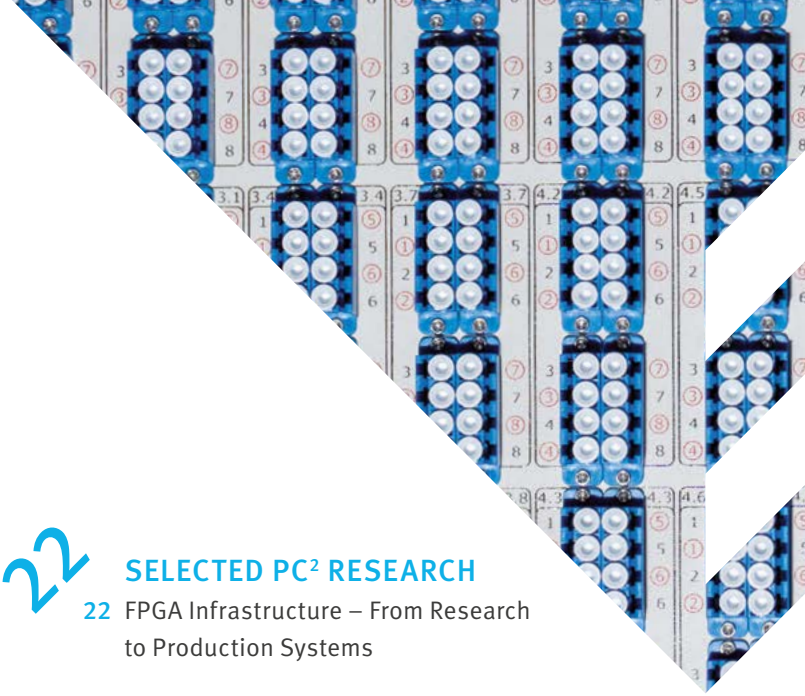
PADERBORN UNIVERSITY

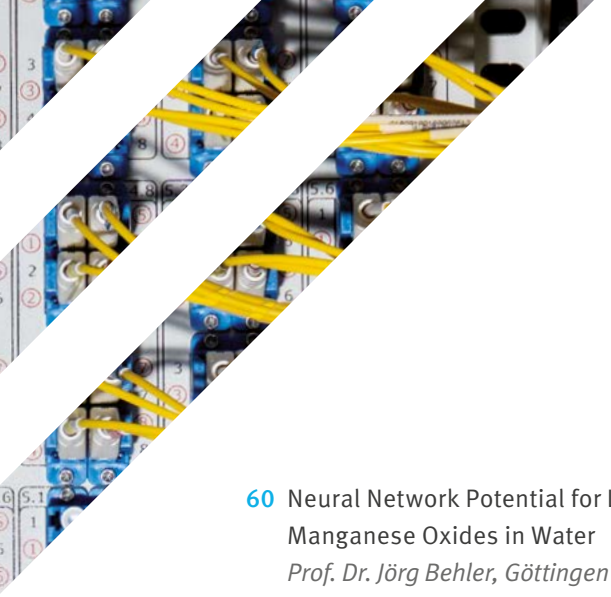
Paderborn Center for Parallel Computing

PROJECTS FACTS RESEARCH HPC TEACHING PEOPLE

ANNUAL REPORT 2017/18/19



CONTENTS



Paderborn Center for Parallel Computing

PREFACE

It is my great pleasure to be able to present the latest PC² research and service report for the period 1/2017–6/2019 for you. Right before the publication of the last report, we had received notice that our Noctua proposal for funding our next generation HPC system and a new computer center building, which will be dedicated to HPC, has been approved by the German Council for Science and Humanities.

The approval of the proposal thereby marked the start of very exciting times for PC²: the expansion and transition to a nationwide HPC center. Since then, the implementation of the Noctua project has progressed according to the ambitious schedule outlined in the proposal. The design of the new computer center is complete and the construction approval has been obtained. The commencement for the construction works is now imminent at the time of writing this report.

PREFACE

In September 2018, we celebrated the inauguration of the first phase of the Noctua supercomputer – a Cray CS500 cluster system with more than 10,000 Intel Xeon CPU cores. This new HPC system is now complementing our previous OCuLUS installation in order to satisfy the urgent demand for more computing resources. Noctua is not only our new workhorse, rather also a pioneering platform for research at the intersection of computational science and computer science by utilizing the deployment of leading-edge FPGA accelerators. PC² was the first academic institution worldwide which received the latest generation Intel Stratix 10 FPGAs in this scale. Another world-breaking initial innovation is the connection of all 128 network ports of the FPGAs by means of a protocol-agnostic full-crossbar optical switch, which enables us to implement arbitrary application-specific interconnection topologies between the FPGAs.

On the services side, we have also made great strides by filling the first batch of additional permanent staff positions which were committed by the University as part of the expansion of PC². We were able to hire two highly qualified HPC experts who will train and support our users for optimizing their HPC codes for our HPC and storage systems. Additionally, their mission also includes collaborative research with the users of our HPC center regarding new methods and tools which are optimized for modern computer architectures. Our research support services will be further expanded with personnel funded by the HPC.nrw competence center for high-performance computing, a project which was recently approved by the North Rhine-Westphalian Ministry of Culture and Science.

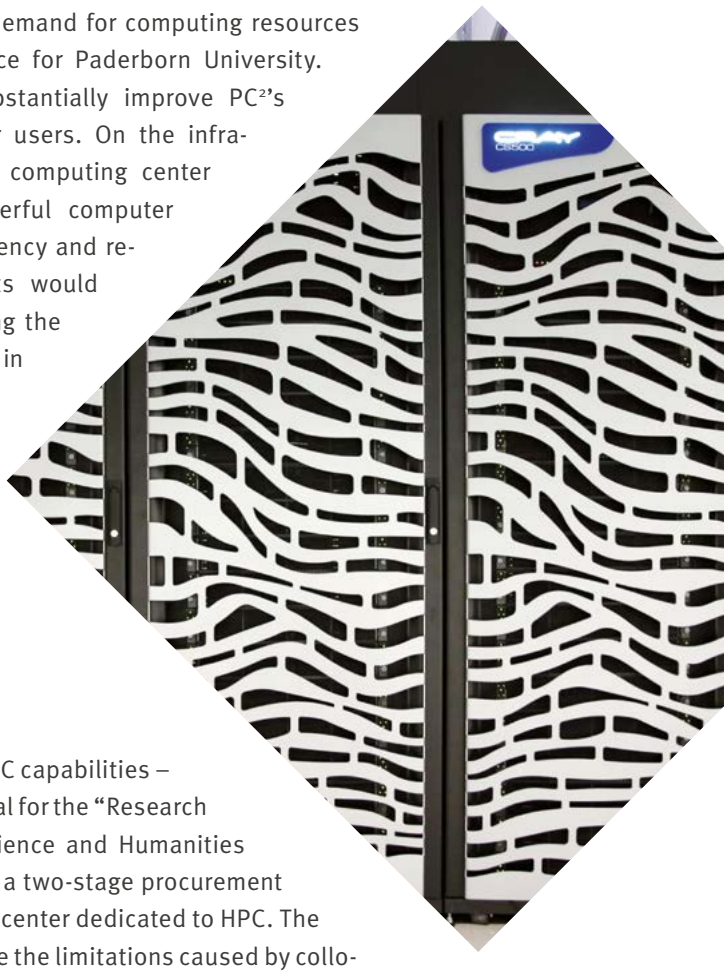
The governance of our center has also been adapted to satisfy the new role and competences of PC². In order to implement the research-guided and competitive access to research infrastructures, which is mandated through the funding of the German Council for Science and Humanities, we have institutionalized our process for obtaining access to computing resources. The newly founded resource allocation board is now responsible for assigning computing time on all HPC systems based on a technical and – for large-scale projects – a scientific peer-review of the application. This process ensures quality-controlled and fair access for external and internal users. In this report, you will find summaries of the research projects which have been approved by the resource allocation board in the first public call for computing time proposals in Spring 2019.

Finally, and most importantly, I would like to thank our funding agencies, collaborations partners, and the University Executive Board. Without their support, neither the development of PC² nor the excellent research of our users, which was enabled by our infrastructure, would have been possible.

Prof. Dr. Christian Plessl
Managing director and chairman of the board

THE NOCTUA PROJECT – A DATA CENTER DEDICATED TO HPC

In 2016, Paderborn University's Executive Board and the PC² Management Board discussed how to optimally address the rapidly growing demand for computing resources and the strategic importance of computational science for Paderborn University. The outcome of this discussion was a plan to substantially improve PC²'s capability to provide HPC resources and services for users. On the infrastructure side, the plan foresaw an upgrade of the computing center facility in such a way that significantly more powerful computer systems can be operated at an increased level of efficiency and reliability. These technical infrastructure improvements would be complemented by additional personnel for operating the HPC systems and HPC experts for supporting researchers in the effective use of the HPC systems through consulting and collaborations. This decision fell on fertile ground at the North Rhine-Westphalia Ministry of Arts and Sciences, which subsequently declared their support for the plan and ambition of Paderborn to act as a nationwide HPC service center.



PROPOSAL FOR RESEARCH BUILDING

The first step for implementing the expansion of PC²'s HPC capabilities – denoted as the Noctua Project – was to prepare a proposal for the "Research Infrastructure" program of the German Council for Science and Humanities (Wissenschaftsrat). The proposal consists of two parts: a two-stage procurement of a new HPC system and the construction of a new data center dedicated to HPC. The motivation for building a new data center was to eliminate the limitations caused by collocating the existing HPC systems operated by PC² with the servers operated by the University's Central IT Service Unit (IMT) in a data center which was designed for traditional air-cooled servers. The new data center will completely focus on operating HPC systems with their specific high density and cooling requirements and a power and cooling redundancy level adjusted to HPC services.

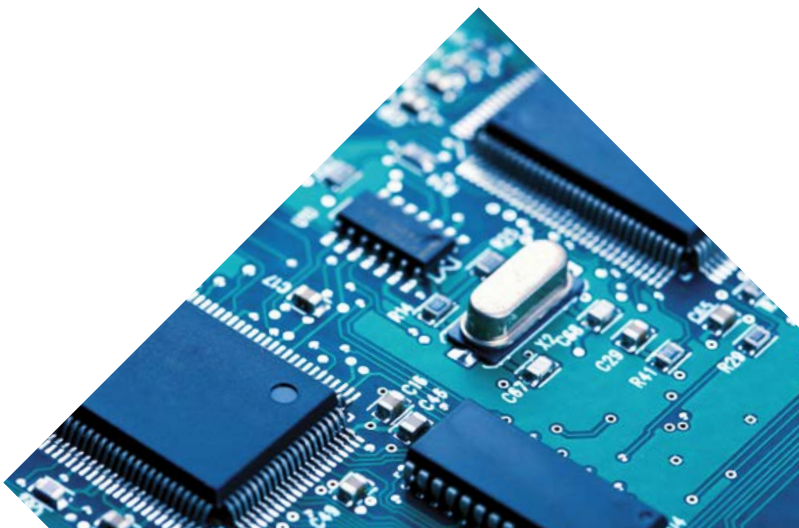
To be able to achieve best in class energy efficiency, the new data center will be designed for warm water cooled servers, which can operate almost exclusively with free cooling i.e. without power hungry compression refrigerators. To deliver the acutely needed increase for computing resources to our users in a timely manner, the first stage of the Noctua HPC system would be installed in the existing data center. The second stage of the system will then be installed in the new data center after the end of construction.

DECISION OF THE JOINT SCIENCE CONFERENCE (GWK)

After a positive evaluation of a pre-proposal, the full proposal was submitted in January 2017 to the German Council for Science and Humanities. Following the recommendation by the Council for Science and Humanities in May 2017, the Joint Science Conference (Gemeinsame Wissenschaftskonferenz, GWK) approved funding of the Noctua Project in June 2017. The Council for Science and Humanities had issued a remarkable recommendation with highest ratings for our proposal.

The German Federal Government and the North Rhine-Westphalia Regional Government will jointly provide a total of 25.4 Million Euros from 2018 to 2022. A total of 10 Million Euros will be invested in a new high-performance computer in two stages. For the construction of the modern and particularly energy-efficient data center, which is anticipated to be completed in 2020, an amount of 15.4 Million Euros is provided.

For Paderborn University, this proposal with the new data center is the first success in the research infrastructure program of the Council for Science and Humanities. Prof. Dr. Christine Silberhorn, at that time Vice President for research stated “With Noctua we are able to establish the best-possible conditions for interdisciplinary research at the cross section of applications, methods and computing systems research and we are well prepared for future requirements. For Paderborn University, this

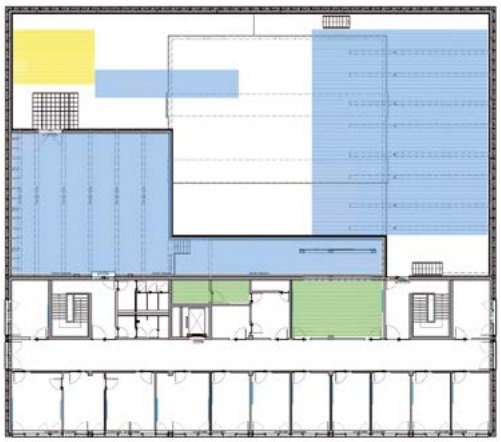


VISUALIZATION AND FLOOR PLANS OF THE PLANNED HPC DATA CENTER

Project partners: Paderborn University, Paderborn Center for Parallel Computing, Bau- und Liegenschaftsbetrieb (BLB) NRW, and DC-CE RZ-Beratung GmbH & Co.KG

1st floor

2nd floor



HPC Systems
Electr. Power
Cooling
Fire protection
Technical Operation

is an additional important step towards increasing the international visibility of its top-level research. We are very proud to become one of the most powerful university HPC centers in Germany with our new research infrastructure."

PADERBORN UNIVERSITY BECOMES A FULL MEMBER OF THE GAUSS-ALLIANZ

This funding commitment also influenced additional perspectives for Paderborn University. The leading scientific supercomputer centers of Germany are merged in the Gauß-Allianz to promote research and development in the field of HPC and to coordinate the HPC-related activities in Germany. Paderborn University, represented by PC², was a founding associated member of the Gauß-Allianz. Based on the decision of the Joint Science Conference to approve the funding of the Paderborn University for a new national-level HPC system, the Gauß-Allianz member status of the Paderborn University was subsequently raised from associated member to full member. With the status of a full member of the Gauß-Allianz, PC² enters the top 10 of German HPC centers. PC² is now therefore in a position to compete with the other national-level HPC centers for HPC funding.

INSTALLATION OF NOCTUA STAGE 1

The public procurement process for the first stage of the Noctua HPC system was awarded to the company Cray with a contract for a CS500 cluster system. The Cray CS500 is installed in the computer room of PC² located in the data center in building O and was inaugurated in September 2018. This system delivers triple the performance of the previous flagship system, OCuLUS. The new HPC system is deployed with 272 dual-processor compute nodes powered by Intel's latest generation Xeon Skylake CPUs. The installed processors, each with 20 cores, are the highest-performing parts of Intel's Xeon Gold portfolio. Overall, the system provides a total of 11,000 cores and 51 TByte of main memory. The system is connected by a 100 Gbps Intel OmniPath interconnect for supporting highly parallel MPI applications. Additionally, Noctua features a Cray ClusterStor L300N storage appliance. The combination of Lustre, GridRAID and the NXD flash accelerator technology provides 720 TByte of highly reliable storage and high bandwidth for I/O-intensive compute jobs. With this HPC System, the PC² users once again have the latest HPC technology with the most powerful computing nodes available.

A distinctive feature of the Noctua system is the deployment of 32 Field-Programmable Gate Array (FPGA) accelerators featuring the latest generation Intel Stratix 10 FPGAs, placing it at the very top of academic HPC production systems with state-of-the-art FPGAs. The selected FPGAs, each with 5,760 variable-precision DSP blocks, are well suited to floating-point heavy scientific computations. The four communication ports of the FPGAs are directly connected via optical links to a 320 port optical switch. A first set of applications which benefit from FPGA acceleration are currently ported and re-

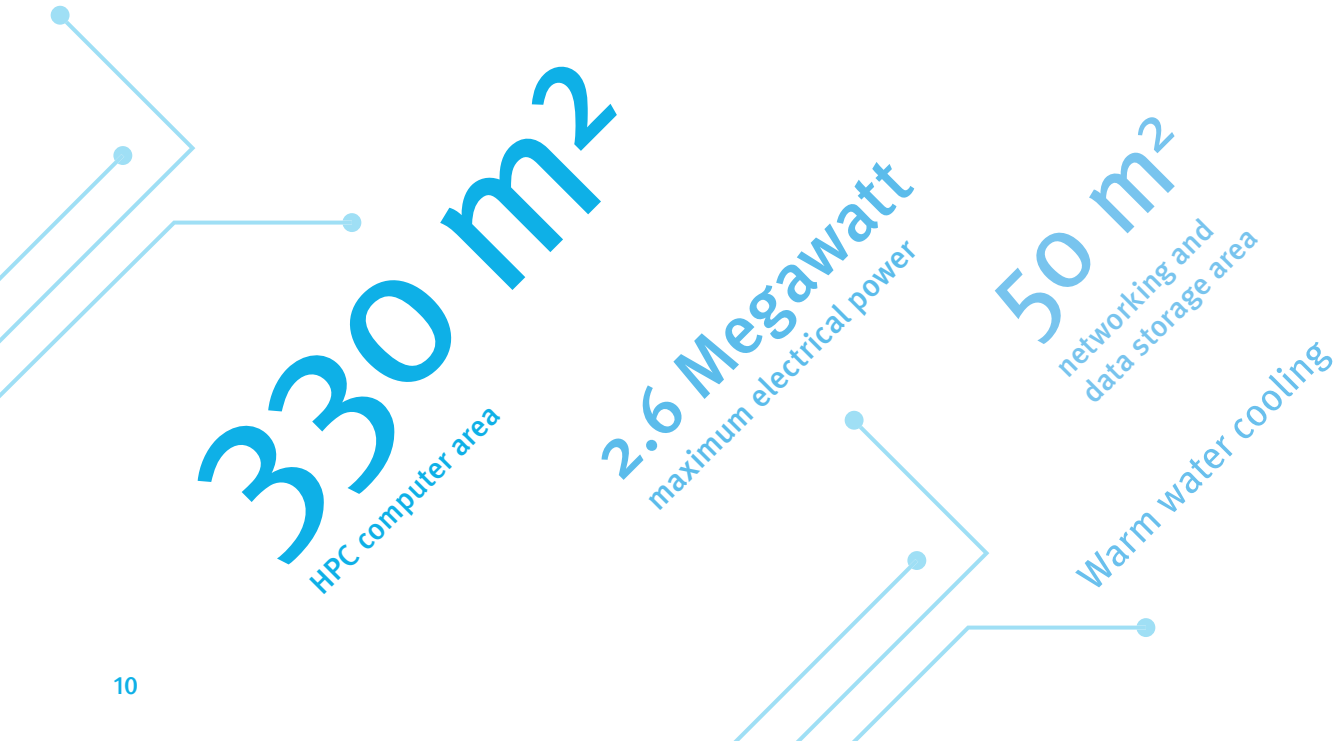
engineered in close cooperation with computational scientists. This infrastructure will be used to study the potential of FPGAs for energy-efficient scientific computing, enabling PC² to maintain its leading role in establishing this technology in HPC.

HPC DATA CENTER BUILDING X

The construction of the HPC data center is scheduled to be begin in 2019 and will be completed in early 2021. The building is located at Mersinweg (Building X) and will consist of two integrated parts, the computer center and two levels of office space and learning areas.

The design goals of our new data center are environmental sustainability, low total cost of ownership, and flexibility to support future HPC systems. To achieve best of class energy efficiency, we will remove a very large fraction of the heat dissipated by the HPC systems using warm water cooling with a flow temperature of approximately 35°C. Considering the climate in Paderborn, we can use extremely efficient, compressor-free cooling almost all year round. An auxiliary compressor cooling system with lower capacity is available to supply cold water for conventional air-cooled IT components, such as storage systems, and to support the free cooling system during the hottest hours of the year. All major components of the cooling facilities are implemented with an N+1-redundancy. The high temperature water from the return flow will be used for heating the rest of the building and a neighboring building. The main power supply is also

SPECIFICATION FOR THE COMPUTING CENTER



optimized to strike a good balance between energy efficiency, cost and availability, by using an N+1-redundancy uninterruptible power supply backed up by an emergency diesel engine generator only for central components of the HPC system and facility infrastructure. To enable our computer center to adapt to the presently unknown operating conditions for the future, we have partitioned the whitespace into three logical segments, which can be independently configured to different temperature levels. Two segments are always usable for the productive HPC system during regular operation. The third segment is available to build up the first stage of a successor system, which may use different temperature levels. The building is designed also with extensibility for the technical infrastructure in mind by providing spare rooms for installing equipment for increasing the capacity of cooling and power supply, and even office space by adding up to two additional floors to the office wing. A direct network connection will enable us to jointly use the existing facilities in building O from the new data center.

NOCTUA STAGE 2

The second stage of the Noctua HPC system is planned to be installed in 2021, closely following on from the end of the construction of the HPC data center building X. This implies that the procurement process has to start in early 2020. In the time before, the final configuration of the HPC system must be balanced between actual user requirements and technical opportunities.

SPECIFICATION FOR THE OFFICE PART OF THE BUILDING

190 m²
Teaching and seminar rooms, student lab, social rooms

60 m²
Data center control room and IT workshop

300 m²
15 offices (1–3 pers. per office)

REPORT FROM THE RESOURCE ALLOCATION BOARD

Computing time on our HPC systems is allocated by the Resource Allocation Board for a period of 12 months based on a technical examination and, for large projects, a scientific evaluation by external reviewers. Applications for small projects can be submitted at any time and are continuously evaluated. There are two calls for proposals per year for large projects.

In the most recent call 2019-1, the Resource Allocation Board awarded 156 million core-hours to 59 computing projects. In total, 13 large and 46 small projects were approved including 19 external projects from principal investigators not affiliated with Paderborn University.

The supported projects are predominantly from the domains of condensed matter physics, physical chemistry, electrical and mechanical engineering and computer science. The call in April 2019 was the first call where users could apply for resources on our new Noctua system. 21 projects have been allocated 80 million core-hours on this system alone. Three projects have been assigned 10 million or more core-hours on Noctua:

- **Condensed matter physics:**
  "Photonic materials from ab-initio theory"
  with 17 million core-hours on Noctua

- **Physical chemistry:**
  "DFTB calculations on water catalysis"
  with 14.4 million core-hours on Noctua

- **Computer science:**
  "On-the-fly machine learning"
  with 9.9 million core-hours each on
  Noctua and on OCuLUS

We were very pleased to have received so many high-quality proposals from a large variety of different scientific disciplines and institutions. Particularly encouraging is that 7 projects using FPGA resources will be funded. This indicates the emerging interest for this accelerator technology which is a key competence of our center. We have also seen a steeply increasing interest in GPUs confirming the trend to use accelerators and which is something we will consider for future HPC system procurements.

Prof. Dr. Thomas D. Kühne
Chairman of the Resource Allocation Board

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 – for Tier 2 workloads – also nationwide. The system administrators and technical advisers employed by PC² support researchers to be able to utilize the HPC systems effectively and provide guidance with porting and optimizing their scientific codes.

The current main HPC system is the 10,000-core Noctua cluster which was put into operation in 2018. In addition, PC² operates smaller, subsidiary HPC systems which are either dedicated for specific research projects or are customized to support workloads which do not suit the Noctua cluster, such as GPU-based computing, cloud or throughput computing applications.

An overview of the main computing systems which have been in operation in the reporting period is shown in the tables below. The research systems are presented in the article “FPGA Infrastructure”.

COMPUTING SYSTEM ACCESS

Academic users from North Rhine-Westphalia can apply for free of charge access to all publicly available systems. Researchers from other states of Germany can only apply to the Tier 2 system. Computing time on the HPC systems is allocated by the Resource Allocation Board for a period of 12 months. Users can apply for large projects (› 2 million core hours) twice per year with proposal submission deadlines in March and September. Applications for small projects can be submitted at any time.

Access to dedicated purpose systems can be granted on a case by case basis. Commercial users are also welcome but may have to pay a fee for using the systems.

ADDITIONAL TECHNICAL INFORMATION AND APPLICATION FORMS

Additional technical information regarding the HPC infrastructure, installed software, access to the systems, computing time application forms and the current call for proposals can be found in the “HPC Services” section of the PC² website.

PRODUCTION SYSTEMS

NAME/ PURPOSE	SUPPLIER	YEARS OF OPERATION	NUMBER OF NODES	NUMBER OF CORES	MEMORY PER NODE	PROCESSOR TYPES	INTER-CONNECT
Noctua **Tier 2 System** **Main HPC System**	Cray	Since 2018	272	10,880	192 GIB	Intel Xeon Gold 6148 FPGA Accelerators	Omni-Path 100Gbps Direct FPGA interconnect 4x 40 Gbps
OCuLUS **Tier 3 HPC System** **Subsidiary HPC demand**	Cluster Vision	Since 2013	616	9,920	64 GIB, 256 GIB, 1 TIB, 4 TIB	Intel Xeon E5-2670, Intel Xeon E5-4670 GPU Accelerators	InfiniBand QDR
Arminius+ **Subsidiary HPC demand**	Fujitsu	2010–2018	60	720	36 GiB	Intel X5650 2.67 GHz	InfiniBand QDR
High Throughput Cluster	Various	2009–2018	–	~ 650	Up to 8 GiB	Intel or AMD x86-64	1 Gbps Ethernet
OpenStack Cloud	Teuto.net	Since 2016	4	64	256 GiB	Intel Xeon E5-2640v3	10 Gbps Ethernet

FILE SYSTEMS

TYPE	MANUFACTURER	YEARS OF OPERATION	CAPACITY	PROTOCOLS	AVAILABLE ON
Network Attached Storage	Isilon	Since 2009	200 TB	NFS, CIFS	All systems
Parallel File System	BeeGFS	Since 2013	500 TB	BeeGFS	OCuLUS
Parallel File System	Lustre	Since 2018	720 TB	Lustre	Noctua

FACTS AND FIGURES

ca. 40
Preinstalled HPC Software Applications

750 TFlop/s
Linpack Performance

ca. 80
User Projects

1.4 PByte
Mass Storage Capacity

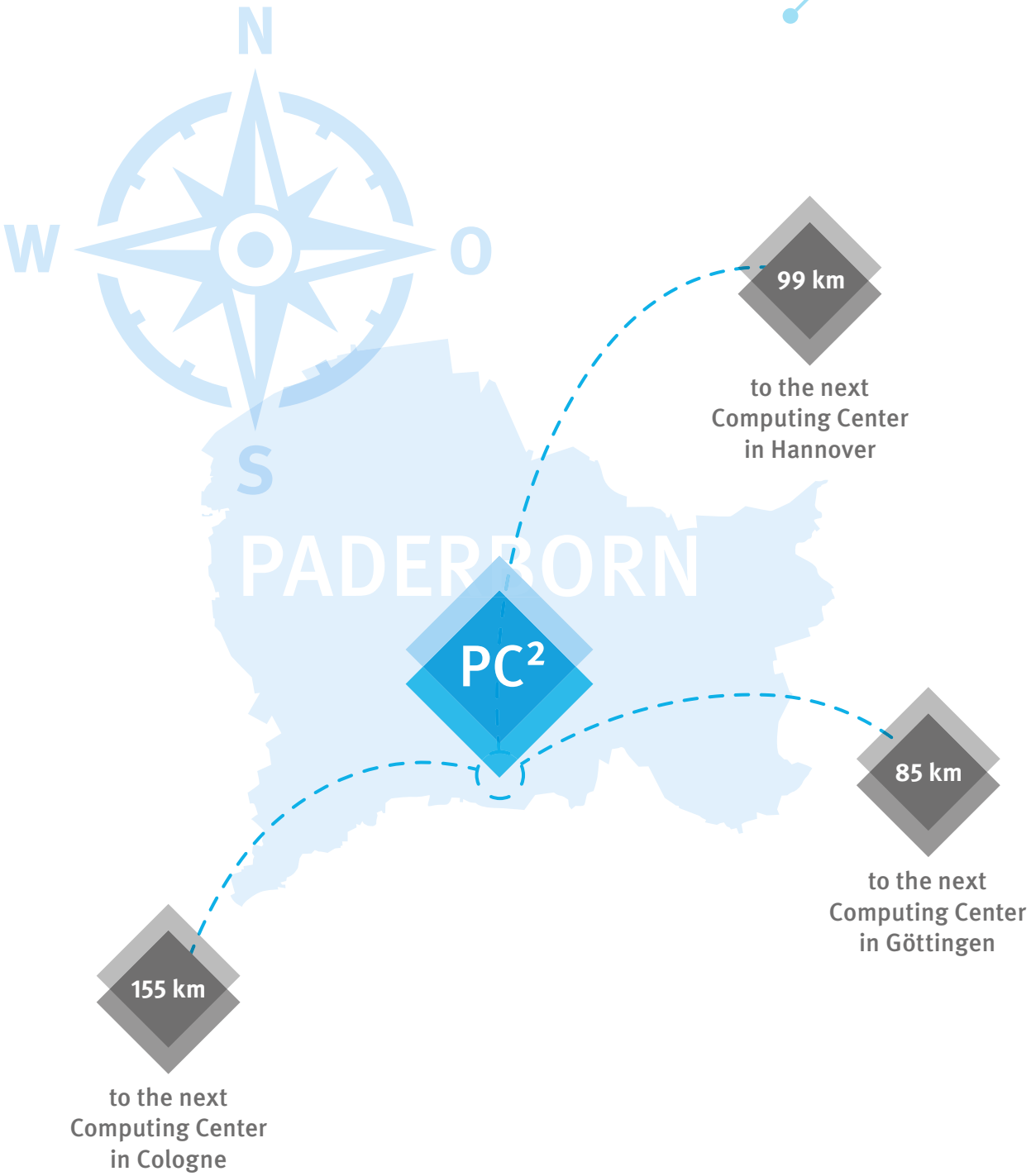
22,000
Processor Cores

952
Cluster Nodes

49
GPU Accelerators

100 TByte
Main Memory

58
FPGA Accelerators


N
W
O
S
PADERBORN
PC²
99 km
to the next
Computing Center
in Hannover
85 km
to the next
Computing Center
in Göttingen
155 km
to the next
Computing Center
in Cologne

BOARDS AND EMPLOYEES

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 June 2019.

Prof. Dr. Michael Dellnitz
Department of Mathematics

Prof. Dr. Jens Förstner
Department of Electrical Engineering

Dipl.-Inf. Axel Keller
Paderborn Center for Parallel Computing
Representative of technical and administrative personnel

Dr. Tobias Kenter
Paderborn Center for Parallel Computing
Representative of scientific personnel

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

Oliver Kruse
Student representative

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)

Prof. Dr. Marco Platzner
Department of Computer Science

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

Prof. Dr. Wolf Gero Schmidt
Department of Physics

Dr. Jens Simon
Paderborn Center for Parallel Computing
Representative of scientific personnel

Prof. Dr. Andrea Walther
Department of Mathematics

ADVISORY BOARD

The PC² management board is supported by an advisory board in order to promote its trans-regional character. The advisory board is filled with representatives of science, industry and ministerial administration, providing professional insight for strategic decisions.

Dr. Christoph Hagleitner
Manager Accelerator Technologies
IBM Research Zurich, Switzerland

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

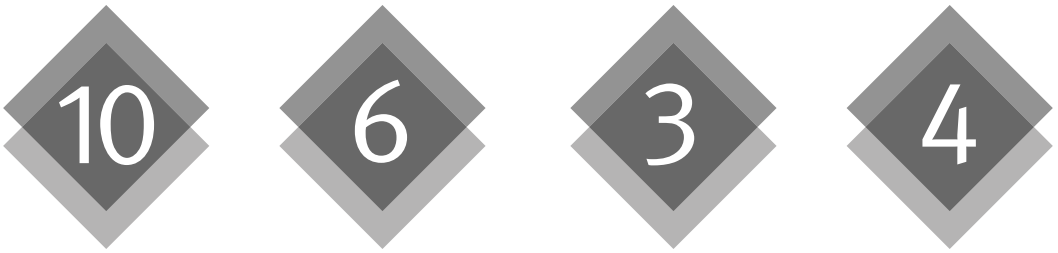
Prof. Dr. Alexander Reinefeld
Scientific Director
Zuse Institute, Berlin, Germany

Marie-Christine Sawley, PhD
Director Exascale Computing Research Lab
Intel, Paris, France

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

PC² STAFF

In the years 2017, 2018 and 2019, PC² employed



research associates

administrative and technical staff

trainees

students and graduate assistants

Dipl.-Inf. Bernard Bauer

Philipp Borkowski

M.Sc. Paolo Gorlani

Selina Dettmer

Dipl.-Inf. Axel Keller

Michaela Kemper

Dr. Tobias Kenter

Dipl.-Ing. Andreas Krawinkel

M.Sc. Michael Laß

Gopinath Mahale

M.Sc. Marius Meyer

Holger Nitsche

Prof. Dr. Christian Plessl

M.Sc. Arjun Ramaswami

M.Sc. Heinrich Riebler

Dr. Robert Schade

Dr. Jens Simon

M.Sc. Gavin Vaz

Marcel Wilkowksy

Nils Winnwa

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

Oliver Kruse

Maxim Ritter

Erik Messerli

Rushikesh Nagle

FPGA INFRASTRUCTURE – FROM RESEARCH TO PRODUCTION SYSTEMS

FPGA acceleration can provide performance gains and energy savings which are especially required in the HPC domain. FPGAs are still expanding quickly in terms of performance, mostly through area scaling, and there are a variety of PCIe-based FPGA accelerator cards available with dedicated memory and network connectivity. However, unlike GPUs, FPGAs are still novel territory for HPC vendors, which up to now requires special expertise to specify and operate HPC systems with FPGAs.

PC² has a unique background regarding FPGA research and operations in the German HPC landscape and beyond. During recent years, multiple generations of state-of-the-art HPC systems which are specifically tailored to FPGA acceleration have been, or are still, operated at PC² (reference to list on extra page). On top of ever-increasing capacity of the FPGAs, these systems provided practical experience with different development flows, system level integration of the FPGAs and, more recently, also multi-FPGA operations.

With the installation of Noctua, PC² was the first academic institution to receive Stratix 10 FPGAs in production quality and volume. In contrast to the previous FPGA research systems, the 16 FPGA-nodes, each with two BittWare 520N cards, are now available to all HPC users of PC² that can make use of FPGA acceleration. The system is a consequent step forward in terms of individual and aggregate FPGA performance, with only the DSP blocks delivering up to 32 x 10 TFLOPs of single precision compute throughput. Scalability over multiple FPGAs is supported by a unique direct interconnect topology which was implemented on top of the system setup which was procured from Cray. OpenCL was selected as the FPGA development flow which is currently best suited for the HPC community and appropriate integration with the workload manager enables users to retain FPGA bitstreams in production while new tool versions are deployed. In the next sections, we will look at workload manager integration, interconnect and programming support in more detail. Two projects which make special use of that infrastructure are presented in the “User Projects” part of this report.

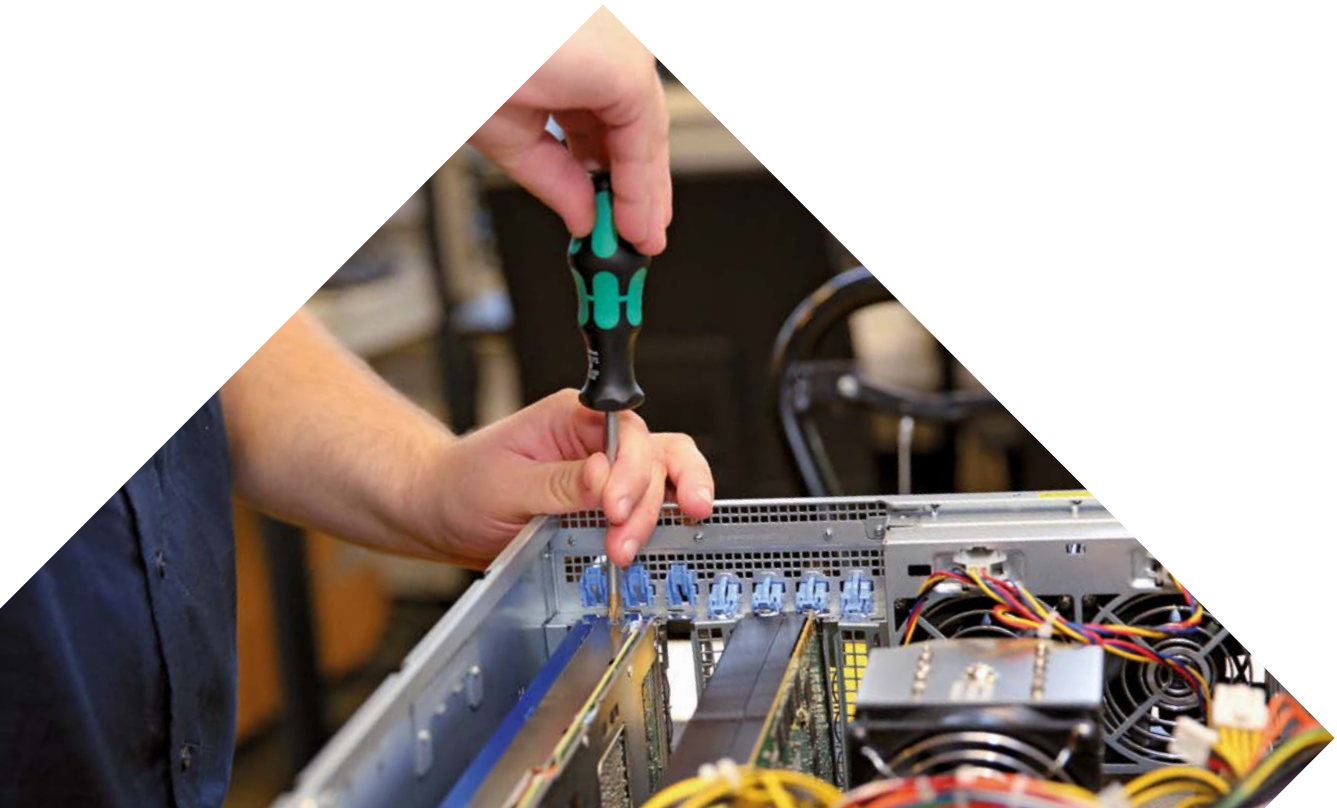
ON DEMAND VERSION CONFIGURATION OF FPGA NODES

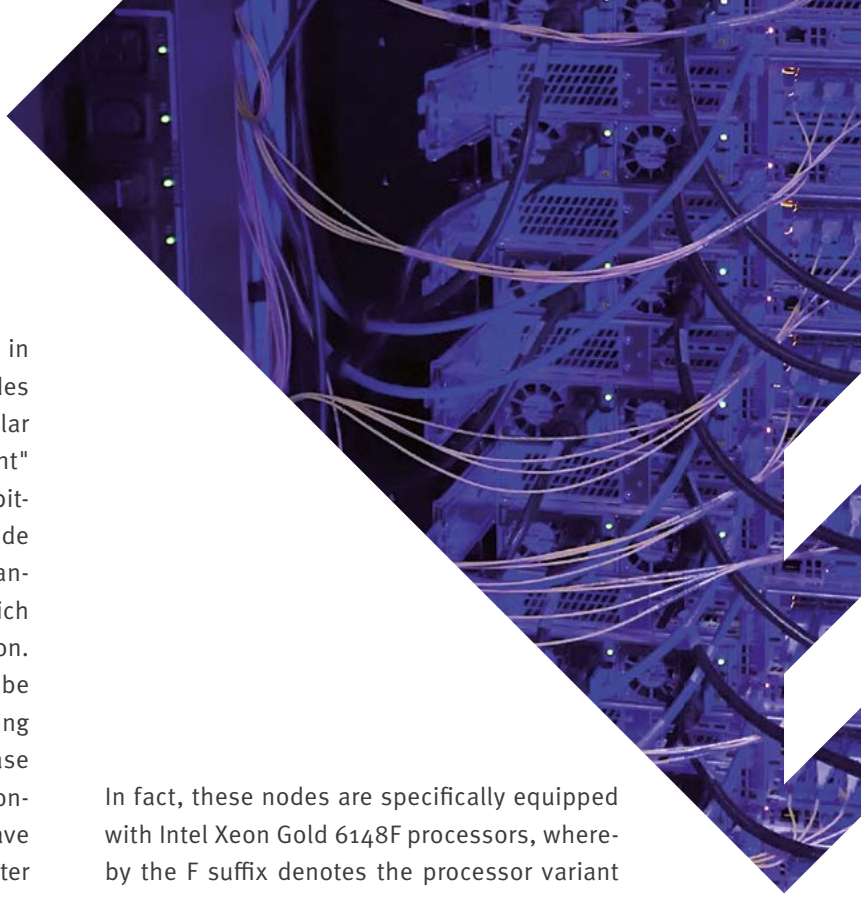
From our experience with previous FPGA systems, we have identified two requirements for a production system: regular tool updates and the ability to run designs created with previous tool versions. The OpenCL tool chain is still progressing on both ends, the high-level syn-

thesis (HLS) step which translates the OpenCL code to a design in hardware description language (HDL) and the back end flow which maps the HDL design to the physical FPGA resources. The HLS step has been actively evolving with new features and optimizations over the last years and will continue to do so, while the backed synthesis received large amendments for the Stratix 10 architecture and is now undergoing a lot of fine tuning. It is therefore of paramount importance that we receive regular updates and can thereby make them available to all users. Generally, OpenCL designs are source compatible with new tool versions, but since it takes many hours to compile a bitstream with a specific tool version, the capability to reuse existing bitstreams beyond the tool update cycles is highly desirable. This capability is also important for reproducibility of results, just like when using specific compiler versions when compiling HPC codes for comparisons.

In order to use a bitstream which was created with a specific tool version, the FPGAs need to be configured with a matching firmware, a so-called base bitstream. This base bitstream implements the communication with the host CPU via PCIe, provides access to the DDR memory of the FPGA card, and enables quick configuration for the accelerator bitstreams by utilizing partial reconfiguration at program runtime. Finally, the software drivers matching the tool version need to be loaded after the base bitstream is configured.

The solution which was planned during the negotiation stage for Noctua procurement and





implemented during the system installation in collaboration with Cray and BittWare provides this functionality integrated with the regular Slurm workload manager. With a "--constraint" argument, the user specifies which base bitstream and tool version the allocated node or nodes should provide. The workload manager will initially try to allocate nodes which already provide the requested configuration. If this is not possible, then other nodes will be allocated and, transparently to the requesting user, will be configured with the required base bitstream, rebooted to bring up the PCIe connection with the correct settings, and have the matching drivers installed. Therefore, after a few minutes, the allocation request can be served with freshly configured nodes. From the first year of preparation, installation and operation of Noctua, five different variants of base bitstreams and tools are already available in this way. For the next years, two to three updates per year are expected.

DEDICATED FPGA INTERCONNECT

With FPGAs arriving in the HPC domain, scaling of FPGA accelerated codes will become just as important as their contributions to single node performance and efficiency. The conventional approach to integrate accelerators like GPUs into HPC systems are PCIe cards which rely on the host and its networking infrastructure to communicate with other nodes and accelerators. The Noctua FPGA nodes fully support that approach using Intel Omni-Path as high speed network technology which integrates them uniformly with the rest of the Noctua system. In fact, these nodes are specifically equipped with Intel Xeon Gold 6148F processors, whereby the F suffix denotes the processor variant with integrated Omni-Path connectivity, in order to still provide full x16 PCIe slots for both FPGA cards. Applications which offload a part of the node-local calculations to the FPGAs can use this infrastructure to scale up to 16 nodes or 32 FPGAs.

However, FPGAs are also well suited for a more direct integration into high-speed networks. The selected BittWare 520N cards provide four QSFP+ network ports. When connected via electrical or optical QSFP+ pluggable transceivers to another such port on a different FPGA card, the two ports create a direct 40 Gbps point-to-point link which can be used from inside the OpenCL accelerator code. The simple serial transmission through these channels suits the pipelining and data streaming concepts for FPGAs very well and is even frequently used inside single-FPGA designs to exploit task-level parallelism. Hence, with a suitable topology of such serial links, applications can scale over multiple FPGAs without ever requi-

ring latency intensive communication via the hosts. The FPGA nodes, as installed by Cray, provide full physical access to all QSFP+ network ports of every FPGA card but were not procured with an inter-FPGA network. Hence, specific inter-FPGA network topologies have to be created by physical wiring of network ports, which raises the question for which topology should be set up and how to handle cases when a user job only allocates a part of the topology.

A highly flexible solution to support arbitrary topologies was added with the installation of a Calinet 320S Optical Circuit Switch in the first half of 2019. All FPGA ports are now physically connected with 40 Gbps links to the optical switch which serves as a protocol-free and transparent connection layer. Along with a job request, a user can now request any interconnect topology for FPGA-to-FPGA connections and the workload manager will, along with the node allocation, establish the requested connections through the optical switch. With this setup of configurable connections, additional research on the FPGA interconnect can continue without interfering with production jobs which depend on the presence of specific topologies.

Allocating Configured FPGA Nodes and Interconnect Topology

By requesting a node in the FPGA partition with the constraint 19.1.0, the base bitstream and driver for the Intel FPGA SDK for OpenCL 19.1.0 will be provided for this job.

```
srun --partition=fpga --constraint=19.1.0 ./fpga_application
```

When additionally requesting pairwise connections for the FPGA interconnect, the FPGA application on this node can use all four serial channels of one FPGA card to communicate to the respective channels of the other FPGA card.

```
srun --partition=fpga --constraint=19.1.0 --fpgalink="pair" ./fpga_application
```

When multiple nodes, here 16, are allocated, then the user can request direct FPGA connections which create a topology, here a 2D torus, which connects all FPGAs in the selected nodes. In addition to predefined topologies, a job request can also specify every possible individual connection between any of the allocated FPGA cards.

```
srun --partition=fpga --constraint=19.1.0 --nodes=16 --fpgalink="torus" ./fpga_application
```

More details and examples can be found in our technical support wiki.

OVERVIEW OF FPGA PRODUCTION, TESTBED AND RESEARCH SYSTEMS

SYSTEM	OPERATION	CPU	FPGA	TOOLFLOW	FEATURES
PRODUCTION SYSTEMS					
Noctua (Stage 1)	Since 2018	Xeon Gold 6148	Intel Stratix 10 GXG2880	Intel OpenCL	16-nodes each with 2 BittWare 520N cards
TESTBED SYSTEMS					
HARP	Since 2017	Intel BDW+FPGA multi-chip module	Intel Arria 10 GX1150	Intel OpenCL, HDL, OPEA	10-node cluster with 1 BDW+FPGA processor per node
XCL	Since 2017	Xeon E5-1630v4	Xilinx Virtex-7 VX690T + Xilinx Kintex Ultrascale KU115	Xilinx OpenCL	8-node cluster with 2 FPGA cards per node (AlphaData ADM-PCIE-7V3 and ADM-PCIE-8K5)
RESEARCH SYSTEMS					
Micron/Pico Workstation	Since 2016	Intel i7-5930K	Xilinx Kintex Ultrascale KU115	Xilinx OpenCL	FPGA board with Hybrid Memory Cube
IBM S812L	Since 2016	10-core POWER8	Xilinx Virtex-7 VX690T	HDL + CAPI interface	PCIe-attached FPGA card with cache-coherent memory interface
Generic x86 Workstation	Since 2016	Xeon E5-1620 v2	Intel Arria 10 GX1150	Altera OpenCL toolflow	PCIe-attached FPGA card
Generic x86 Workstation	Since 2015	Xeon E5-1620 v2	Xilinx Virtex-7 VX690T	Xilinx OpenCL toolflow	PCIe-attached FPGA card
Maxeler MPC-C	Since 2012	Xeon X5660	Xilinx Virtex-6 SX475T	MaxJ spatial programming language	4 PCIe-attached FPGA cards, MaxRing FPGA interconnect
Convey HC-1	2010-16	Xeon 5138	4x Xilinx Virtex-5 LX330	HDL and existing firmware (personalities)	CPU and FPGA attached via FSB, cache-coherent NUMA
Nallatech SlipStream	2008-10	Xeon 7300 MP	Xilinx Virtex-5 LX110T	HDL	CPU and FPGA attached via FSB
XtremeData XD1000	2006-12	Opteron	Altera Stratix II EP2S180-3	HDL	CPU and FPGA attached via HyperTransport

PROGRAMMING AND SUPPORT

In order to make use of FPGA acceleration, performance critical parts of an application must either be ported to the FPGA or use a library that uses FPGA functions. In both directions, PC² is collaborating in projects with code developers among the users. In the HighPerMeshes project presented later in this report, core parts of complete applications are implemented for FPGA execution and we are working on code generation from a domain specific language. For the CP2K software, FPGA acceleration for frequently used functions like 3D-FFT calculations has been, and is being, developed with a library approach. These projects make use of an OpenCL based toolflow, which is also available for all other users and code owners on our systems.

OpenCL is a host API and C-like accelerator programming language which was originally developed for GPUs. It provides structures for data parallelism and local memory which are also beneficial for mapping algorithms to FPGAs. With the Intel FPGA SDK for OpenCL and other OpenCL compilers targeting FPGAs, it is now easier than ever before to functionally port codes to FPGAs. The functionality can quickly be verified through emulation. The required platform integration with memory controllers, host synchronization and DMA transfers via PCIe and, in our case, serial point-to-point connections is provided through the base bitstreams and can be readily used from OpenCL accelerator code.

In order to profit from offloading to FPGAs, the key is not only functionality, rather also creating a design which exploits the strengths of FPGAs in order to achieve good performance. This part remains challenging also with OpenCL based toolflows. To provide support with usage of the FPGA infrastructure and particularly with performance optimization, in October 2018 Dr. Tobias Kenter took over the role of advisor for FPGA acceleration in PC². In addition to consulting and support for FPGA acceleration on an individual basis, we also organize tutorials on FPGA development for our systems, like in September 2018 by FPGA consulting company El Camino in Paderborn with a two day introduction course, in March 2019 by Tobias Kenter at DATE conference with a focus on comparison between Intel and Xilinx tools, and in May 2019 in Paderborn by Bill Jenkins (Intel) on development flows beyond OpenCL.

DR. TOBIAS KENTER, DOMAIN EXPERT AND CONSULTANT FOR FPGA ACCELERATION

Tobias Kenter received his PhD from Paderborn University in 2016 on the topic of productivity for FPGAs through overlays, compilation approaches and tight coupling between FPGAs and CPUs. Since then he has focused on OpenCL based FPGA development for his research and also for teaching and dissemination. He was involved in the concept, procurement and set-up of the FPGA nodes in Noctua with the goal to make them as user friendly as possible. As PC² HPC consultant for FPGA acceleration, he strives to bring more applications to this exciting technology.

COMPUTATIONAL QUANTUM CHEMISTRY AT PC²

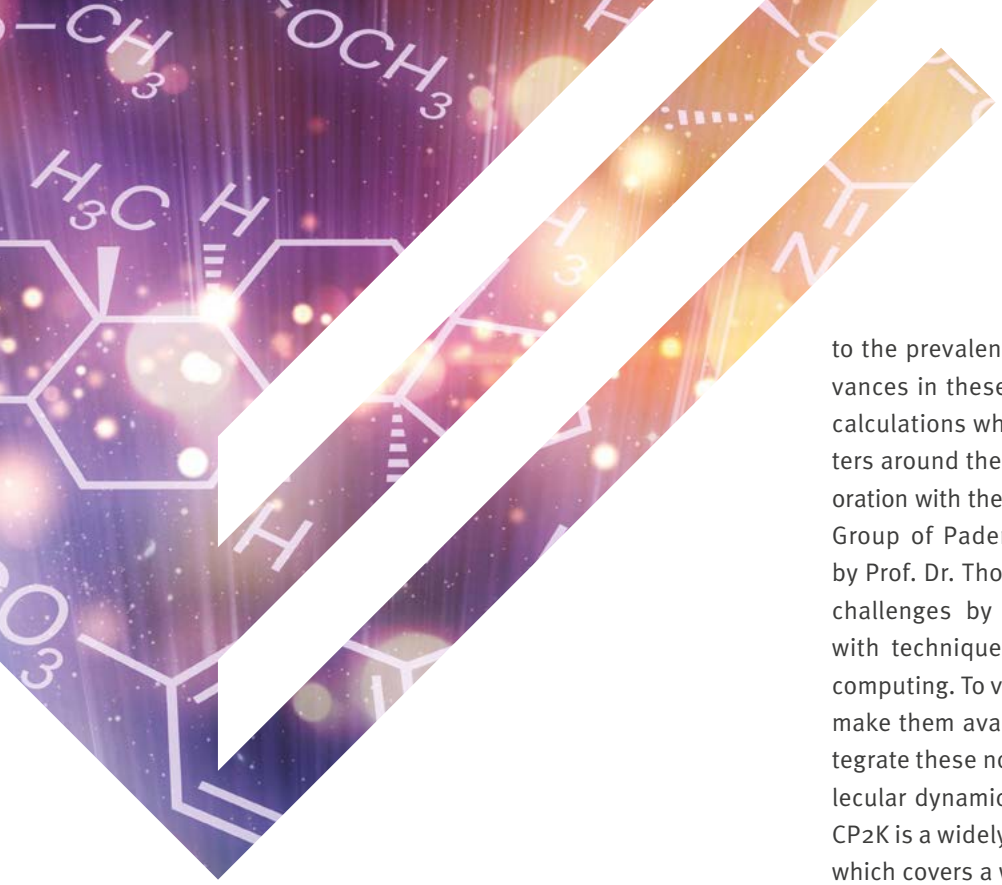
Applications from computational quantum chemistry and condensed-matter physics nowadays dominate the consumed compute time at many high-performance computing centers, which is also the case for PC². The reasons for this high demand are the wide applicability of these ab-initio simulations and the computational complexity of the underlying methods. Ab-initio simulations are highly valuable in order to understand the fundamental physical processes and chemical reactions. Also, many practical applications, such as the development of new or improved materials and technological processes for tackling challenges in areas like battery technology, photovoltaic energy conversion, or energy efficiency require large-scale ab-initio calculations.

The term “ab-initio” or, equivalently, the term “first principles” refers to the goal to only rely on basic laws of nature without including assumptions or experimental measurements. The main modeling method for these ab-initio calculations is density-functional theory (DFT) [1,2]. If also the classical motion of nuclei is considered, then these calculations are called ab-initio molecular dynamics (AIMD) simulations. Path-integral molecular dynamics (PIMD) simulations exceeds the quality but also the numerical cost of AIMD by even treating the nuclei as quantum-mechanical particles.

COMPUTATIONAL ASPECTS OF DFT

The high computational demand of DFT has multiple causes. Fundamentally, the conventional DFT method requires solving an eigenvalue problem, which scales cubically with the number of atoms. That is, the required computational cost increases by a factor of eight when the number of atoms in the system is doubled. Due to this unfavorable algorithmic complexity, only systems with a few hundred atoms can be simulated with conventional DFT algorithms.

Additional refinements or extensions additionally increase the computational demand. For example, for determining many physical properties, computing the solution of a static configuration of atoms is insufficient. Instead, the atomic motion needs to be considered which is achieved by computing the movement of atoms in many small time steps. The computational effort thereby becomes proportional to the length of the simulated time and time step. Additionally, basis sets of different quality can be selected for representing the electronic wave functions. Last but not least, it is also possible to implement more complex and thereby more accurate approximations of the electronic interactions like local and semi-local functionals or hybrid functionals which include some portion of exact exchange.



Hence, the properties of a DFT calculation must be carefully selected so that the desired physics of the system is properly described but the calculation remains feasible with the available computational resources and time. The scalability of DFT calculations in different dimensions such as system size, time span, or basis set quality makes them very suitable for large-scale high-performance clusters and exascale efforts.

ALGORITHMIC DEVELOPMENTS FOR DFT AT PC²

The DFT-related work at PC² is focused on accelerating and improving the energy efficiency of the AIMD simulation of very large systems. This application scenario is motivated by the workload of our HPC systems. However due to the prevalence of DFT calculations, any advances in these directions will also make DFT calculations which are performed at HPC clusters around the world more efficient. In collaboration with the Dynamics of Condensed Matter Group of Paderborn University, which is led by Prof. Dr. Thomas D. Kühne, we tackle these challenges by accelerating DFT calculations with techniques of approximate and custom computing. To validate our contributions and to make them available to the community, we integrate these novel methods into the CP2K molecular dynamics code (http://www.cp2k.org). CP2K is a widely-used open-source application which covers a wide range of methods, such as classical molecular dynamics, ab-initio molecular dynamics, PIMD and others. The Dynamics of Condensed Matter Group at Paderborn University, together with the Department of Chemistry at the University of Zurich, are the main driving forces behind the development of CP2K. A significant percentage of the compute time on our new Noctua system has also been granted to projects which use CP2K.

Most of the large-scale linear algebra performed in CP2K is delegated to the DBCSR sparse-matrix library (Distributed Block Compressed Sparse Row Matrix library, https://www.cp2k.org/dbcsr). This library was formerly a part of CP2K but is now developed more independently to enable using the important advances such as the very efficient matrix-matrix multiplication algorithm or the included acceleration with GPUs also in other programs. Where appropriate, we incorporate our results in DBCSR in order to make our implementation efforts available also for uses beyond CP2K.

During the reporting period, we have contributed to the development of methods for quantum chemistry in four areas:

1. Iterative algorithms for linear-scaling DFT,
2. massively parallel algorithm for approximate matrix functions (Submatrix Method),
3. acceleration of Fast Fourier Transforms with FPGAs, and
4. approximate computing for efficient calculations with reduced-precision arithmetic,

which we will summarize in the following.

ITERATIVE ALGORITHMS FOR LINEAR-SCALING DFT

The previously mentioned cubic scaling of conventional DFT techniques hinders the simulation of large systems. To address this problem, several linear-scaling DFT approaches have been developed, whose computing time grows only linearly with the number of atoms. In linear-scaling DFT calculations, one important operation is the computation of inverse roots of matrices. For example, when using non-orthogonal basis functions, such as Gaussian-type orbitals, the inverse root $S^{-1/2}$ of the overlap matrix S must be computed during the calculation to compensate for the overlap of basis functions. Other approaches require the computation of the matrix-sign function $\mathrm{sign}(A) = A(A^2)^{-1/2}$ during the DFT self-consistency cycles. To prevent the cubic complexity of computing inverse square roots of dense matrices, methods with linear complexity which exploit the sparsity of the matrices are required.

In collaboration with Dorothee Richters (Johannes Gutenberg University of Mainz), Andrea Walter (Institute of Mathematics, Paderborn University) and Thomas D. Kühne (Department of Chemistry, Paderborn University) we have developed a general iterative algorithm for computing the inverse principal p-th root of a symmetric positive definite matrix [3]. The iterative algorithm enables us to compute an approximate solution, which further reduces the computational effort compared to an exact solution. We have recently included this new technique in the CP2K code together with new higher orders of iterative algorithms based on Padé approximations for the matrix-sign function.

MASSIVELY PARALLEL ALGORITHM FOR APPROXIMATE MATRIX FUNCTIONS (SUBMATRIX METHOD)

To advance the development of linear-scaling DFT methods, we have recently derived the submatrix method [4] in collaboration with Stephan Mohr (Barcelona Supercomputing Center), Hendrik Wiebeler and Thomas D. Kühne (Department of Chemistry, Paderborn University). This highly parallelizable method enables the approximate computation of matrix functions such as p-th order roots and the sign function for very large but sparse matrices. The schematic idea of the method is outlined in the infobox.

Although only approximate solutions of matrix functions can be obtained with the original submatrix method, we have recently generalized

it to a series of approximations which systematically converge to the exact solution.

The dimension of the matrices, for which we have to calculate matrix functions in DFT, is proportional to the number of atoms. The decomposition of the matrix functions which act on the whole large sparse matrix into evaluations of matrix functions of much smaller and dense submatrices will therefore enable the acceleration of these operations with FPGAs and GPUs. Especially FPGAs are promising candidates to offload not only individual matrix-matrix multiplications but the evaluation of whole iterative algorithms for matrix functions. The fact that these matrix function only have to be evaluated for small dense matrices also reduces the communication effort between compute nodes and mediates the bottleneck due to the rather slow PCI Express interface between the CPU and accelerators such as FPGAs.

The efforts for including the submatrix method into DBCSR in an efficient way are ongoing.

ACCELERATION OF FAST FOURIER TRANSFORMS WITH FPGAS

Fast Fourier transforms are used in DFT, for example for plane-wave grids or for the efficient evaluation of Ewald summations. A prototype for FPGA-accelerated three-dimensional FFTs was developed by a PC² member in his Master's thesis [5]. This implementation has recently been generalized with a generic and flexible interface for offloading FFTs to FPGAs. This interface has been merged into the development version of CP2K and is scheduled to be included in the next major release.

One future goal is to develop a widely parametrized and auto-tunable FFT implementation with configurable size, dimensions, and data types (real/complex, fixed-point, standard floating-point and custom floating-point). Since FFT is a kernel in many HPC codes, the resulting library will also be usable beyond CP2K and other DFT codes.

Submatrix method

The submatrix method [4] allows for the massively parallel calculation of approximate matrix functions for large sparse matrices. The method achieves this feat by constructing a submatrix for every column of the original large sparse matrix by deleting columns and corresponding rows which have vanishing elements in the column for which the submatrix is constructed. Hence, in the simplest variant of the submatrix method one obtains as many submatrices as columns in the original large matrix. One can then apply the matrix function, like the matrix sign function, inversion, or p-th order roots to the small submatrices. The final result matrix is obtained afterwards by reversing the initial construction procedure of the submatrices.

The sparse input matrix is divided into a set of principal submatrices that can be processed entirely independent of each other. For an N × N input matrix, the operation can be performed in parallel on N processors.

Each column induces its own principal submatrix. To construct the submatrix i, rows that are zero in column i, as well as their corresponding columns, are removed. The resulting submatrices are much smaller and more dense than the original input matrix.

The matrix operation of interest (inversion, sign-function, principial p-th root, etc.) is performed on each submatrix.

Each submatrix contributes one column to the result matrix. The elements from submatrix i that originated from column i of the input matrix are copied back to their original position. The result matrix exhibits the same sparsity pattern as the input matrix.

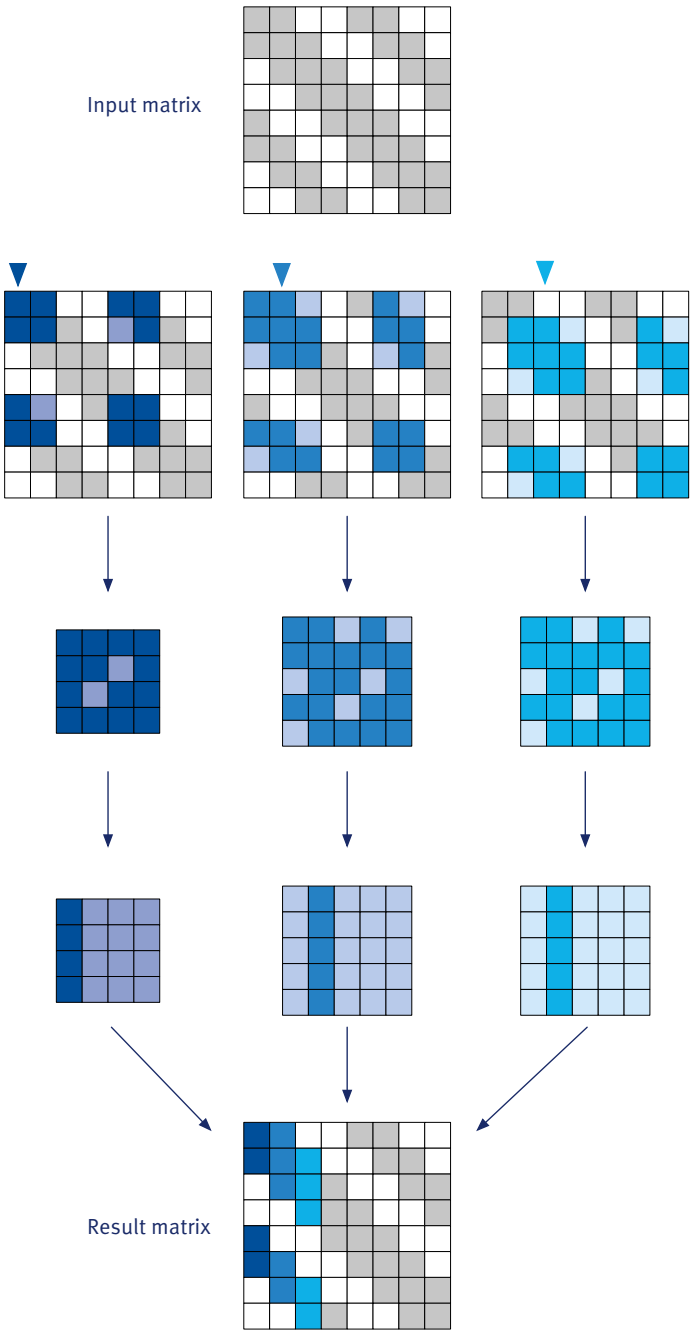


Figure: Schematic representation of the submatrix method from [4].

APPROXIMATE COMPUTING FOR EFFICIENT CALCULATIONS WITH REDUCED-PRECISION ARITHMETIC

Many emerging architectures like GPUs, tensor processing units, or FPGAs can perform arithmetic operations with low-precision number formats such as single (32 bit)/half (16 bit) precision or fixed-point formats much more efficiently than for 64-bit double-precision numbers. Applications which can tolerate the errors introduced by low-precision can thereby profit from substantially higher performance.

Fortunately, DFT calculations can be formulated to be resilient to many forms of numerical errors by exploiting the fluctuation-dissipation theorem. Using a modified Langevin formulation and treating numerical errors in force computations as noise, it is possible to perfectly compensate for the errors and compute a proper finite-temperature canonical ensemble for the atoms. The noise can, for example, be caused by computing FFTs or linear algebra in lower precision on accelerators or by other approximations such as the submatrix method. If the noise created follows a few statistical relations, then the fluctuation-dissipation theorem guarantees that the obtained finite-temperature statistical properties such as the kinetic-energy distribution and pair-correlation functions of atoms are correct within the underlying approximations in DFT.

We have recently shown [6] with the example of liquid silicon at a temperature of 3000 Kelvin that, in the above-described scheme, atomic forces with modeled fixed-point and floating-point noises accurately reproduce the pair-correlation functions of atoms.

DR. ROBERT SCHADE, SCIENTIFIC ADVISOR FOR THEORETICAL CHEMISTRY AND PHYSICS

Robert Schade received his Ph.D. from Georg-August University Göttingen in 2019 for the development of new methods for the ab-initio simulation of materials with strong local electronic correlations. In his Ph.D. work [7], Robert Schade developed a novel method for the description of strong local electronic correlations in solids based on reduced density-matrix functional theory (rDMFT). This work involved the combination of methods from quantum chemistry such as configuration-interaction-based methods, two-particle reduced density-matrix functional theory and variational Monte-Carlo methods with density-functionals in the framework of density-matrix functional theory for solids and molecules. His implementation of this new method in the CP-PAW code (www2.pt.tu-clausthal.de/paw, Clausthal Technical University) resulted in a successful description of homolytic bond breaking in small molecules and the isolating behavior of Nickel-(II)-oxide in the paramagnetic state. Both systems are not correctly described by common density-functional theory with approximate local or semi-local functionals due to the presence of strong electronic correlations. He has also designed a variant of this new method where the computationally heavy part can operate on a gate-based quantum computer. His proof-of-concept calcula-

tions eomploying existing quantum computers showed the merit of the new approach.

At PC², Dr. Schade is engaged in HPC-consulting for scientific users as well as general training of users to empower them to use the available compute resources in an efficient way. In the newly granted HPC competence network for North-Rhine Westphalia (http://hpc.nrw), he serves as the coordinator for the work package which considers the software environments and computer operation. His main research focus is on the design and implementation of new highly parallel algorithms for quantum chemistry and their acceleration with FPGAs.

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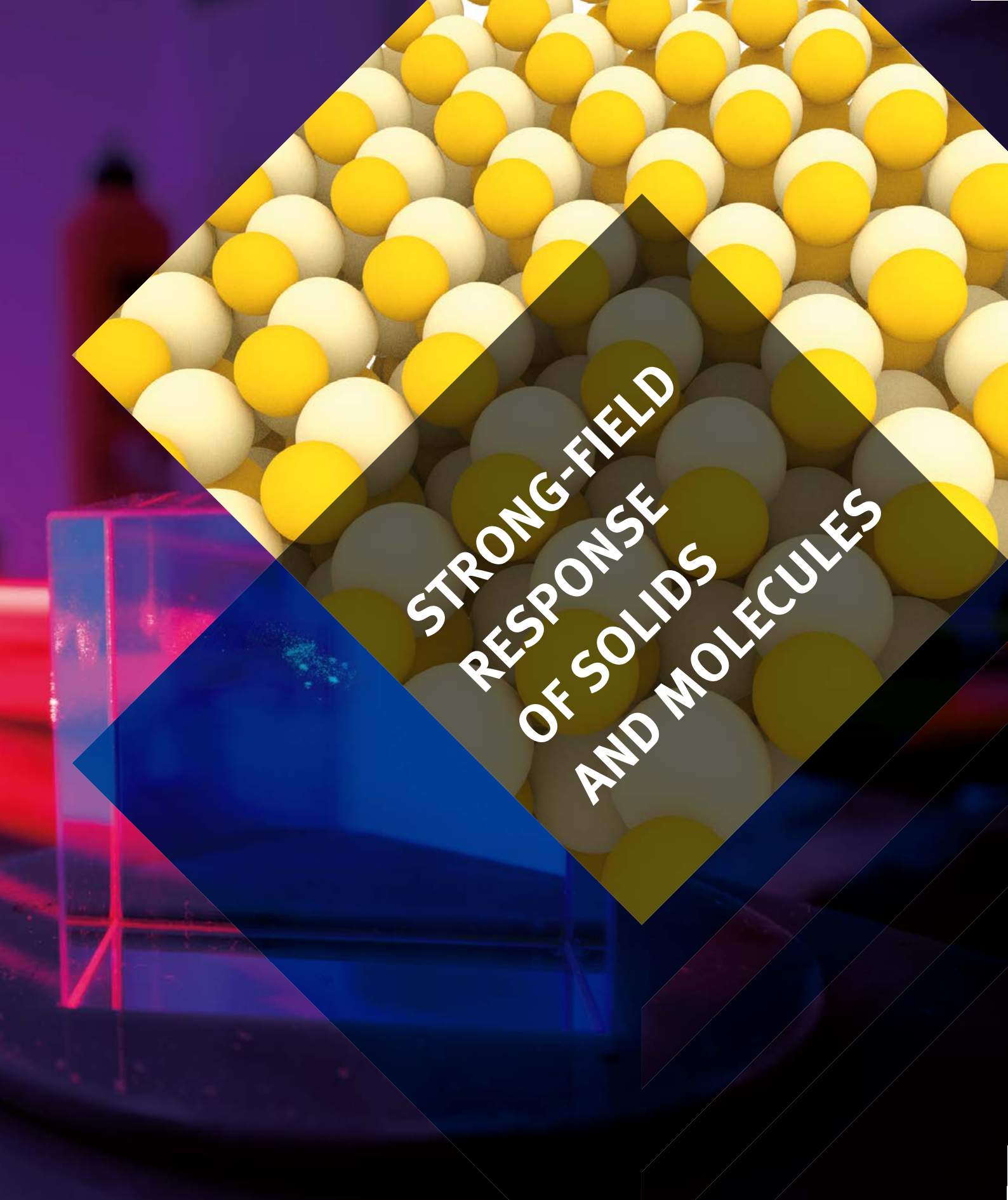
USER PROJECTS

USER PROJECTS

Our HPC systems and HPC user advisors provide computing resources and consulting for projects of a large number of researchers from Paderborn University, academic institutions in North Rhine-Westphalia, and nationwide. During the last allocation period, the use of Noctua and OCuLUS was instrumental for about 60 third-party-funded projects, e.g. projects with DFG-funding from SFB TRR 142, SFB TRR 75, SFB 1375, SFB 901, SFB 765, SFB 1073, FOR 2316, FOR 2457, FOR 2692, SPP 1962 and projects funded from BMBF, ZIM, BMWE, and the European Research Council.

To provide insight into the research of our users, we present three large projects that have been approved in the most recent allocation period in more detail and the remaining large projects with a briefer project overview. In addition to these large scale projects, our resources are also supplying computing time for a large number of projects with lower computing time demands, which are listed and grouped be research area to illustrate the complete spectrum of research enabled by our HPC systems.


STRONG-FIELD
RESPONSE
OF SOLIDS
AND MOLECULES

The interaction of light with matter covers a large number of physical phenomena which we literally see in our everyday life, as it is responsible (amongst other things) for the vision process. Early scientists mostly focused on investigations of electromagnetic radiation in the visible range ("Zur Farbenlehre" J. W. v. Goethe, 1810) and at low intensities, where material polarization responds linearly to incident electromagnetic fields. Although unknown at that time, quantum mechanical effects already resulted in measurable effects such as color alterations of stained glass (e.g. in church windows) when including gold nanoparticles of varying size.

With the advent of tunable, high-intensity light sources, the investigation of nonlinear effects, where the material polarization alters in a nonlinear fashion with electric field of incident light, became accessible.

The interactions of intense light and matter give rise to a plethora of interesting phenomena such as multiphoton absorption/ionization, four-wave mixing, sum and difference frequency generations, optical parametric amplification, laser induced electron diffraction [1,2] or second, third or higher-order harmonic generations.

Spectral signatures, however, become increasingly complex when investigating quantum systems and their dynamics in strong fields since the increasing importance of nonlinear effects requires careful theoretical description and examination. So far, most of our understanding of strong-field effects is based on the simplest atoms and molecules such as H_2 and H_2+ or simple model systems. [3,4]

This project aims at simulating and interpreting the strong-field dynamics of real molecules and larger systems in a rigorous real-space, real-time approach including non-linear strong-field effects such as photoionization and high-order harmonic generation (HHG) of systems ranging from small (chiral) molecules through nanosystems to the condensed phase. The project aims at advancing the theoretical description of light-driven dynamics of multi-electron systems. To this end, we will employ a state-of-the-art numerical description of the strong-field response of solids and molecules based on the real-time, real-space time-dependent density functional theory (rtTDDFT) as implemented in the Octopus program package. The numerical propagation of time-dependent Kohn-Sham orbitals, from which the time-dependent electron density is constructed, is executed in short (attosecond) time steps, typically requiring several ten-thousand consecutive propagation steps for covering a short excitation pulse of about 50–100 fs duration. This comprehensive microscopic description of light-matter interaction enables a detailed investigation of nonlinear effects such as high harmonic generation (HHG) or photo electron emission.

In an exemplary way, we present initial results of simulations of HHG from CdSe nanoparticles performed at Noctua PC² computer cluster. (Higher) harmonic generation is a process, in which atoms and molecules interacting with high intensity laser pulses emit radiation at frequencies which are multiples of the incident laser frequency. For small gas-phase systems, HHG is usually explained via the so-called three-step model, which includes (1.) tunnel-

ing ionization of an electron out of the potential well of the atom/molecule and (2.) acceleration of the electron due to interaction with the external field. For an intense, time-dependent incident laser field, the electron may return to the parent ion, where it has a possibility to (3.) recombine and emit the accumulated kinetic energy in a coherent short burst of electromagnetic radiation – the HHG. Due to the coherent nature of the high energetic radiation, HHG is the routine method to generate attosecond pulses.

In solids, the HHG processes are much more complex since electrons do not freely propagate through space but propagate in the conduction band(s), giving rise to inter currents and intra-band currents, forming the basis of HHG. Although much more challenging for theoretical scientific efforts, solids, however, provide a promising route towards bright and compact HHG sources since their electron density is much higher than that of gas phase systems.

We have so far performed simulations of CdSe nanoparticles with different particle sizes (4–64 atoms on Noctua, corresponding to about 0.5–1.5 nm diameter). HHG spectra are simulated in a rigorous real-time, real-space approach. The incident laser field parameters are chosen corresponding to recent experiments from our experimental collaborators. The field strength (intensity) of the field is such that most likely, ionization is suppressed, thereby restricting HHG to effects of electron and hole dynamics within the nanoparticles.

Figure 1 shows the different employed structures including spherical boxes of varying size which were discretized with an equidistant grid of 0.3 a.u. resolution, resulting in more than 7,000,000 mesh points. Electron dynamics were propagated for >100 fs (17600 steps of about 6 as). A complex absorbing boundary at the periphery of the simulation box monitored electronic density leaving the nanoparticle. As the integrated electronic charge (i.e. number of electrons) of the system did not significantly alter during simulation runs, we assured that the resulting HHG spectra originate only from the current dynamics within the nanoparticles. Simulations were performed including rota-

Prof. Dr. Stefanie Gräfe

Stefanie Gräfe is professor for Theoretical Chemistry at the Friedrich Schiller University Jena. Her research interests are focused on the theoretical description and simulation of light-matter interaction, including processes induced or driven by intense and/or extremely short light pulses.

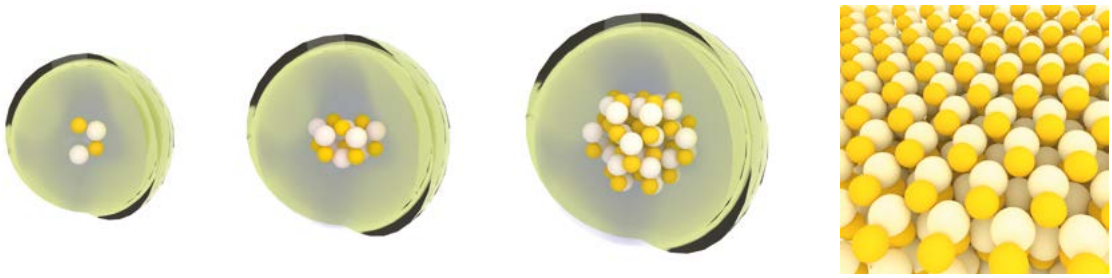


Figure 1: Investigated structures of CdSe nanoparticles of different size (4–64 atoms, corresponding to 0.5–1.5 nm diameter). Spherical simulation environments for finite-difference calculations are shown around the structures. Reference calculations employed bulk CdSe with periodic boundary conditions.

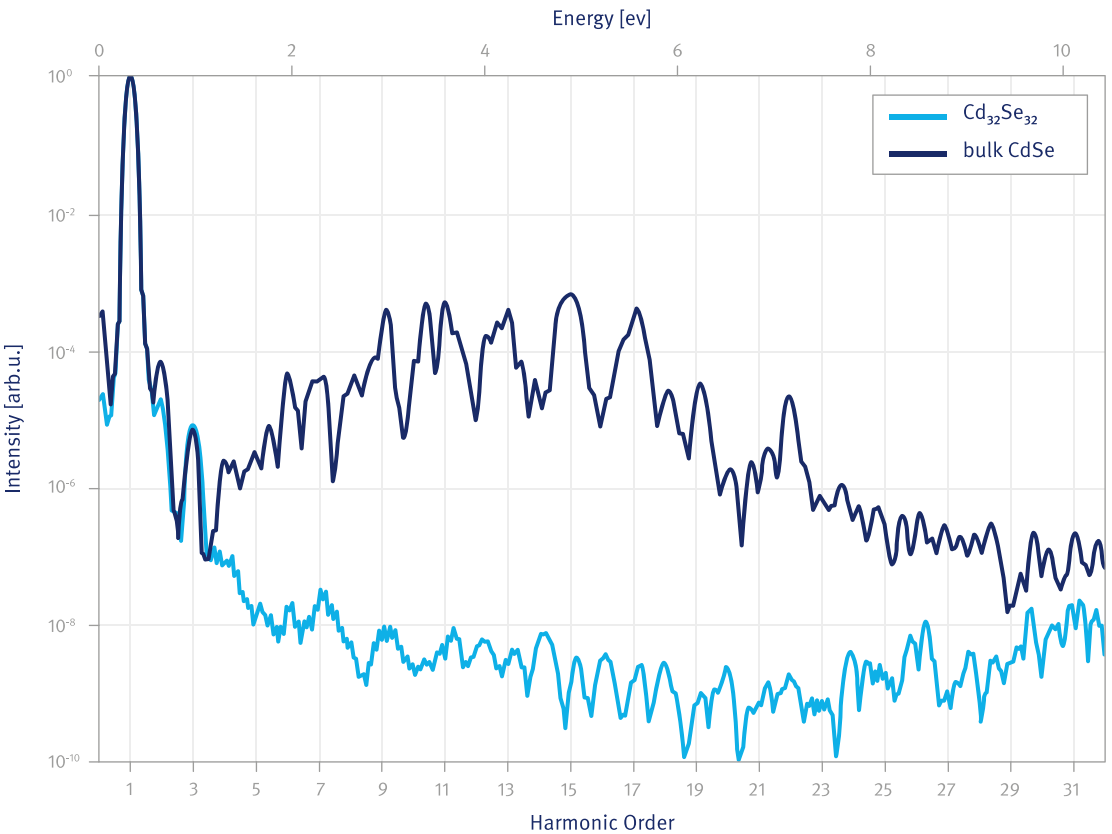


Figure 2: HHG spectra of bulk CdSe and 64-atom (1.5 nm) CdSe nanoparticle.

tional averaging over multiple orientations of the nanoparticle. The resulting HHG spectrum of a 64-atom nanoparticle is shown in comparison to a bulk simulation of CdSe using periodic boundary conditions in Figure 2.

The simulation of bulk CdSe clearly shows peaks low orders (1st – the fundamental – and the 3rd harmonic order). From 5th to 9th order the signal is rather noisy, which might be due to a high joint density of states in this energy window. For higher energies, clear peaks of odd harmonics are visible up to the 17th harmonic.

In contrast to this, the HHG spectrum of 1.5 nm (64 atom) CdSe nanoparticles looks very different. Clearly, the confinement significantly reduces the contribution of high orders (>5) to the spectrum. Our goal is a systematic investigation of the effect of different laser and material parameters on the resulting HHG spectra using a rigorous state-of-the-art ab-initio approach based on the rtTDDFT. As computation of the spectra is extremely demanding (up to 100,000 CPU hours per simulation run), HPC facilities such as the PC² computer cluster are of utmost importance for our work.

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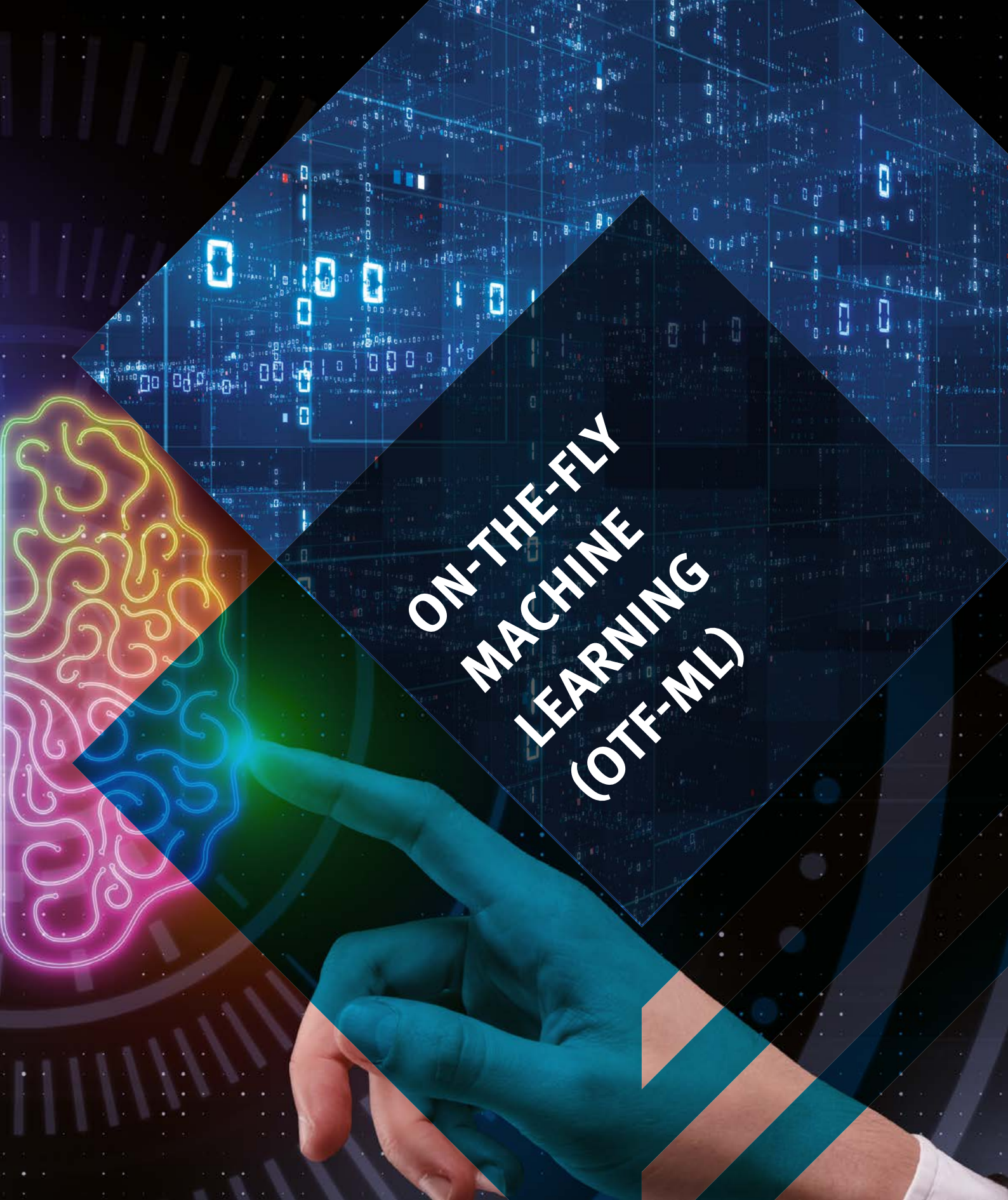
ON-THE-FLY
MACHINE
LEARNING
(OTF-ML)

Most sub-fields of computer science deal with the creation of algorithms or parts thereof such as data structures. On an abstract level, an algorithm can be seen as a function mapping inputs to outputs. Originally and still today, many algorithms are carefully designed manually in order to accomplish a certain task such as finding the shortest path from one point to another in a graph. This requires the designer to have both a strategy available for solving the task of interest and, equally importantly, tobe able to describe formally how this strategy works. Unfortunately, there exist problems for which algorithm designers, or even humans in general, are unable to describe the strategy they use for solving it. For example, the task of discriminating images which show either a cat or a dog is not a too hard task for most people, or even children. But describing how this problem is solved is a completely different story. Hence, a formal description of the identification process is deemed impossible, and the classical manual algorithm design approach is unsuitable for such problems.

Machine learning can be viewed as an alternative approach to creating such a system which returns a desired output for a given input. Instead of manually specifying the behavior of the system, machine learning deals with inducing such a system, usually called model, from supplied data. In its most basic form, this data consists of example pairs of inputs and outputs of the system to be constructed.

Due to the extensive digitalization of almost all areas of life (e.g., Industry 4.0, social media platforms, IoT, ...) vast amounts of data are generated daily, and the trend is still rising. To make use of the information contained in such data, the latter has to be acquired, analyzed and processed for the task in question. In a subsequent step, a machine learning model has to be tailored to and trained using the preprocessed data. This results in a sequence of successively executed algorithms, also referred to as machine learning pipeline. The execution of the latter is then usually followed by representation and/or interpretation of the associated results of the model.

Research in the area of data science has raised many different algorithms for each step of this pipeline, which in turn provide degrees of freedom in the form of parameters which enable fine-tuning to the respective data. Altogether, this results in a wide variety of possible candidates (»1050 [1, 2, 3]). Unfortunately, there is also no algorithm of choice for each step which is the best across all kinds of datasets but the right choice highly depends on the specified task and respective data.

As a consequence, for each new task, such a pipeline has to be designed from scratch to achieve satisfying performance, which requires expertise in data science.

However, most developers, let alone end users, in application domains are neither data scientists nor machine learning experts and the number of experts in this field is severely limited so that the demand for the expertise cannot be satisfied nearly. Accordingly, there exists an urgent need for tools which are both easy to use and also provide high quality ML

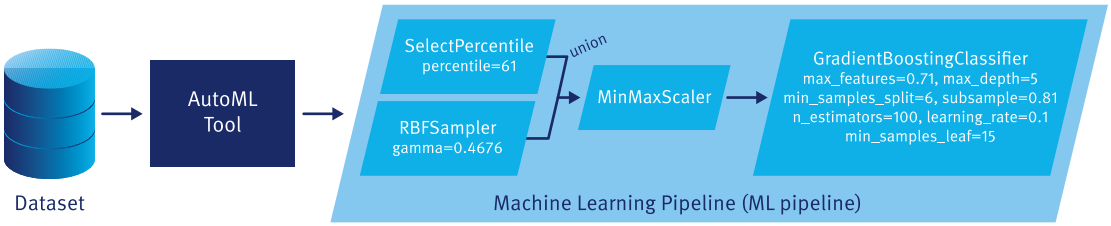

Figure 1: Instead of manually specifying the behavior of a system f generating a desired output y for a given input x, machine learning deals with inducing such a system, usually called model, from supplied data and prior knowledge

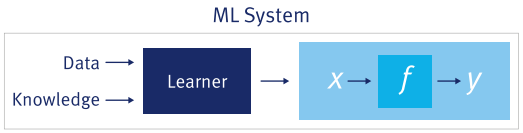

Figure 2: AutoML tools take a dataset (the data of the user, describing the desired system's behavior) as an input and return a pipeline of machine learning algorithms tailored to the specifics of the respective dataset.

solutions to end users without requiring constant interaction with an ML expert. Ideally, such a tool automates the whole process of creating an ready for operation ML system starting from data preprocessing, the choice of a model class, the training and evaluation of a model and finally ending with the representation and interpretation of the results. The research field of automated machine learning (AutoML) has emerged from this demand and vision.

In the last couple of years, AutoML has established itself as a hot and influential topic. Despite the short history of AutoML, impressive results could be obtained by AutoML tools such as Auto-WEKA [1], auto-sklearn [2], and TPOT [4]. Quite recently, we have advanced the state of the art in AutoML by another tool called ML-Plan [3, 5, 6, 7] which performs competitive and, in several cases, is even superior to the already existing approaches. While the approaches differ significantly in the way that they search for the most appropriate candidate, these tools have one thing in common. During the search, several potential solutions have to be trained and evaluated on the actual data, which is already computationally intensive for a single candidate and usually it is necessary to consider several of them. In fact, the training and evaluation of an ML pipeline can take up to several hours or even days.

Parallelization of the evaluation of ML pipelines cannot help to search the space of possible solutions exhaustively, since the complexity of the search space is far too high. Within a given time frame, however, parallelization has a positive effect on the quality of the returned solution, as multiple candidates can be con-

sidered simultaneously, normally several hundreds or even thousands of such pipelines need to be considered in a single run.

Accordingly, to advance research in this field, enormous amounts of computational resources are required as such tools need to be evaluated thoroughly on a broad spectrum of different datasets. These resources are gratefully provided, in our case, by PC². We intensively used PC² clusters for conducting experiments to investigate new methods and techniques in order to further improve the solution quality and efficiency of our AutoML tool ML-Plan. Due to the increasing amount of competitors, AutoML scenarios and benchmark datasets, we plan to ramp up our experiments to over 2000 CPU years in the upcoming months.

Moving AutoML to a cloud environment and providing machine learning functionality on-the-fly as a service, it becomes an application domain of "On-The-Fly Computing" which we refer to as "On-The-Fly Machine Learning" (OTF-ML) [8, 9]. The homonymous collaborative research center (CRC) 901 "On-The-Fly Computing" deals with the automatic on-the-fly configuration and provision of individual IT services out of base services which are available on world-wide markets. ML-Plan has been developed within the scope of the CRC 901 at Paderborn University and constitutes the core of our vision for OTF-ML. On the one hand, with OTF-ML, we want to enable end users who do not necessarily have sufficient hardware resources to run AutoML on their own devices in order to use machine learning functionality tailored to their needs. Alternatively in a cloud environment, there are more degrees of freedom to scale, for example by running more candidate evaluations in parallel, by distrib-uting the entire search process or by sharing resources between similar requests. PC² forms the foundation for all future work in this direction.

Prof. Dr. Eyke Hüllermeier

Eyke Hüllermeier is a professor in the Department of Computer Science at Paderborn University, where he heads the Intelligent Systems and Machine Learning Group, a member of the Heinz Nixdorf Institute, and a Director of the Software Innovation Campus Paderborn. He received his PhD in 1997 and a habilitation degree in 2002. Prior to joining Paderborn University in 2014, he held professorships at the Universities of Dortmund, Magdeburg and Marburg.

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QUANTUM
STATE-RESOLVED
HIGH-DIMENSIONAL
REACTION
DYNAMICS WITH
NON-ADIABATIC
TRANSITIONS

Most sub-fields of computer science deal with the creation of algorithms or parts thereof such as data structures. On an abstract level, an algorithm can be seen as a function mapping inputs to outputs. Originally and still today, many algorithms are carefully designed manually in order to accomplish a certain task such as finding the shortest path from one point to another in a graph. This requires the designer to have both a strategy available for solving the task of interest and, equally importantly, as well as being able to describe formally how this strategy works. Unfortunately, there exist problems for which algorithm designers, or even humans in general, are unable to describe the strategy they use for solving it. For example, the task of discriminating pictures which show either a cat or a dog is not a too hard task for most people, or even children.

But describing *how* this problem is solved is a completely different story. Hence, a formal description of the identification process is deemed impossible and the classical manual algorithm design approach is unsuitable for such problems.

Specifically, the project focuses on the accurate first principle description of elementary reaction processes. While a fully quantum state-resolved level of understanding has been achieved for triatomic and selected tetratomic reactions, extending this level of understanding towards reactions involving a larger number of atoms is a challenging subject. Reactions of methane with atoms such as H, Cl, O, or F are prototypical examples extensively studied by fundamental research focusing on the detailed

Prof. Dr. Uwe Manthe

Uwe Manthe has been professor for Theoretical Chemistry at Bielefeld University since 2004. His primary research interests are quantum effects in chemical reaction dynamics. Additionally, he is workingon the development of efficient numerical methods for quantum molecular dynamics simulations, which requires solving extremely high-dimensional differential equations.

understanding of chemical reactivity. Furthermore, these reactions are important processes in atmospheric and combustion chemistry.

Crossed molecular beam techniques, awarded the 1986 Nobel Prize in chemistry, facilitate experimental studies of elementary chemical reactions at the level of quantum state resolution. Two collimated beams of dilute gas-phase atoms or molecules are prepared in selected quantum states and intersect in a vacuum chamber so that individual reactive collisions can be detected. The direction and velocity of the resulting scattered products are measured to provide information about the partitioning of energy among different quantum states of the product molecules. Modern experiments studying reactions of methane with different atoms yielded impressive results, highlighting the complexity of polyatomic reaction dynamics at a quantum state-resolved level. Reactive resonance in the $Cl+CH_4$ reaction [1] or a counterintuitive mode-selective chemistry in $F+CHD3 \rightarrow HF+CD3/DH+CHD_2$ reaction [2] are prominent examples.

While impressive progress has been achieved in experimental studies, the accurate theoretical description of the reactions with methane is still a challenging task. Detailed wave packet dynamics calculations studying reactions of methane with Cl or F atom had to rely on reduced dimensional models considering up to eight active coordinates. Only the reaction of methane with the H atom could be studied in full dimensionality [3]. These calculations relied

Dr. Bin Zhao

Bin Zhao has been a postdoctoral researcher in Prof. Dr. Uwe Manthe's group since 2017. His primary research interest is quantum reaction dynamics, focusing on the development of fundamental theory and efficient numerical methods in order to facilitate the study of various quantum effects in reaction systems with three to six atoms.

on the multi-configurational time-dependent Hartree (MCTDH) approach [4], which facilitates numerically efficient high-dimensional wave packet dynamics calculations.

All high-level calculations described above rely on the Born-Oppenheimer (BO) approximation. The reaction is described as a collective motion of all nuclei on a multi-dimensional landscape given by a single adiabatic potential energy surface (PES). Non-adiabatic transitions between different electronic states cannot be described in this approximation. However, atoms such as F and Cl show electronically degenerate ground states due to the presence of incompletely filled p orbitals, and the reaction of methane with F(^{2}P) or Cl(^{2}P) atoms occurs on coupled conically intersecting PESs. Rigorous theory therefore has to explicitly consider non-adiabatic electronic transitions in these reactions. Accurate coupled diabatic PESs describing the F(^{2}P)/Cl(^{2}P)+CH_4 reactions have recently been developed. [5]

Using the computational resources of the Noctua cluster at PC², large-scale wave packet dynamics calculations can be extended to study the effect of non-adiabatic transition in the reaction of methane with F and Cl atoms. Previous theoretical work regarding these reactions considered only the lowest adiabatic PES and ignored non-adiabatic transitions resulting from vibronic and spin-orbit couplings. The present project will overcome this limita-

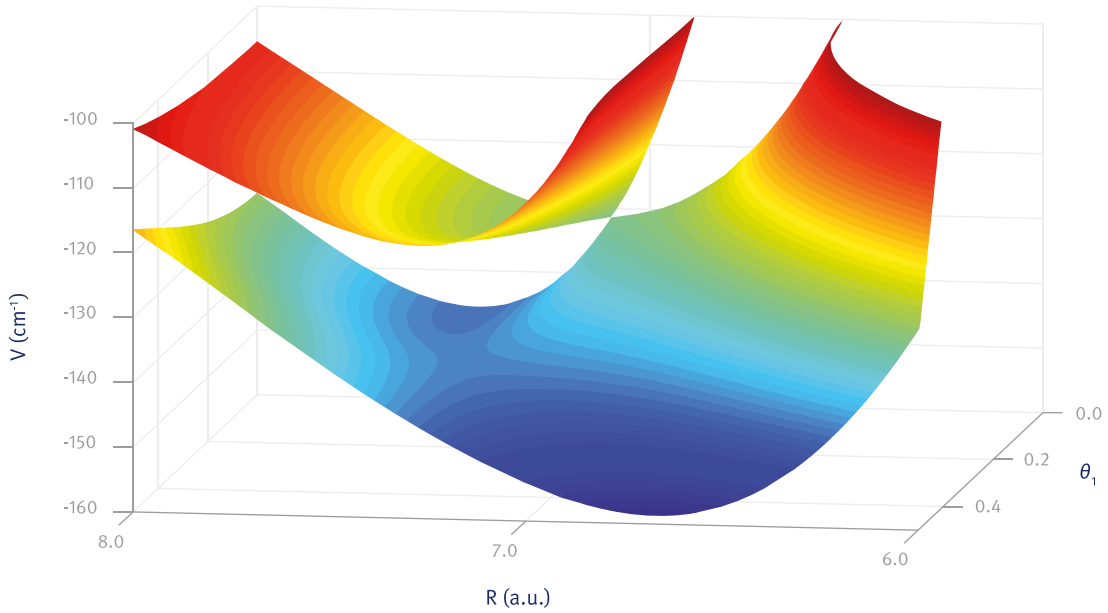

Figure 1: Conical intersection in the entrance channel of the F+CH_4 reaction.

tion. For the first time, quantum state-resolved scattering calculations including non-adiabatic transitions will be performed for reactions with more than three to four atoms. The calculations will provide unprecedented information about the effects of non-adiabatic transitions on the reactions of open shell atoms with polyatomic molecules. These results will help to develop concepts which will explain how non-adiabatic effects affect the state-specific chemistry occurring in these systems.

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EFFICIENT AND ACCURATE DFTB CALCULATIONS TO UNRAVEL THE CHEMISTRY OF ON-WATER CATALYSIS

Water plays a determining role to life. It is present in a vast number of processes in biochemistry and the mechanistic for how water affects such processes is still a matter of active research. Despite the fact that water is the solvent of choice for nature to implement its syntheses, its role in synthetic organic chemistry is less important: water is not a popular solvent choice.

Our research is aimed at using state-of-the-art first-principle simulations to obtain a detailed picture of the atomic structure and dynamics at the water/organic interface of the Diels-Alder on-water reactions. We use a combination of a low-cost quantum computational chemical method, specifically the density functional tight binding scheme DFTB (originating here at Paderborn University), and an efficient linear scaling method which enables us to compensate for numerical noise while sampling the exact Boltzmann distribution. This would lead to achieve more efficient, yet still accurate,

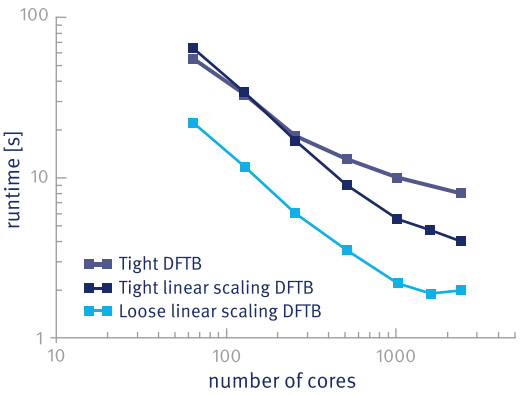
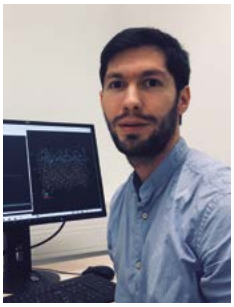


Figure 1: performance comparison of a full DFTB calculation and linear scaling DFTB with two different precisions.



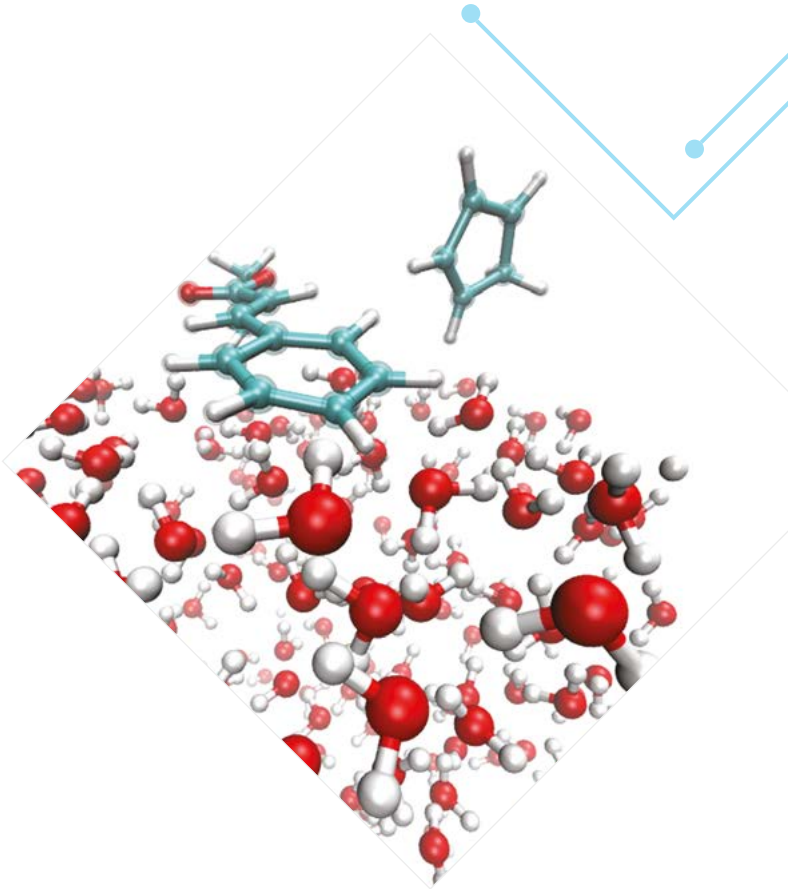
Dr. Andrés Henao Aristizábal

Andrés Henao Aristizábal is a postdoctoral researcher in the group of Prof. Dr. Thomas D. Kühne, dynamics of condensed matter. His research is focused on the use of low-cost ab initio methods to study chemical reactions in the liquid/liquid interface sponsored by an Alexander von Humboldt fellowship. He previously obtained a Bachelor Degree in Physics Engineering in Colombia and a M.Sc and Ph.d in Computational Physics in Barcelona, Spain.

simulations with a DFTB level of description for a realistic water/organic system, and in fact for a range of condensed matter applications which are only feasible to date using classical molecular dynamics or for too small system-sizes using ab-initio calculations.

The results obtained will be compared to sum frequency generation experiments which are specific to detect the interfacial properties to establish the correlations between the structure and hydrogen bond strength at the water/organic interface.

This project is developed within the research group of Prof. Dr. Thomas D. Kühne, dynamics of condensed matter, which focuses on the development and application of novel ab-initio molecular dynamics methods.



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AA


NEURAL NET-
WORK POTENTIAL
FOR LITHIUM
MANGANESE
OXIDES IN WATER

Lithium intercalation compounds are important cathode materials in batteries. The lithium manganese oxide spinel $Li_xMn_2O_4$, with $0 < x < 2$, is a prominent example which provides advantages such as low costs and non-toxicity.

However, an accurate description of $Li_xMn_2O_4$ by first-principle methods such as density functional theory (DFT) is far from trivial due to its complex electronic structure. It has been found that the local density approximation as well as the generalized gradient approximation are unable to describe $Li_xMn_2O_4$ correctly. We have performed an extensive benchmarking for different $Li_xMn_yO_z$ systems using the hybrid PBE0, HSE06 functionals and the recently developed local hybrid PBEor functional. We have found that these functionals yield energetic, structural, electronic, and magnetic properties which are correspond well with experimental measurements. The computational costs of PBEor are significantly lower than those for the other hybrid functionals, because PBEor relies on on-site Hartree-Fock exchange only.

Apart from the electronic structure, a second challenge is the requirement for large systems to perform simulations for realistic structural models including, for example, defects. Employing DFT directly in form of ab initio molecular dynamics is unfeasible because of the high costs. We will overcome this problem by employing an efficient and accurate machine learning potential based on neural networks. The high-dimensional neural network potential will enable high-level theoretical studies of the dynamics at finite temperatures which will address, for example, the lithium diffusion process.

Prof. Dr. Jörg Behler

Jörg Behler graduated in chemistry at the University of Dortmund. In 2004, he obtained his PhD at the Fritz-Haber-Institute in Berlin. After a postdoctoral residence at ETH Zürich, he established his own research group at the Ruhr-Universität Bochum in 2007. In 2013, he was awarded the Hans G. A. Hellmann prize for his work on the development of high-dimensional neural network potentials. He received his venia legendi in 2014. He has been a full professor for theoretical chemistry at the University of Göttingen since 2017.

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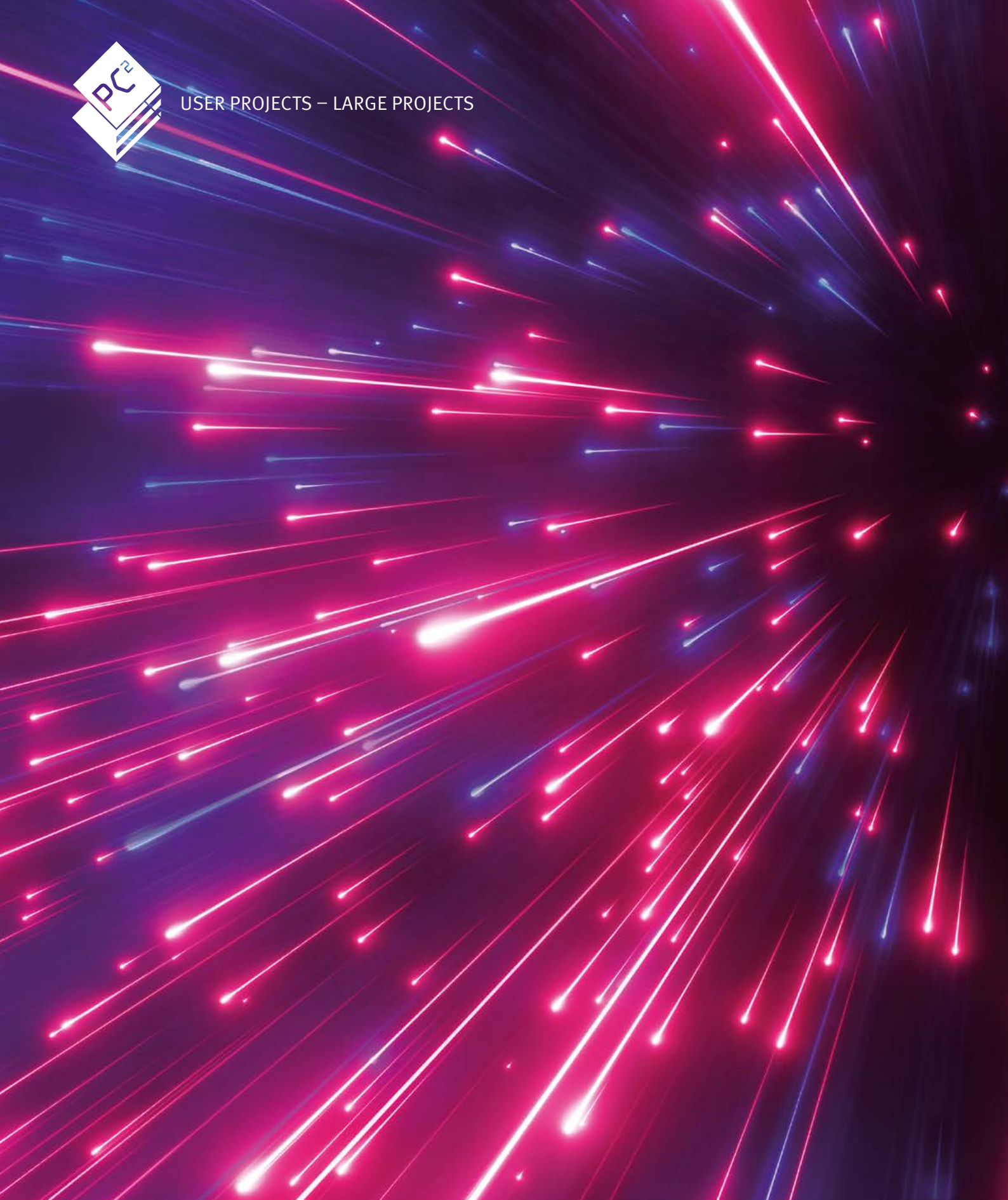

USER PROJECTS – LARGE PROJECTS

HIGH-PERFORMANCE SIMULATIONS OF LIGHT SCATTERING ON PARTICLES AND IN DENSE MEDIA

Optical measurements of light scattered from various kinds of particles like dust, droplets, or ice particles and powder-like media provide information about their physical properties, such as e.g. their morphology and composition. This approach is utilized in different fields e.g., in remote sensing of the aerosols and soils on Earth and the Solar System bodies, observations of cosmic dust, noninvasive biological tissue diagnostics and optical particle characterization in industrial applications.

Retrieval of the information regarding the scatterers, i.e. solution of the inverse problem, requires knowledge of optical properties for all the variety of particles. The problem becomes even more complicated when such particles form dense powder-like media with high degrees of packing density where multiple scattering plays important role. This kind of an electromagnetic problem is multi-scale and requires significant computational resources.

We utilize the Discontinuous Galerkin Time Domain (DGTD) method for numerical simulations to study optical properties of isolated random irregular particles and densely packed multi-particle structures. The DGTD method is based on unstructured meshing and has very good parallel scalability properties, which is an advantage when solving large problems. Our parallel light scattering code shows nearly perfect scaling for at least 4000 CPU cores.

Utilizing this highly scaling code on PC² HPC systems enable us to study the influence of factors such as particle size, material and packing density, on the formation of the scattering angle dependencies of intensity and polarization of light scattered from model structures.

Prof. Dr. Jens Förstner

Jens Förstner is head of the Theoretical Electrical Engineering (TET) group at Paderborn University. He studied Physics and Computer Science at Philipps Universität Marburg and University of Kent at Canterbury/UK. During his PhD at Technical University Berlin and his postdoctoral studies at University of Arizona, he focused on simulating nanophotonic structures, he led an Emmy Noether research group on “Computational Nanophotonics” and was appointed at Paderborn University in 2013.

Model of a densely packed
cluster of irregular particles

(a)

(b)

(c)

Figure 1:
(a) Model of an irregular particle with rough surface.
(b) Model of a densely packed cluster of irregular particles.
(c) Numerical solution of light pulse propagation through an irregular particle.

Reference

Y. Grynko, Y. Shkuratov, and J. Förstner
Light scattering by irregular particles much larger than the wavelength with wavelength-scale surface roughness, *Opt. Lett.*, 14, 3491–3493, 2016


HIGH-
PERFORMANCE
DISTRIBUTED
MEMORY
PROGRAMMING ON
RECONFIGURABLE
HARDWARE

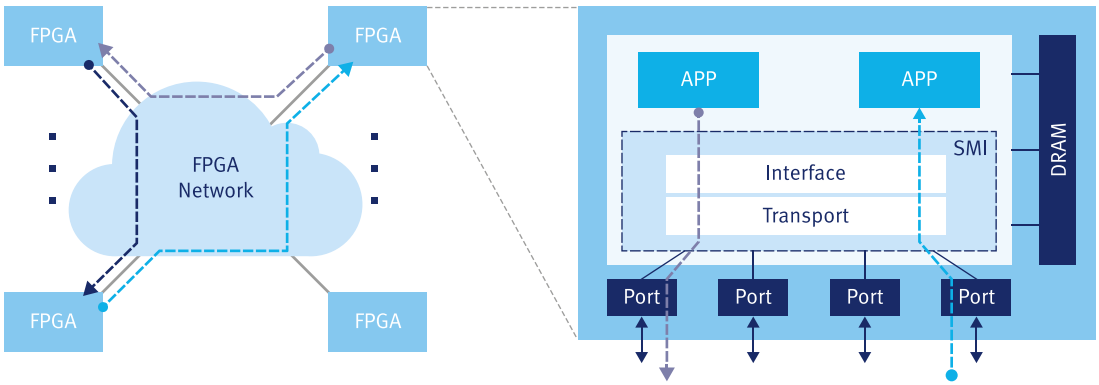
Distributed memory programming is the established paradigm used in high-performance computing (HPC) systems, requiring explicit communication between nodes and devices. When FPGAs are deployed in distributed settings, communication is typically handled either by going through the host machine, sacrificing performance, or by streaming across fixed device-to-device connections thereby sacrificing flexibility. In this collaboration between PC² and the Scalable Parallel Computing Lab (SPCL) at ETH Zurich, we address the requirement for a distributed memory programming model for multi-FPGA systems.

We propose the Streaming Message Interface (SMI): a communication model and API which unifies explicit message passing with a hardware-oriented programming model, facilitating minimal-overhead, flexible, and productive inter-FPGA communication. Instead of bulk transmission, messages are streamed across the network during computation, enabling communication to be seamlessly integrated into pipelined designs. Using SMI, programmers are able to implement distributed, scalable HPC programs on reconfigurable hardware, without deviating from best practices for hardware design.

The unique hardware setup of the Noctua cluster at PC² enables us to prototype SMI on a dedicated FPGA interconnect. By utilizing point-to-point QSFP connections between the Nallatech 520N FPGA boards, we were able to implement runtime-configurable routing, with support for arbitrary network topologies. We have already successfully shown low-latency streaming communication between eight FPGAs using SMI, and continue to explore larger systems and network topologies due to the newly installed optical switches in the cluster.

Prof. Dr. Torsten Höfler

Torsten Höfler is an Associate Professor of Computer Science at ETH Zürich, Switzerland. He chairs the "Collective Operations and Topologies" working group at the MPI Forum, authored chapters of the MPI-2.2/-3.0 standards and has published numerous peer-reviewed scientific articles. His research interests revolve around performance-centric software development and include scalable networks, parallel programming techniques and performance modeling.



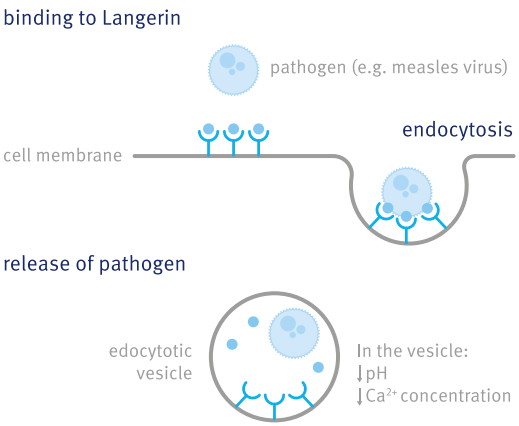
Multi-FPGA programming with SMI

Reference

Tiziano De Matteis, Johannes de Fine Licht, Jakub Beraneck, Torsten Hoefler
Streaming Message Interface: High-Performance Distributed Memory Programming on Reconfigurable Hardware
Accepted at the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'19)

INVESTIGATION OF PH-DEPENDENT CA(II)-BINDING AFFINITY IN LANGERIN

To trigger an immune response against an infection caused by viruses or bacteria, the invading pathogens need to be captured and transferred to the immune system. The transmembral C-type lectin receptor Langerin is one of the receptors in humans that recognizes pathogens like HIV by binding to glycans on their surface. A calcium(II)-ion in the Langerin binding pocket is crucial for the binding. The extracellular binding event takes place within a pH-neutral environment. The pathogen is subsequently encapsulated in an endocytotic vesicle. The pH drops to approximately 6.5 to 5.5 in the vesicle . This acidic pH lowers the binding constant of calcium(II) to Langerin. The loss of calcium in turn triggers the release of the pathogen, which is then additionally processed by the immune system. The following puzzle arises: The calcium(II)-ion is coordinated by glutamate and aspartate residues, which have a pKa of approx. 4. The coordinating residues are not therefore very sensitive to the drop in pH from 7 to about 6. How then is the pH-dependent calcium(II)-affinity implemented by the protein scaffold?

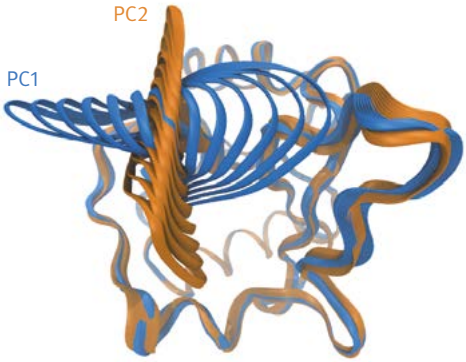


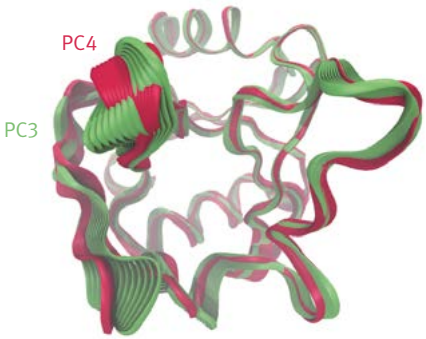
Recognition and capture of a pathogen by C-type lectin Langerin.

We already identified histidine H294, which has a pKa value around 6, as one of possibly more pH-sensors which influence the calcium(II)-binding affinity and, due to that, facilitate the release of pathogen-ligands in the cell-inside. The side chain of this residue, however, has no direct contact to the primary binding site and therefore represents an allosteric site that regulates the protein activity over a yet unknown mechanism.

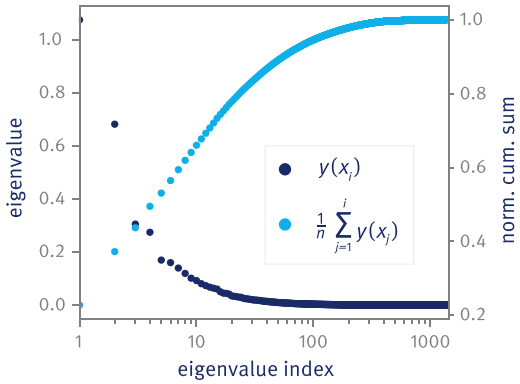
Jun.-Prof. Dr. Bettina Keller

Bettina Keller is a junior professor for “Theoretical Chemistry” at the Freie Universität Berlin. Her research focuses on the development of computational methods for the analysis of time-series data, in particular for the analysis of molecular-dynamic simulations. She uses these methods to elucidate the dynamics of complex molecular systems. In 2018, she was awarded the G.A. Hellmann prize for Theoretical Chemistry.





A principal component analysis of Langerin shows the movement of the short loop. The short loop is involved in sensing the drop in pH and in regulating the pH-dependent Ca^{2}+-affinity.



Eigenvalue spectrum of the covariance matrix (dark blue) and normalised cumulative variance (light blue).

We intend to elucidate the exact mechanism of pH-dependent calcium(II)-binding in Langerin on an atomic level by a combination of classical all-atom molecular dynamics simulations, steered molecular dynamics experiments and the construction of Markov state models. Up to now there does not exist, to our knowledge, any rigorous explanation of such a mechanism in Langerin or a related protein. It would greatly improve the understanding of this important receptor and its close relatives.

Reference

J. Hanske, S. Aleksić, M. Ballaschk, M. Jurk, E. Shanina, M. Beerbaum, P. Schmieder, B.G. Keller, C. Rademacher
Intradomain Allosteric Network Modulates Calcium Affinity of the C-Type Lectin Receptor Langerin
J. Am. Chem. Soc. 138 (**2016**), Pages 12176–12186


USER PROJECTS – LARGE PROJECTS

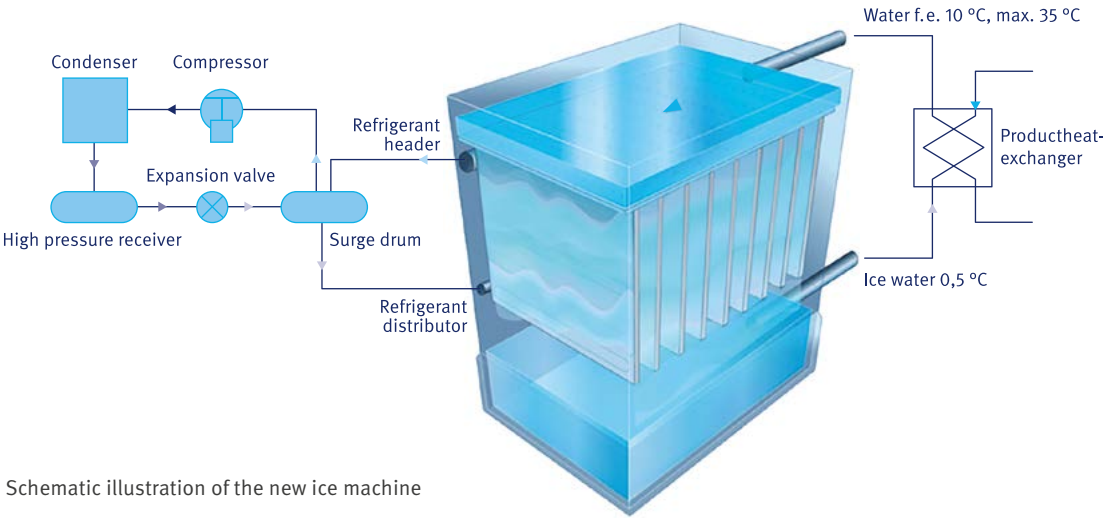

CFD
SIMULATIONS OF
HEAT AND MASS
TRANSPORT
IN MULTIPHASE
FLOWS

Foodstuff industry companies produce ice in form of ice shards directly at the manufacturing site in order to implement product cooling. Recently, a new ice machine design (compare with Figure 1) enabling more energy-efficient ice production has been proposed; it is characterized by lower operating and maintenance costs compared to conventional designs. The key components of the new machines are panels made of pillow-like plates, which are arranged as vertically aligned and parallel to each other. Water is supplied to the outer pillow-plate surface as a thin liquid film, while a working medium at a temperature below the water freezing point, is directed through the inner channels of the pillow-plate panels. As a result, water freezes on the outer panel surface due to the latent heat dissipation to the working medium flowing inside the pillow-plate panels. As soon as the desired thickness of the ice layer is reached, a warm working medium is guided through the inner channels so that the ice layer detaches from the pillow-plate surface, falls down and is processed into shards by a crusher.

Pillow-plate panels represent a quite new type of heat transfer equipment, and therefore, their thermo-hydraulic characteristics are still not fully captured. This is why appropriate design equations for the new ice machines are missing, resulting in certain design uncertainties preventing exploitation of their full potential. To overcome this problem, we have applied advanced numerical methods, the so-called Computational Fluid Dynamics, to study the film flow on the outer surface of the pillow-plate panels as well as the ice formation process. The simulations belong to the class of multiphase flow, which is very demanding and requires significant computational power. We executed our simulations with the aid of two commercial software tools, ANSYS Fluent and SIEMENS PLM Star-CCM+, in parallel on up to 1024 cpu cores.

Prof. Dr. Eugeny Kenig

Eugeny Kenig obtained his PhD degree in 1985 from the Russian Academy of Sciences. From 1994–95, he was an Alexander von Humboldt Fellow at the University of Dortmund. He subsequently worked at the Universities of Dortmund and Essen as well as at the BASF chemical company. He finished his habilitation in Dortmund in 1999 and accepted a call for the professor position in Paderborn in 2008. He is director of Fluid Process Engineering, focusing on integrated separation processes, micro-separation units and on problems of process-related energy efficiency.



Schematic illustration of the new ice machine

References

1. R.F. Engberg, M. Wegener, E.Y. Kenig. **Numerische Simulation der konzentrationsinduzierten Marangoni-Konvektion an Einzeltropfen mit verformbarer Phasengrenze** *Chem. Ing. Techn. 86*, 185–195 (2014)
2. R.F. Engberg, M. Wegener, E.Y. Kenig. **The impact of Marangoni convection on fluid dynamics and mass transfer at deformable single rising droplets – A numerical study** *Chem. Eng. Sci. 116*, 208–222 (2014)
3. R.F. Engberg, M. Wegener, E.Y. Kenig. **The influence of Marangoni convection on fluid dynamics of oscillating single rising droplets.** *Chem. Eng. Sci. 117*, 114–124 (2014)
4. R.F. Engberg, M. Wegener, E.Y. Kenig. **A systematic CFD-based method to investigate and optimise novel structured packings.** *Chem. Eng. Sci.* 122 452–464 (2015)
5. R.F. Engberg, E.Y. Kenig. **An investigation of the influence of initial deformation on fluid dynamics of toluene droplets in water.** *Int. J. Multiphase Flow* 76 144–157 (2015)
6. M. Piper, A. Zibart, E. Djakow, R. Springer, W. Homberg, E.Y. Kenig **Heat transfer enhancement in pillow-plate heat exchangers with dimpled surfaces: A numerical study** *Appl. Therm. Eng.* 153, 142–146 (2019)


USER PROJECTS – LARGE PROJECTS

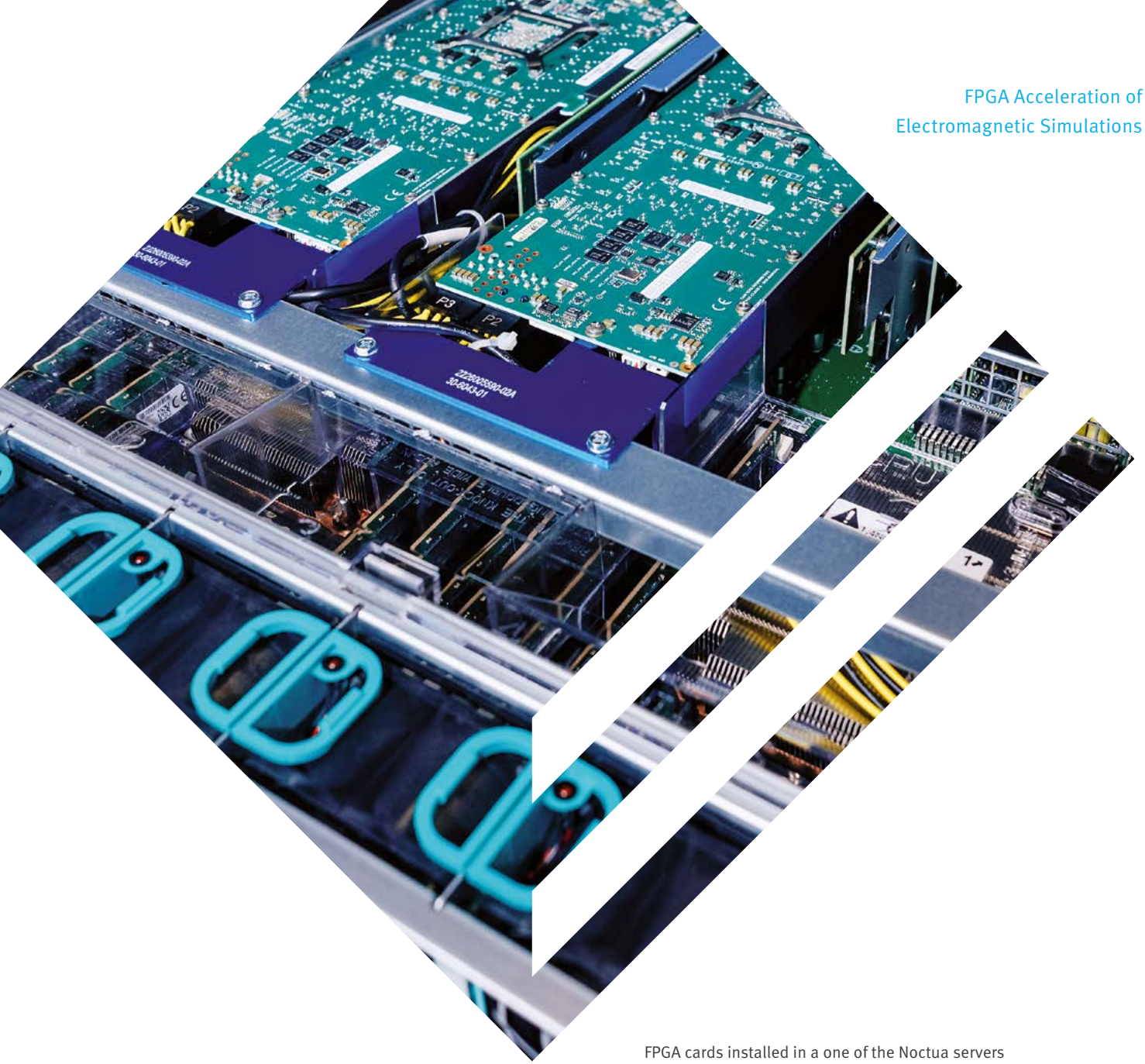

FPGA
ACCELERATION
OF ELECTRO-
MAGNETIC
SIMULATIONS

Simulations of electromagnetic effects in novel materials and surfaces contribute a significant workload to our HPC systems. In order to improve performance and energy efficiency of these workloads, we have investigated them as a target for FPGA acceleration by looking at applications which operate on unstructured meshes and use the Discontinuous Galerkin method. In an initial extensive case study, we found out that several characteristics enable these applications to profit well from the flexibility of FPGA architectures. A single FPGA of the previous Arria 10 generation is now outperforming the two-socket CPU nodes of the previous HPC Oculus cluster by around 1.5–2x at much lower power consumption. With the availability of multiple FPGA nodes connected with high speed interconnect, we scaled this application to up to 32 Stratix 10 FPGAs by communicating through the host via MPI. Multiple FPGAs create the possibility to solve larger problem sizes or smaller problem sizes faster, but the parallel efficiency still left room for improvement. The addition of direct FPGA-to-FPGA interconnect provides the foundation for such improvement. In initial designs on 2 and 4 FPGAs, the efficiency problems were resolved and significant headroom for more communication-intensive scenarios was indicated.

In the collaborative BMBF-funded project *HighPerMeshes*, we are working on generalizing these case studies towards more applications regarding unstructured meshes by using a domain-specific language (DSL) embedded in C++. The manually-optimized designs will be complemented by code generation for FPGAs and other targets. Scaling is achieved transparently to the application writer through distributed execution of suitable loop structures within the DSL.

Dr. Tobias Kenter

Tobias Kenter received his PhD from Paderborn University in 2016 on the topic of productivity for FPGAs through overlays, compilation approaches and tight coupling between FPGAs and CPUs. Since then he has focused on the acceleration of scientific applications on FPGAs using OpenCL based development flows from Intel and Xilinx. With his research, he strives to establish more rigorous, HPC-like performance models and evaluation in the FPGA community.



FPGA cards installed in a one of the Noctua servers

Reference

[1] Tobias Kenter, Gopinath Mahale, Samer Alhaddad, Yevgen Grynko, Christian Schmitt, Ayesha Afzal, Frank Hannig, Jens Förstner and Christian Plessl. **OpenCL-based FPGA Design to Accelerate the Nodal Discontinuous Galerkin Method for Unstructured Meshes.** In *Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM)*, 2018, IEEE.


HYDROSURF

The project is based on the results of recent theoretical and experimental investigations regarding the acidic character of the hydrophobic air-water interface, hinting that proton hopping processes at the air-water interface occur preferentially via water-wires oriented parallel to the surface plane which lead to an increase of the residence time of the proton at the interface, thereby resulting in an interface which is more acidic than that of bulk water.

These water-wires have been shown to be the direct consequence of the specific HB-structure which is formed at the air-water interface in order to maximize water-water H-Bonds, consisting in an extended & continuous 2D-H-Bond-Network, with more than 90% of interfacial water being interconnected through H-Bonds all oriented parallel to the surface. Since the 2D-H-Bond-Network is formed at the hydrophobic air-water interface in order to maximize water-water H-Bonds, similar highly

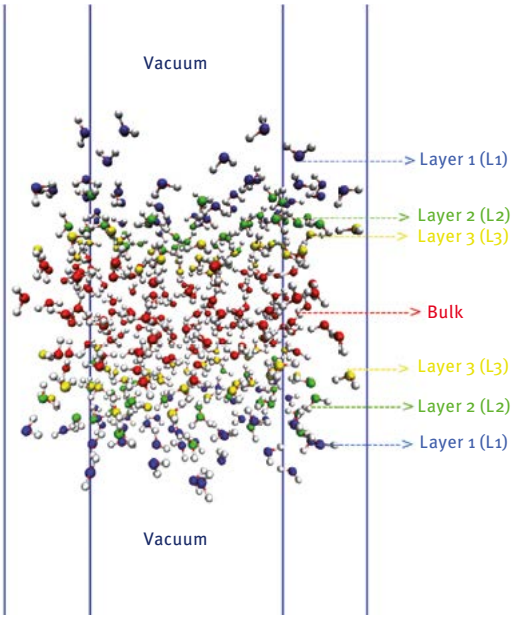


Figure 1: Model of the simulated air-water Interface. The bulk-like water molecules in the middle are shown in red, whereas the surfaces molecules, which are at the core of our investigation are, depending on the layer where they are located, colored in blue, green and yellow respectively.

Prof. Dr. Thomas D. Kühne

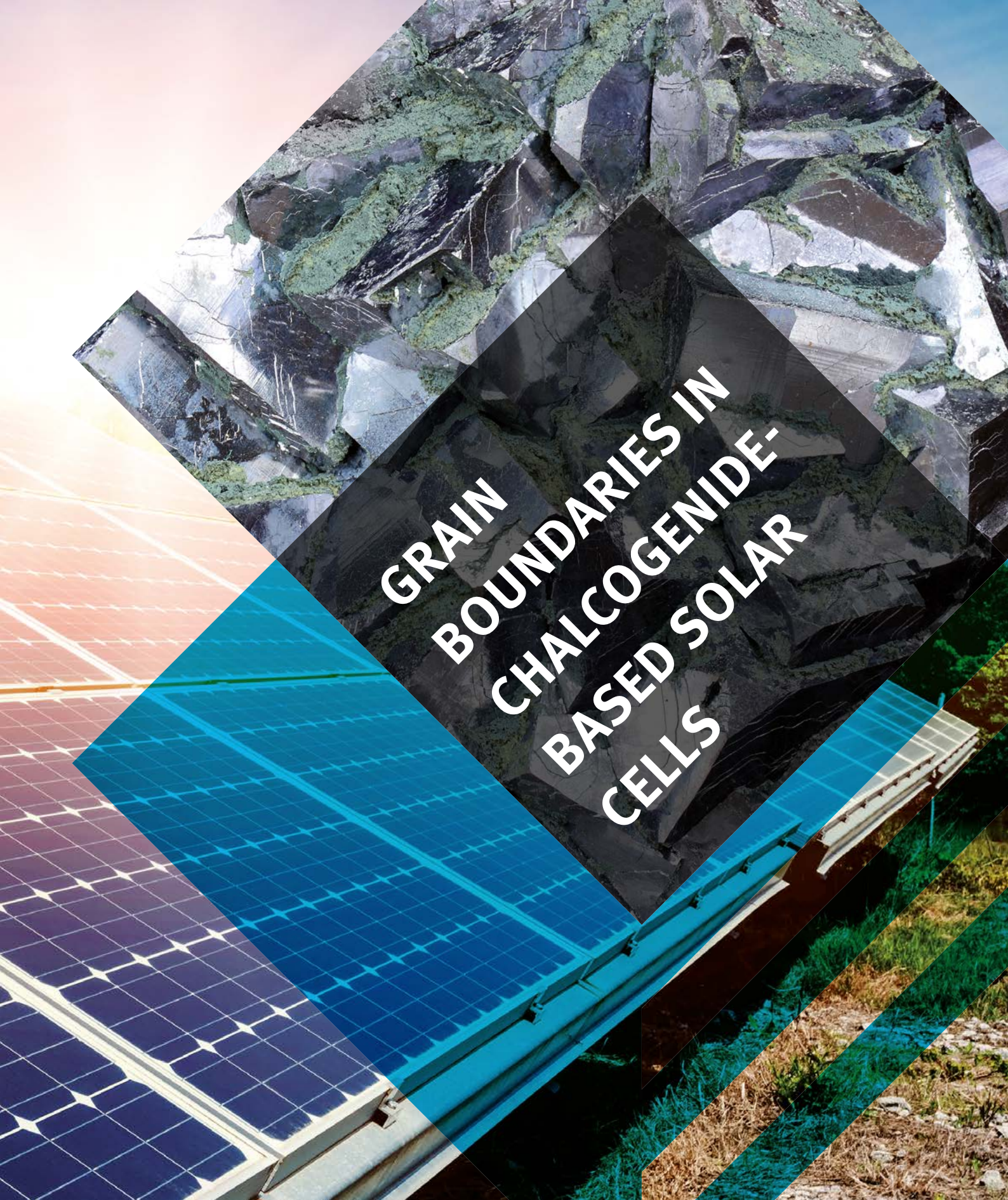
Thomas D. Kühne is currently professor for theoretical chemistry at Paderborn University. He was previously an assistant professor for theoretical chemistry at the University of Mainz and a post-doctoral research fellow in the condensed matter physics group at Harvard University. In 2003 he received his BSc in Computer Science, in 2005 MSc in Computational Science and Engineering and in 2008 his Dr. Sc. ETH degree in Theoretical Physics, all from the Swiss Federal Institute of Technology. He is an expert in the development of computational methods for ab-initio molecular dynamics and electronic structure theory, as well as the application of such techniques to investigate relevant questions regarding Chemistry, Biophysics and Material Sciences.

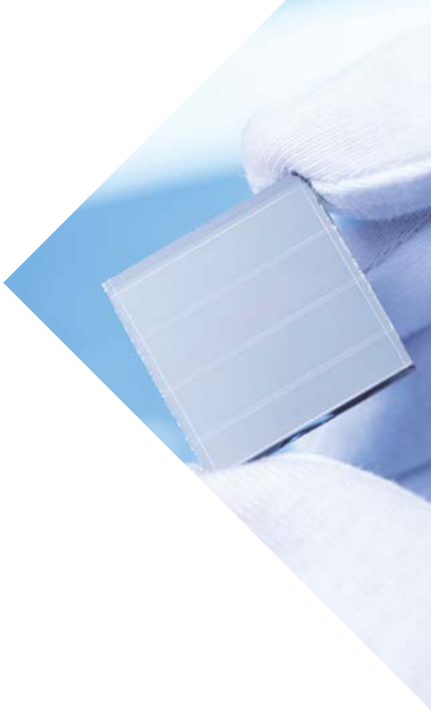
interconnected and preferentially oriented networks are expected to form at other aqueous interfaces, where water is in contact with "sufficiently hydrophobic" surfaces. At these interfaces, if the formation of the 2D in-plane water-wires is verified, then it will lead to the pivotal conclusion that hydrophobic interfaces are systematically acidic regions, with essential consequences for the chemical reactivity at these interfaces.

The validation of this hypothesis is the primary objective of the proposed theoretical work. Once this is achieved through DFT-MD simulations, including quantum nuclei DFT-MD simulations for a complete structural characterization and rationalization of the impact of nuclei quantum effects on the proton hopping mechanism and on the water-wires at hydrophobic aqueous interfaces, then the second objective is the identification of SFG/IR/Raman spectroscopic markers for interfacial protons at these interfaces, which can be in turn be experimentally probed, thereby providing definitive markers for surface acidities still missing in the literature.

Reference

N. K. Kaliannan, A. H. Aristizábal, H. Wiebeler, F. Zysk, T. Ohto, Y. Nagata, and T. D. Kühne. **Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface.** *Mol. Phys.* (2019).


GRAIN BOUNDARIES IN CHALCOGENIDE-BASED SOLAR CELLS



Thin-film solar cells based on Cu (In,Ga)Se_2 (CIGSe) have the highest efficiency among the second-generation solar cells. In contrast to silicon-based solar cells, the efficiency of CIGSe cells with a polycrystalline absorber exceeds the efficiency of their monocrystalline counterpart. This is remarkable, because the performance of optoelectronic devices is typically considered to be worse for polycrystalline semiconductors. Generally, grain boundaries (GB) are expected to create deep gap levels which act as recombination centers and are detrimental for the solar-cell performance. Regarding this fact, it is highly desirable to understand the effect of GBs on the properties of absorbers.

In this study, we investigate the energetics and electronic structure of GBs in the presence of point defects in CIGSe and similar absorber materials such as CdTe and $Cu_2ZnSnSe_4$. Three GB models are considered to model the GBs in these materials. The formation of intrinsic, alkali atoms and oxygen point defects at the GBs of chalcogenide-based absorber materials will be studied. Furthermore, we aim to study the diffusion mechanisms of the impurities as well as the self-diffusion of constituent elements along the grain boundaries employing nudged elastic band (NEB) calculations and adaptive kinetic Monte Carlo (aKMC).

Dr. Hossein Mirhosseini

Hossein Mirhosseini is the head of the multiscale modeling of energy materials group at Paderborn University involved in multidisciplinary projects collaborating with partners from academics and industry. The group investigates promising materials for energy harvesting (solar and thermoelectric energy), energy storage (batteries and hydrogen storage) and photocatalytic applications.

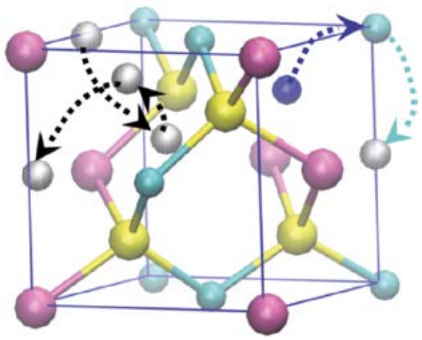


Figure 1: Diffusion mechanisms in the $CuInSe_2$ lattice.

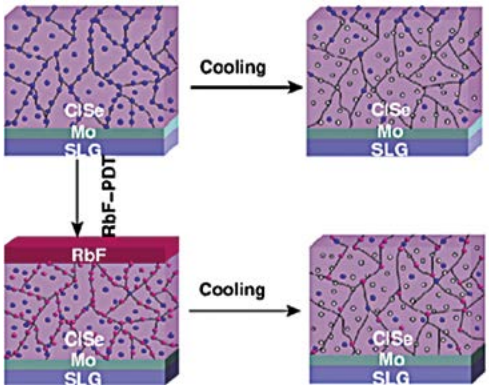


Figure 2: Diffusion of light (blue) and heavy (red) alkali atoms in polycrystalline $CuInSe_2$.

Reference

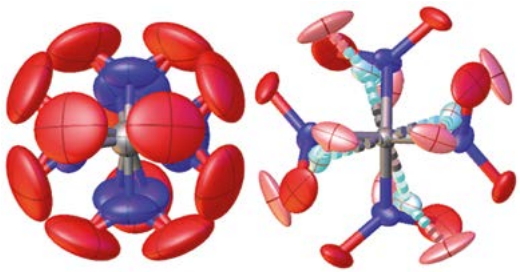
M. Chugh, T. D. Kühne, and H. Mirhosseini
Diffusion of Alkali Metals in Polycrystalline $CuInSe_2$ and their Role in the Passivation of Grain Boundaries
ACS Appl. Mater. Interfaces 11, 14821 (2019)

DFG CORE FACILITY – GAS ELECTRON DIFFRACTION AND SMALL MOLECULE STRUCTURE CENTER (GED@BI)

Gas-phase electron-diffraction is one of the most powerful methods to investigate chemical structures in an unperturbed state and therefore free of intermolecular forces for example in liquids or crystals. X-ray diffraction (XRD) is a routine technique in chemistry nowadays, yet the basic principles of gas-phase electron-diffraction (GED) are the same. The comparison of structures in different phases tells us about intermolecular forces and how molecules become distorted in the solid state. Gas-phase structures are unperturbed by such forces and can therefore be compared with quantum-chemical results of free molecules and thereby serve as reference for development of new theoretical methods.

In this project, we investigate and seek to understand intramolecular interactions which influence the structure, reactivity and stability of different molecules in the context of London dispersion forces, halogen bonding, intramolecular stacking interactions and closed shell metallophilic interactions. An essential part of our work regarding evaluation of gas-phase electron diffraction data utilizes state-of-the-art quantum-chemical resources (in terms of Hardware and Software) which are provided by the PC² HPC-Systems.

A recent result which illustrates our work is the structural chemistry of tetranitromethane, which was repeatedly investigated for more than 70 years but we could only now describe the dynamics structure in the gas and the complicated disorder in the crystalline state [1].



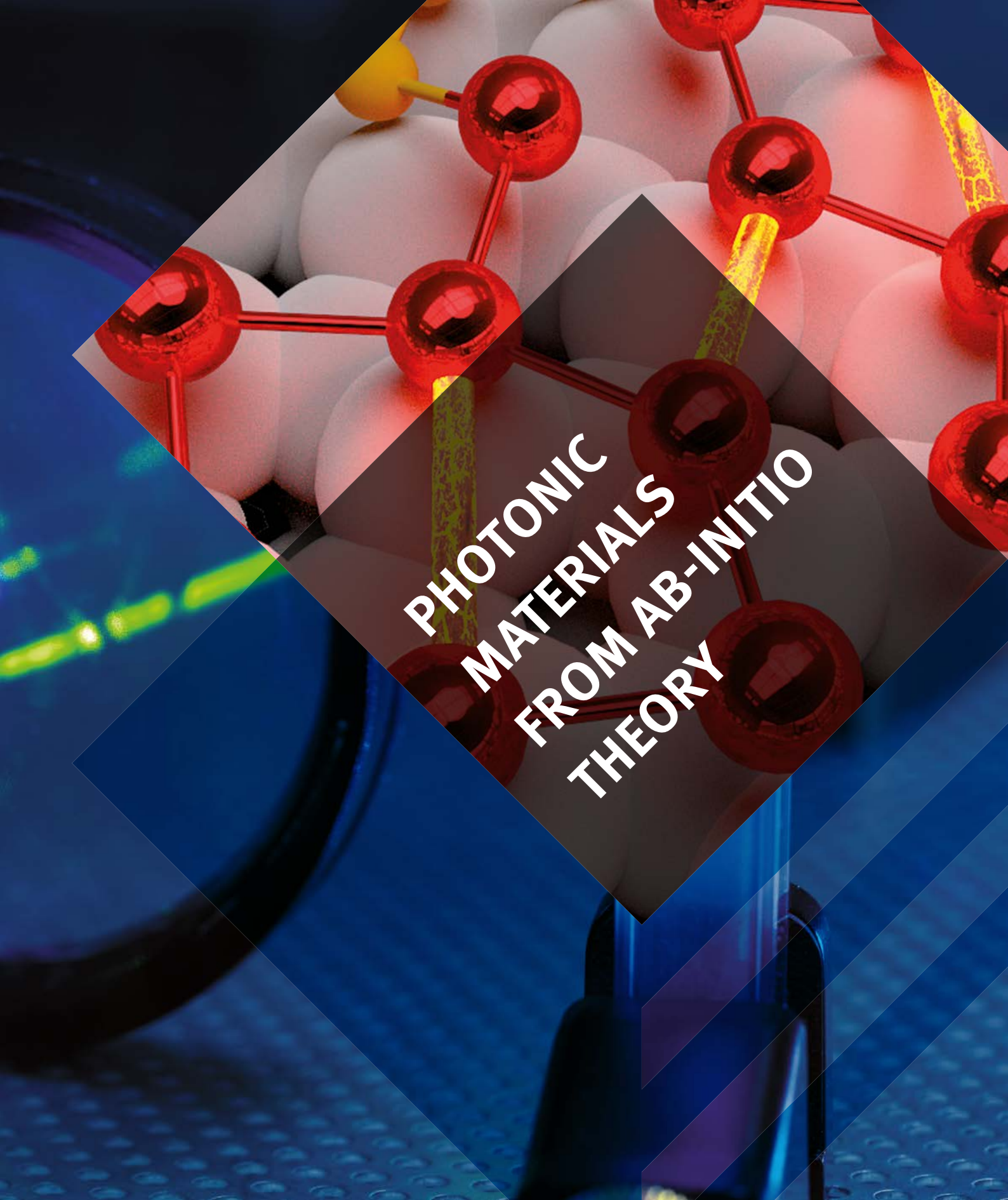
Two models of disorder for solid tetranitromethane

Prof. Dr. Norbert W. Mitzel

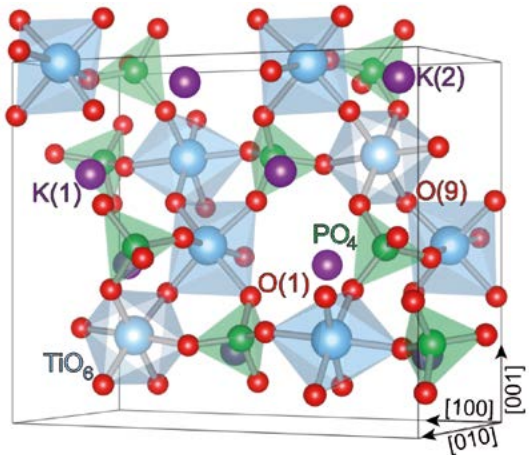
Norbert W. Mitzel, Prof. of Inorganic and Structural Chemistry, Bielefeld University, studied chemistry at TU München, completed his PhD with H. Schmidbaur, learned structural chemistry techniques as a Marie-Curie fellow with D.W.H. Rankin (University of Edinburgh). Following his habilitation at TUM in 2002, he then went to the University of Münster as professor of inorganic chemistry and to Bielefeld in 2007. His research interests are Lewis acid chemistry, weak interactions and structural chemistry in different phases.

Reference

Y.V. Vishnevskiy, D.S. Tikhonov, J. Schwabedissen, H.-G. Stammler, R. Moll, B. Krumm, T. M. Klapoetke, and N. W. Mitzel.
Tetranitromethane: A Nightmare of Molecular Flexibility in the Gaseous and Solid States.
Angew. Chem. Int. Ed. 2017, 56, 9619–9623.


PHOTONIC
MATERIALS
FROM AB-INITIO
THEORY

Accurate parameter-free calculations of optical response functions for real materials and nanostructures still represent a major challenge for computational materials science. Our project concentrates on the development and application of ab-initio methods which provide access to linear and nonlinear optical spectra. It explores, on the atomistic level, how the material structure, its composition and defects but also external parameters like stress, temperature or magnetic fields influence the optical response. In addition, we explore how optical excitations modify the material electronic and atomic structure as well as the time dynamics of optical excitation and de-excitation. The project thereby leads to a better understanding of existing materials and contributes to the design of new photonic materials.

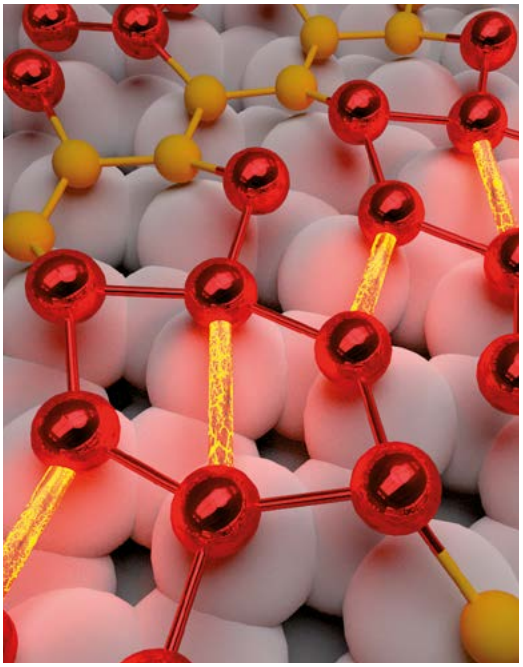


Potassium titanyl phosphate (KTP) is a nonlinear optical material which is intensively investigated in our project. Its unit cell is shown above.

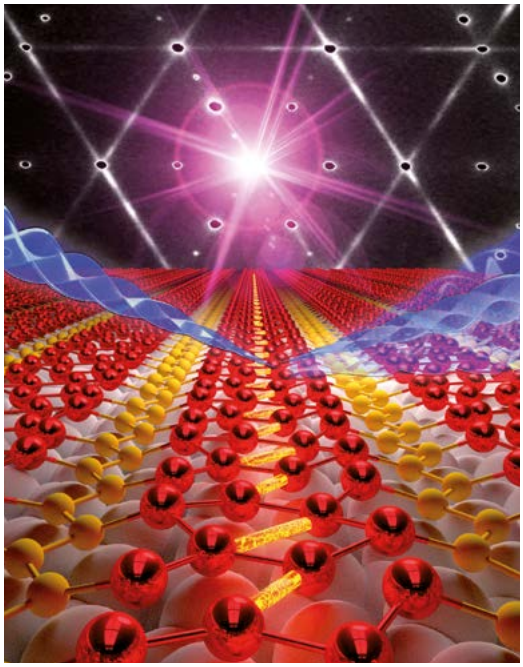
Our calculations start from an accurate description of the structural and electronic ground-state properties within density-functional theory (DFT). Time-dependent DFT in conjunction with a Berry-phase formulation of the dynamical polarization accounts for many body effects in the optical response in an efficient way without recourse to virtual orbitals. More precise schemes based on many body perturbation theory, such as the GW approximation for the quasiparticle energies or the Bethe-Salpeter equation (BSE) for the linear optical response, are be used to benchmark the TDDFT results. Both zero-point vibrations

Prof. Dr. Wolf Gero Schmidt

Wolf Gero Schmidt has been heading the Theoretical Material Physics Group at Paderborn University since 2006. Previously, Schmidt worked, inter alia, at the Massey University in Auckland, New Zealand. Current research areas include theoretical description and numerical modeling of optical and electronic excitations in semiconductors and ferroelectrics, mesoscopic electron transport and phase transitions in low-dimensional systems.



Optically induced bond breaking in silicon substrate-stabilized indium nanowire.



Time-resolved electron diffraction enables measuring the time dynamics of optically induced phase changes.

and thermal lattice vibrations are included in the calculations. The computational methods developed in our project are applied to a wide range of II-VI, III-V and nitride semiconductors and nanostructures as well as ferroelectric materials such as potassium titanyl phosphate, which are shown below.

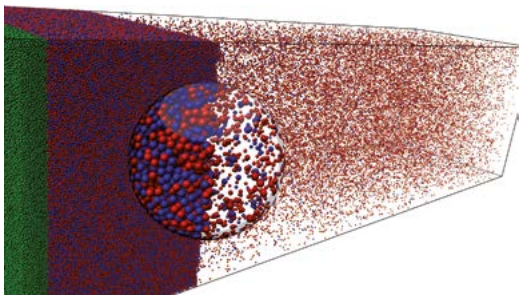
Reference

C.W. Nicholson, A. Lücke, W.G. Schmidt, M. Puppin, L. Rettig, R. Ernstorfer, M. Wolf.
"Beyond the molecular movie: Dynamics of bands and bonds during a photoinduced phase transition"
Science 362, 821 (2018).


LARGE-SCALE
MOLECULAR
DYNAMICS
SIMULATIONS

In modern thermodynamics, not only equilibrium conditions, but also the dynamics of non-equilibrium processes are studied because of their importance for processes in nature and technical applications. To cover such non-equilibrium scenarios, it is necessary to consider systems with a large number of particles. For this purpose, our group combines thermodynamics and statistical physics with high-performance computing to develop suitable computational tools, namely ms2 and ls1 mardyn.

In this project, large-scale molecular dynamics simulations are used to investigate transition processes, like the evaporation of a liquid. The excellent scalability of the simulation tool ls1 mardyn, which is parallelized with MPI either using domain decomposition or k-d tree-based decomposition, is exploited here. Scenarios imitating stationary evaporation processes are studied with a detailed view on the interface region between liquid and vapor in systems



Snapshot of a stationary simulation of evaporation into vacuum. The system consisted of a liquid and a vapor phase, connected through a planar interface. To the left, the liquid was extended by a reservoir, deployed for replenishment and thereby to attain stationary conditions. Particles constituting the reservoir, forward and backward particle flux are colored green, red and blue, respectively.

Prof. Dr. Jadran Vrabec

Jadran Vrabec is Professor for Thermodynamics and Process Engineering at the Technical University of Berlin. His work is centered around molecular modeling and simulation for process and energy engineering applications. After studying process engineering at the Ruhr-University of Bochum, he also accepted his PhD there in 1996. He became a group leader for molecular thermodynamics at the University of Stuttgart, where he received his habilitation in 2007. Between 2009 and 2018, he was Professor for Thermodynamics and Energy Technology at Paderborn University.

under global non-equilibrium. The evaporating liquid is exposed to gaseous atmospheres with pressures lower than those under equilibrium conditions, leading to a pressure gradient which drives the evaporation process. The variation of the counter pressure, including the case of vacuum with zero pressure, will be assessed. To evaluate the influence of the liquid on the evaporation process, the parameters of the quadrupolar two-center Lennard-Jones model for molecular anisotropy and polarity will be varied, retaining all other conditions of the simulation scenario as constant. A set of different model fluids will therefore be analyzed, which comprises three real components (N_2, O_2, CO_2). This study will lead to new physical insights into evaporation processes, which are of major importance for energy and process engineering.

Reference

René Spencer Chatwell, Matthias Heinen, Jadran Vrabec
Diffusion-limited evaporation of a binary liquid film
International Journal of Heat and Mass Transfer 132 (2019) 1296–1305


FURTHER
RESEARCH
PROJECTS

FURTHER RESEARCH PROJECTS

In the following, we present an overview of the projects in the small category that have been approved since the introduction of the new resource allocation process in April 2019.

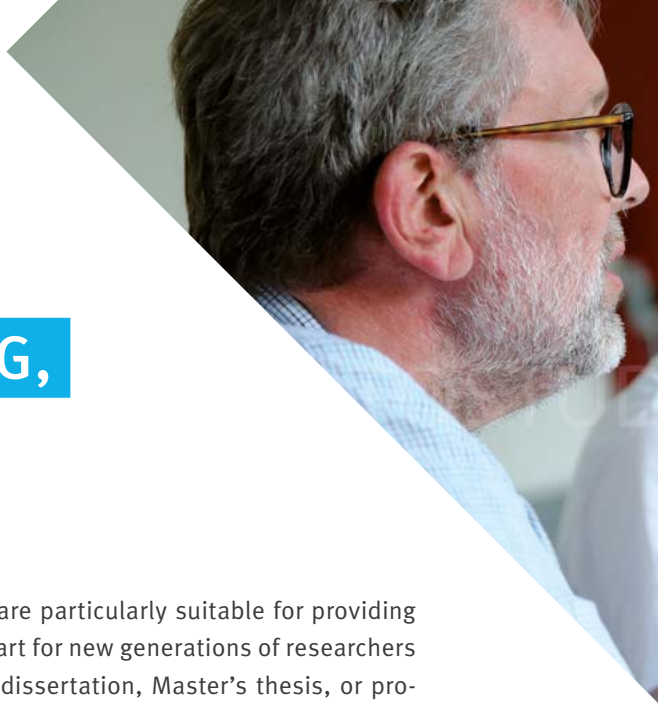
PRINCIPAL INVESTIGATOR	INSTITUTION	TITLE
CHEMISTRY		
Prof. Dr. Matthias Bauer	Paderborn University	(TD)DFT investigations on transition metal complexes for (photo)catalytic applications
Prof. Dr. Thomas Bredow	University of Bonn	Modeling of catalytically active surfaces of VO2
Prof. Dr. Sonja Herres-Pawlis	RWTH Aachen University	Catalysis with transition metal complexes
Prof. Dr. Jan Paradies	Paderborn University	Quantum Mechanical Description of FLP and Heteriacne Systems
Prof. Dr. René Wilhelm	Paderborn University	Properties of Organometallic Compounds and Interactions with Biomolecules
PHYSICS		
Dr. Thorsten Deilmann	University of Münster	Trions and excitons in magnetic monolayers and multi-layer materials
Prof. Dr. Andreas Klümper	University of Wuppertal	Plateau to plateau transitions of the integer quantum Hall effect
Prof. Dr. Torsten Meier	Paderborn University	Integrated measurement-induced nonlinearity with superconducting detectors
		Multi-dimensional nonlinear Bloch oscillations and related phenomena
		Modeling nonlinear-optical properties of semiconductors using DFT bandstructures
Prof. Dr. Peter Kratzer	University of Duisburg-Essen	Ab-initio simulation of electronic excitation and relexation
Prof. Dr. Peter Reimann	Bielefeld University	Modelling quantum systems by random matrices
Prof. Dr. Stefan Schumacher	Paderborn University	Nonlinear polarition dynamics in Semiconductor Microcavities
		Microscopic theory of charge generation in conjugated polymers
Jun.-Prof. Dr. Polina Sharapova	Paderborn University	Integrated nonlinear SU (1,1) interferometer
Dr. Wolfgang Unger	Bielefeld University	Lattice QCD in Strong Coupling Regime

PRINCIPAL INVESTIGATOR	INSTITUTION	TITLE
ENGINEERING		
Prof. Dr.-Ing. Joachim Böcker	Paderborn University	Investigation of Artificial Neural Networks for Temperature Estimation in PMSMs
Prof. Dr. Jens Förstner	Paderborn University	Nonlinear wavefront control with dielectric metasurfaces
		Linear and nonlinear optical properties of plasmonic/dielectric nanostructures
		Optical Waveguide Antennas for Directive Emission of Light
Prof. Dr. Reinhold Häb-Umbach	Paderborn University	Multichannel speech separation
		Unsupervised and semisupervised learning from speach and audio
Prof. Dr. Sybille Hellebrand	Paderborn University	Fast-than-AT-Speed-Test (FAST)
Prof. Bernd Henning	Paderborn University	Determination of accoustic material parameters
Prof. Dr.-Ing. Ulrich Hilleringmann	Paderborn University	EEWISE – EMC for Emergent Wireless Systems
Prof. Dr.-Ing. Werner Homberg	Paderborn University	Optimierungsbasierte Hybridauslegung (HyOpt) P4
Prof. Dr. Eugeny Kenig	Paderborn University	CFD Simulations of Heat and Mass Transport in Multiphase Flows
Prof. Dr.-Ing. Gerson Meschut	Paderborn University	DigiBody
Prof. Dr.-Ing. Volker Schöppner	Paderborn University	Numerical process simulation of fluid flow in screw extruders
Prof. Peter Schreier	Paderborn University	Deep learning for medical image processing
Prof. Dr. Walter Sextro	Paderborn University	Fahrwerkkonzept für einen energieeffizienten, verschleißarmen Reifen-Fahrbahn-Rollkontakt
Prof. Dr.-Ing. Ansgar Trächtler	Paderborn University	Instable Vibrations in Washing Machines
Prof. Dr. Thomas Tröster	Paderborn University	Automotive Lightweight Design
MATHEMATICS AND COMPUTER SCIENCE		
Prof. Dr. Falko Dressler	Paderborn University	Simulations of radio networks
Prof. Dr. Gregor Engels	Paderborn University	Wikidata Quality Assurance
		3D ML – Machine Learning
Prof. Dr. Torsten Höfler	ETH Zürich	A programming model and scalable applications for multi-FPGA systems
		COSMO FPGA
Prof. Dr. Eyke Hüllermeier	Paderborn University	Online Bandit Algorithms and Learning of Choice Functions
Prof. Dr. Friedhelm Meyer auf der Heide	Paderborn University	SFB901 On-The-Fly Computing

PRINCIPAL INVESTIGATOR	INSTITUTION	TITLE
MATHEMATICS AND COMPUTER SCIENCE		
Prof. Dr. Axel Ngonga	Paderborn University	Finding the holistic ranking of very large Knowledge Graphs
Dr. Sebastian Peitz	Paderborn University	Data-based control of complex systems
Prof. Dr. Marco Platzner	Paderborn University	Approximate Computing: CIRCA
Prof. Dr. Christian Plessl	Paderborn University	Linear-scaling DFT methods
		Teaching and Training for FPGA Acceleration in HPC Systems
		HPC User Training
		HighPerMeshes
Prof. Dr. Daniel Quevedo	Paderborn University	Reinforcement Learning and Optimization for Large Sstems and Manufactoring
Prof. Dr.-Ing. Sabine Roller	University of Siegen	High-order Direct Accoustics of Rigid Body Movement
Prof. Dr. Carsten Schulte	Paderborn University	Error Correction of Gaze Data
Oliver Walter	Paderborn University	Unsupervised and semisupervised learning for Speech recognition
Prof. Dr. Andrea Walther	Paderborn University	Veronika Schulze: MoMeCha
		Olga Ebel: HyLa
ECONOMICS		
Prof. Dr. Herbert Dawid	Bielefeld University	GROWINPRO: Growth Welfare Innovation Productivity
Prof. Oliver Müller	Paderborn University	SODA LAB
		Data Analytics
Prof. Dr. Kevin Tierny	Bielefeld University	Automatic Parallel Algorithm Configuration and Selection
LIFE SCIENCE		
Prof. Dr. Volker Knoop	University of Bonn	DNA and RNA analyses of early land-plant organelles and associated factors
HUMANITIES		
Prof. Dr. Michaela Geierhos	Paderborn University	Plattformübergreifende Ermittlung qualifizierbarer Bewertungsdimensionen via Text Mining


TRAINING AND TEACHING


TRAINING
AND
TEACHING



HPC TRAINING, TEACHING, AND WORKSHOPS

The effective use of high-performance computers is of key importance for achieving top-class results in computational sciences and for ensuring the efficient use of our HPC systems. It is therefore a central aspect of our mission to train the researchers and students in using and programming our HPC infrastructure. For this purpose, we provide training in various formats which are tailored to the target audience.

Our HPC Qualification Program provides researchers and students with a set of currently four regularly offered courses which cover subjects from Linux and HPC introduction to performance engineering for scientific programs. These compact, half or full-day training courses are particularly suitable for providing a kick-start for new generations of researchers for their dissertation, Master's thesis, or project work. In order to provide forums for the scientific exchange between our users, we also organize research area-specific or computing technology-specific workshops and courses. Our training events and workshops are generally open to all members of German research institutions and are announced by the nationwide Gauss-Allianz HPC Calendar Portal (https://hpc-calendar.gauss-allianz.de/en). Finally, for students of Paderborn University, HPC-related subjects are taught as part of the curriculum of the Computer Science and Computer Engineering programs by PC² members.

HPC QUALIFICATION PROGRAM

Empowering more researchers to use high-performance computing resources is one of the main missions of PC². Our new HPC Qualification Program for researchers and students (http://go.upb.de/pc2hpctrain) is tailored to this goal with courses composed of lectures and hands-on sections. The program is repeated every term and is accompanied by self-assessment tests enabling potential participants to judge their level of experience.

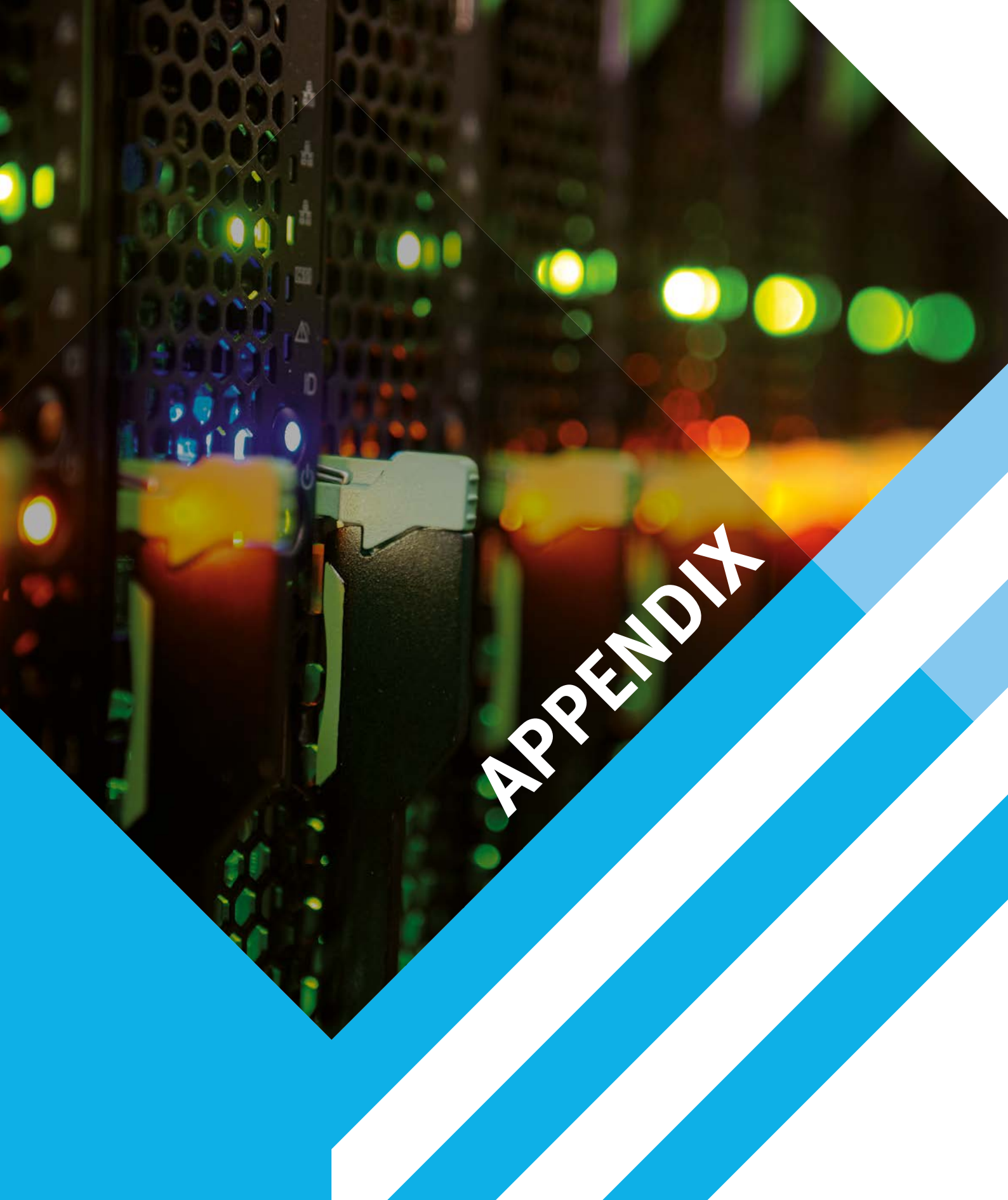
Our HPC Qualification Program currently consists of five training modules which build on one another to enable users to enter at any stage of HPC experience. For example, the first course is a basic Linux introduction course on one afternoon for users who have never used a UNIX-like operating system and the shell. The second course titled "HPC Introduction Course" then informs about the available computing resources, compute time proposals, workload manager, job scripts, and running parallelized programs. This afternoon course enables users to execute existing programs on the cluster systems available at PC². The third course is a full-day course and covers advanced topics of HPC. It lays the foundation for performance engineering by teaching about the many levels of hierarchy in a modern HPC cluster system. Subjects covered in this course include profiling, scaling analysis, pinning, software container and accelerators. The fourth course on "Performance Engineering" then concentrates on source code (and sometimes even assembler instructions) for the discussion of bottlenecks and performance patterns. The previously described four courses prepare researchers for specialized workshops which we organize and see as the fifth step in our course program. One example is a Cray user workshop covering the Cray performance tools.

RECENT WORKSHOPS

HPC TRAINING: PARALLELIZATION WITH MPI AND OPENMP Workshop on parallelization with MPI and OpenMP with lectures and hands-on exercises held by HPC-specialist Rolf Rabenseifner.	February 5–7, 2018
FPGA WORKSHOP: BEST PRACTICES FOR OPENCL DESIGN WITH STRATIX 10 Workshop for experience exchange about design patterns for programming Intel Stratix 10 FPGAs with OpenCL on BittWare FPGA cards. Held in cooperation with Richard Chamberlain of BittWare.	August 16, 2018
CP2K USER TUTORIAL: COMPUTATIONAL SPECTROSCOPY 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.	August 27–29, 2018
FPGA TRAINING: WORKING WITH OPENCL FOR INTEL FPGAS Two day training on FPGA design with OpenCL for Intel FPGAs for beginners conducted by Wolfgang Loewer of FPGA consulting specialist El Camino. Introduction regarding the main programming flow for the Stratix 10 FPGAs in Noctua with a combination of general concepts of OpenCL for FPGAs with hands-on exercises.	September 24–25, 2018
PC² USER MEETING Annual meeting to provide a platform for scientific exchange and networking between users of the PC² infrastructure. Scientific talks by Dominik Marx, Jadran Vrabec and Jens Förstner. Update by PC² staff regarding upgrades to the HPC infrastructure.	December 10, 2018
SPRING MEETING OF THE ZKI AK-SC 2019 Spring meeting of the ZKI Work Group on Supercomputing (Frühjahrstagung des ZKI Arbeitskreises Supercomputing 2019) with contributed talks and workshops relating to the current status and progress of high-performance computing in Germany.	March 14–15, 2019
PRODUCTIVE DESIGN FOR INTEL FPGAS – COMBINING HLS WITH LOWER-LEVEL TOOLS Advanced training regarding programming models for designing FPGA accelerators with Intel high-level design tools. Special emphasis complementing the high-productivity OpenCL-based design flow with other approaches e.g. DSP Builder and HLS Compiler. Held by Intel FPGA specialist Bill Jenkins.	May 20, 2019

RECENT LECTURES AND COURSES ON HPC TOPICS TAUGHT BY PC² MEMBERS

LECTURE: HIGH-PERFORMANCE COMPUTING (MASTER CS, CE)	Prof. Dr. Christian Plessl	Regularly every Winter term
LECTURE: ARCHITEKTUR PARALLELER RECHNERSYSTEME (MASTER CS, CE)	Dr. Jens Simon	Regularly every Summer term
LECTURE: COMPUTER ARCHITECTURE / RECHNERARCHITEKTUR (BACHELOR CS, CE, EE)	Prof. Dr. Christian Plessl	Winter terms since 2018/2019
PROJECT GROUP: FBENCH: DEFINING AND OPTIMIZING OPENCL BENCHMARKS FOR FPGAS	Dr. Tobias Kenter, Prof. Dr. Christian Plessl, Marius Meyer	Winter term 2019/2020 and Summer term 2020
PROJECT GROUP: CUSTONN2 – CUSTOMIZING NEURAL NETWORKS ON FPGAS Focus: Scaling over multiple Stratix 10 FPGAs using dedicated interconnect	Dr. Tobias Kenter, Prof. Dr. Christian Plessl	Winter term 2018/2019 and Summer term 2019
PROJECT GROUP: CUSTONN – CUSTOMIZING NEURAL NETWORKS ON FPGAS Focus: Topology-specific code generation for Xilinx and Intel FPGAs	Dr. Tobias Kenter, Prof. Dr. Christian Plessl	Summer term 2017 and Winter term 2017/2018



APPENDIX

PUBLICATION LIST

2019

- **CIRCA: Towards a Modular and Extensible Framework for Approximate Circuit Generation.**
  L. M. Witschen, T. Wiersema, H. Ghasemzadeh Mohammadi, M. Awais, and M. Platzner.
  Microelectronics Reliability, 99:277–290, 2019. doi:10.1016/j.microrel.2019.04.003.

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- **Higher-Order Contributions and Nonperturbative Effects in the Nondegenerate Nonlinear Optical Absorption of Semiconductors using a Two-Band Model.**
  W.-R. Hannes and T. Meier. *Physical Review B*, 2019. doi:10.1103/physrevb.99.125301.

- **Molecular Doping of PCPDT-BT Copolymers: Comparison of Molecular Complexes With and Without Integer Charge Transfer.**
  C. Dong and S. Schumacher. 2019.

- **Optical Vortex Core Switching in Spinor Polariton Condensates.**
  M. Pukrop, S. Schumacher, and X. Ma. 2019.
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  A. Bocchini, S. Neufeld, U. Gerstmann, and W. G. Schmidt.
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- **Deep Reinforcement Learning for Scheduling in Large-Scale Networked Control Systems.**
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- **Water Splitting Reaction at Polar Lithium Niobate Surfaces.**
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  L. M. Witschen, H. Ghasemzadeh Mohammadi, M. Artmann, and M. Platzner.
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- **Stepwise Growth of Ruthenium Terpyridine Complexes on Au Surfaces.**
  S. K. Peter, C. Kaulen, A. Hoffmann, W. Ogieglo, S. Karthäuser, M. Homberger, S. Herres-Pawlis, and U. Simon. *The Journal of Physical Chemistry C*, 123(11):6537–6548, 2019.
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- **Intensity-Dependent Degenerate and Non-Degenerate Nonlinear Optical Absorption of Direct-Gap Semiconductors.**
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  A. Schulz, C. Wecker, and E. Kenig. In *Jahrestreffen der ProcessNet-Fachgruppe Computational Fluid Dynamics*, 2019.

- **Stofftransport bei der Tropfenbildung.**
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- **Excited-State Band Mapping and Momentum-Resolved Ultrafast Population Dynamics in In/Si(111) Nanowires Investigated with XUV-Based Time- and Angle-Resolved Photoemission Spectroscopy.**
  C. W. Nicholson, M. Puppin, A. Lücke, U. Gerstmann, M. Krenz, W. G. Schmidt, L. Rettig, R. Ernstorfer, and M. Wolf. *Physical Review B*, 2019. doi:10.1103/physrevb.99.155107.

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- **Controlling the Strength of Interaction between Carbon Dioxide and Nitrogen-Rich Carbon Materials by Molecular Design.**
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- **A Branch and Bound Approach for Large Pre-Marshalling Problems.**
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- **Accurate Sampling with Noisy Forces from Approximate Computing.**
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- **Enhancement of the Local Asymmetry in the Hydrogen Bond Network of Liquid Water by an Ultrafast Electric Field Pulse.**
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- **Numerical Simulation of Forced Convection in a Microchannel with Realistic Roughness of 3D Printed Surface.**
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