann, K. Kinoshita, C. Boeddeker, M. Delcroix, R. Haeb-Umbach, in: Interspeech, 2021.

- **Controlling the Emission Time of Photon Echoes by Optical Freezing of Exciton Dephasing and Rephasing in Quantum-Dot Ensembles**
  M. Reichelt, H. Rose, A.N. Kosarev, S.V. Poltavtsev, M. Bayer, I.A. Akimov, C. Schneider, M. Kamp, S. Höfling, T. Meier, in: Proc. Ultrafast Phenomena and Nanophotonics XXV, 2021.

- **Theoretical Analysis and Simulations of Two-Dimensional Fourier Transform Spectroscopy Performed on Exciton-Polaritons of a Quantum-Well Microcavity System**
  H. Rose, J. Paul, J.K. Wahlstrand, A.D. Bristow, T. Meier, in: Ultrafast Phenomena and Nanophotonics XXV, 2021.

- **Neighboring Atom Collisions in Solid-State High Harmonic Generation**
  R. Zuo, A. Trautmann, G. Wang, W.-R. Hannes, S. Yang, X. Song, T. Meier, M. Ciappina, H.T. Duc, W. Yang, Ultrafast Science 2021 (2021).

- **Bright Correlated Twin-Beam Generation and Radiation Shaping in High-Gain Parametric Down-Conversion With Anisotropy**
  M. Riabinin, P. Sharapova, T. Meier, Optics Express 29 (2021).

- **Nondegenerate Two-Photon Absorption in ZnSe: Experiment and Theory**
  L. Krauss-Kodytek, W.-R. Hannes, T. Meier, C. Ruppert, M. Betz, Physical Review B 104 (2021).

- **Microscopic Analysis of High Harmonic Generation in Semiconductors With Degenerate Bands**
  L.H. Thong, C. Ngo, H.T. Duc, X. Song, T. Meier, Physical Review B 103 (2021) 085201.

- **Controlled Growth of Ordered Monolayers of N-Heterocyclic Carbenes on Silicon**
  M. Franz, S. Chandola, M. Koy, R. Zielinski, H. Aldahhak, M. Das, M. Freitag, U. Gerstmann, D. Liebig, A.K. Hoffmann, M. Rosin, W.G. Schmidt, C. Hogan, F. Glorius, N. Esser, M. Dähne, Nature Chemistry (2021) 828–835.

- **Electronic Structure of the Si(111)3×3B Surface From Theory and Photoemission Spectroscopy**
  H. Aldahhak, C. Hogan, S. Lindner, S. Appelfeller, H. Eisele, W.G. Schmidt, M. Dähne, U. Gerstmann, M. Franz, Physical Review B (2021).

- **Spin Polarization, Electron–Phonon Coupling, and Zero-Phonon Line of the NV Center in 3C-SiC**
  H. Jurgen von Bardeleben, J.-L. Cantin, U. Gerstmann, W.G. Schmidt, T. Biktagirov, Nano Letters 21 (2021) 8119–8125.

- **Surface Localized Phonon Modes at the Si(553)-Au Nanowire System**
  J. Plaickner, E. Speiser, C. Braun, W.G. Schmidt, N. Esser, S. Sanna, Physical Review B (2021).

- **InP and AlInP(001)(2 × 4) Surface Oxidation From Density Functional Theory**
  I.A. Ruiz Alvarado, M. Karmo, E. Runge, W.G. Schmidt, ACS Omega (2021) 6297–6304.

- **Optoelectronic Sampling of Ultrafast Electric Transients With Single Quantum Dots**
  A. Widhalm, S. Krehs, D. Siebert, N.L. Sharma, T. Langer, B. Jonas, D. Reuter, A. Thiede, J. Förstner, A. Zrenner, Applied Physics Letters 119 (2021) 181109.

- **Adatom Mediated Adsorption of N-heterocyclic Carbenes on Cu(111) and Au(111)**
  M. Jain, U. Gerstmann, W.G. Schmidt, H. Aldahhak, Journal of Computational Chemistry 43 (2021) 413–420.

- **Potassium Titanyl Phosphate Z- and Y-Cut Surfaces From Density-Functional Theor**
  S. Neufeld, A. Bocchini, W.G. Schmidt, Physical Review Materials (2021).

- **All-Optical Beam Steering Using the Polariton Lighthouse Effect**
  S.M.H. Luk, H. Vergnet, O. Lafont, P. Lewandowski, N.H. Kwong, E. Galopin, A. Lemaitre, P. Roussignol, J. Tignon, S. Schumacher, R. Binder, E. Baudin, ACS Photonics (2021) 449–454.

- **Atomically Thin Sheets of Lead-Free 1D Hybrid Perovskites Feature Tunable White-Light Emission from Self-Trapped Excitons**
  P. Klement, N. Dehnhardt, C.-D. Dong, F. Dobener, S. Bayliff, J. Winkler, D.M. Hofmann, P.J. Klar, S. Schumacher, S. Chatterjee, J. Heine, Advanced Materials 33 (2021).

- **Microscopic Insights into Charge Formation and Energetics in n-Doped Organic Semiconductors**
  C.-D. Dong, S. Schumacher, The Journal of Physical Chemistry C 125 (2021) 21824–21830.

- **Generating Two-Mode Squeezing With Multimode Measurement-Induced Nonlinearity**
  M. Riabinin, P. Sharapova, T. Bartley, T. Meier, Journal of Physics Communications (2021).

- **Electron Polarons in Lithium Niobate: Charge Localization, Lattice Deformation, and Optical Response**
  F. Schmidt, A.L. Kozub, U. Gerstmann, W.G. Schmidt, A. Schindlmayr, Crystals 11 (2021).

- **Polaronic Enhancement of Second-Harmonic Generation in Lithium Niobate**
  A.L. Kozub, A. Schindlmayr, U. Gerstmann, W.G. Schmidt, Physical Review B 104 (2021).

- **Ultrafast Electric Control of Cavity Mediated Single-Photon and Photon-Pair Generation With Semiconductor Quantum Dots**
  D. Bauch, D.F. Heinze, J. Förstner, K. Jöns, S. Schumacher, Physical Review B 104 (2021) 085308.

- **Quantifying Quantum Coherence in Polariton Condensates**
  C. Lüders, M. Pukrop, E. Rozas, C. Schneider, S. Höfling, J. Sperling, S. Schumacher, M. Aßmann, PRX Quantum (2021).

- **GaInP/AlInP(001) Interfaces from Density Functional Theory**
  L. Meier, W.G. Schmidt, Physica Status Solidi (b) 259 (2021).

- **Structuring Coflowing and Counterflowing Currents of Polariton Condensates in Concentric Ring-Shaped and Elliptical Potentials**
  F. Barkhausen, M. Pukrop, S. Schumacher, X. Ma, Physical Review B 103 (2021).

- **Split-Ring Polariton Condensates as Macroscopic Two-Level Quantum Systems**
  Y. Xue, I. Chestnov, E. Sedov, E. Kiktenko, A.K. Fedorov, S. Schumacher, X. Ma, A. Kavokin, Physical Review Research 3 (2021).

- **Explanation as a Social Practice: Toward a Conceptual Framework for the Social Design of AI Systems**
  K.J. Rohlfing, P. Cimiano, I. Scharlau, T. Matzner, H.M. Buhl, H. Buschmeier, E. Esposito, A. Grimminger, B. Hammer, R. Haeb-Umbach, I. Horwath, E. Huellermeier, F. Kern, S. Kopp, K. Thommes, A.-C. Ngonga Ngomo, C. Schulte, H. Wachsmuth, P. Wagner, B. Wrede, IEEE Transactions on Cognitive and Development Systems 13 (2021) 717–728.

2020

- **Non-Adiabatic Transitions in the Reaction of Fluorine With Methane**
  B. Zhao, U. Manthe, The Journal of Chemical Physics (2020).

- **Hybrid Density Functional Theory Benchmark Study on Lithium Manganese Oxides**
  M. Eckhoff, P.E. Blöchl, J. Behler, Physical Review B (2020).

- **Multistable Circular Currents of Polariton Condensates Trapped in Ring Potentials**
  F. Barkhausen, S. Schumacher, X. Ma, Optics Letters (2020).

- **Realization of All-Optical Vortex Switching in Exciton-Polariton Condensates**
  X. Ma, B. Berger, M. Aßmann, R. Driben, T. Meier, C. Schneider, S. Höfling, S. Schumacher, Nature Communications (2020).

- **Externally Controlled Lotka-Volterra Dynamics in a Linearly Polarized Polariton Fluid**
  M. Pukrop, S. Schumacher, Physical Review E (2020).

- **Learning Choice Functions via Pareto-Embeddings**
  K. Pfannschmidt, E. Hüllermeier, in: Lecture Notes in Computer Science, Springer, 2020.

- **Minimizing Crane Times in Pre-Marshalling Problems**
  C. Parreño-Torres, R. Alvarez-Valdes, R. Ruiz, K. Tierney, Transportation Research Part E: Logistics and Transportation Review (2020).

- **Hyper-parameterized Dialectic Search for Non-linear Box-Constrained Optimization with Heterogenous Variable Types**
  M. Sellmann, K. Tierney, in: Lecture Notes in Computer Science, Cham, 2020.

- **A Genetic Algorithm for Finding Realistic Sea Routes Considering the Weather**
  S. Kuhlemann, K. Tierney, Journal of Heuristics (2020).

- **cOn-The-Flyd Calculation of the Vibrational Sum-Frequency Generation Spectrum at the Air-Water Interface**
  D. Ojha, T.D. Kühne, Molecules 25 (2020).

- **Disordered Crystals From First Principles II: Transport Coefficients**
  T. Kühne, J.J. Heske, E. Prodan, Annals of Physics 421 (2020) 168290.

- **Insight From Energy Decomposition Analysis on a Hydrogen-Bond-Mediated Mechanism for On-Water Catalysis**
  M.A. Salem, T.D. Kühne, Molecular Physics (2020) 1–6.

- **Correlating Facet Orientation, Defect-Level Density and Dipole Layer Formation at the Surface of Polycrystalline CuInSe2 Thin Films**
  A. Elizabeth, H. Conradi, S. K. Sahoo, T. Kodalle, C. A. Kaufmann, T. Kühne, H. Mirhosseini, D. Abou-Ras, H. Mönig, Acta Materialia 200 (2020).

- **Nonlinear Dielectric Properties of Random Paraelectric-Dielectric Composites**
  V. Myroshnychenko, S. Smirnov, P.M.M. Jose, C. Brosseau, J. Förstner, Acta Materialia 203 (2020) 116432.

- **Electrochemical N2 Reduction to Ammonia Using Single Au/Fe Atoms Supported on Nitrogen-Doped Porous Carbon**
  S.K. Sahoo, J.J. Heske, M. Antonietti, Q. Qin, M. Oschatz, T. Kühne, ACS Applied Energy Materials 3 (2020) 10061–10069.

- **Comparison of Feature Selection Techniques to Improve Approximate Circuit Synthesis**
  K. Chandrakar, Comparison of Feature Selection Techniques to Improve Approximate Circuit Synthesis, 2020.

- **Preselection Bandits**
  V. Bengs, E. Hüllermeier, in: Proc. Int. Conf. on Machine Learning, 2020, pp. 778–787.

- **Multi-Armed Bandits with Censored Consumption of Resources**
  V. Bengs, E. Hüllermeier, ArXiv:2011.00813 (2020).

- **Investigation of the Surface Equivalence Principle on a Metal Surface for a Near-Field to Far-Field Transformation by the N**
  S. Lange, D. Schroder, C. Hedayat, C. Hangmann, T. Otto, U. Hilleringmann, in: Proc. Int. Symp. Electromagnetic Compatibility (EMC EUROPE), IEEE, 2020.

- **Far-Field Prediction Combining Simulations With Near-Field Measurements for EMI Assessment of PCBs**
  D. Schroder, S. Lange, C. Hangmann, C. Hedayat, in: Tensorial Analysis of Networks (TAN) Modelling for PCB Signal Integrity and EMC Analysis, 1st ed., IET, 2020, pp. 315-346 (32).

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