

Innovatives Supercomputing in Deutschland

InSiDE

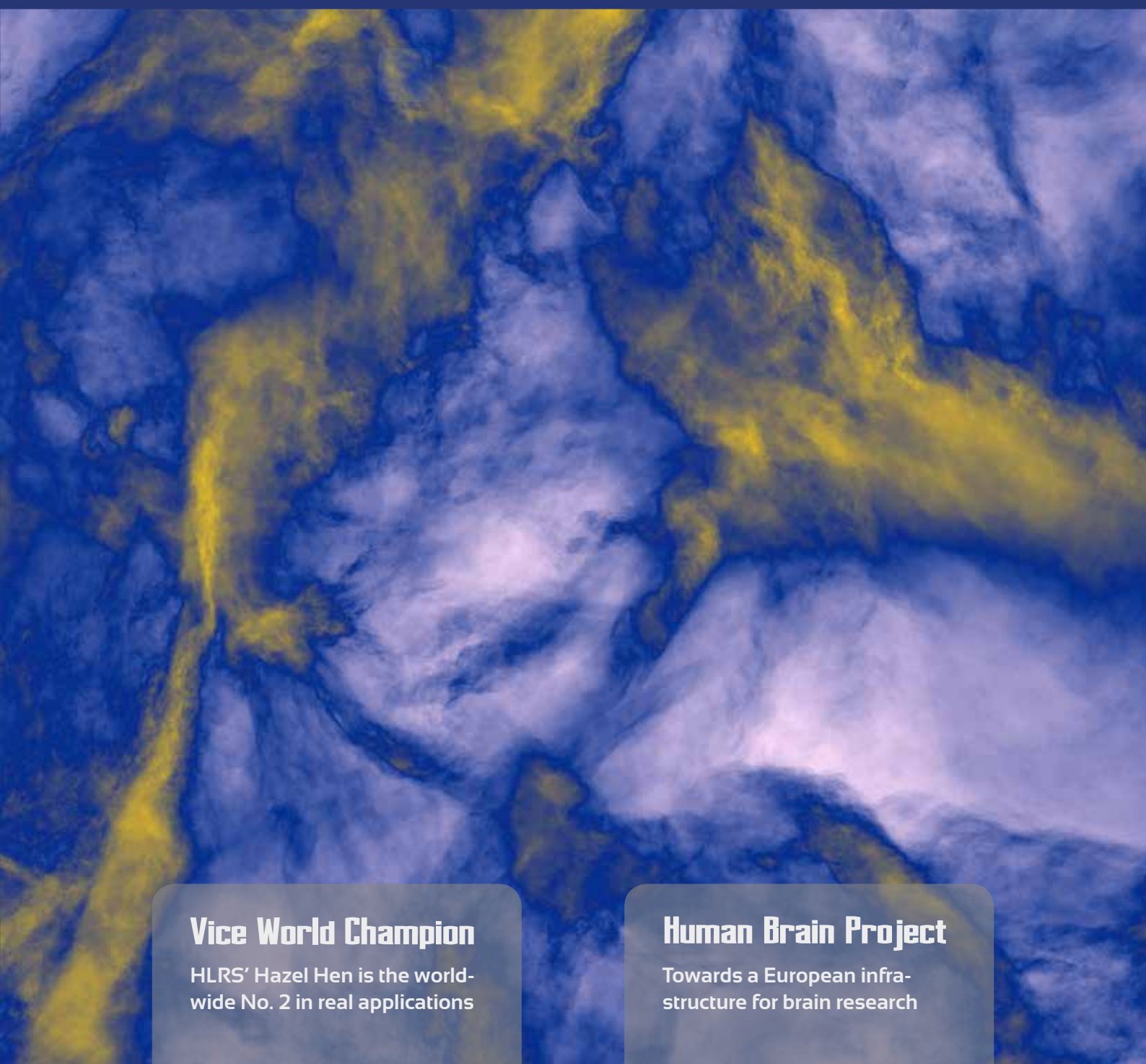
Autumn 2016

Innovative
HPC
in Germany

Vol. 14 No. 2

Turbulence Simulations

The world's largest terrestrial & astrophysical applications



Vice World Champion

HLRS' Hazel Hen is the world-wide No. 2 in real applications

Human Brain Project

Towards a European infrastructure for brain research

Imprint



Prof. Dr. A. Bode
Publisher of InSiDE,
Director of LRZ



Prof. Dr. Dr. Th. Lippert
Publisher of InSiDE,
Director of JSC



**Prof. Dr.-Ing. Dr. h.c. mult.
Prof. E. h. M. M. Resch**
Publisher &
Editor in chief of InSiDE,
Director of HLRS

Editor

F. Rainer Klank, HLRS
klank@hlrs.de

Design

Felicitas Knapp, HLRS
knapp@hlrs.de

Printing

DCC Document Competence Center
Siegmar Kästl e.K., Ostfildern

Cover picture

Christoph Federrath,
Research School of Astronomy and Astrophysics, Australian National University

If you would like to receive InSiDE regularly, please send an e-mail with your postal adress to F. Rainer Klank: klank@hlrs.de

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InSiDE

InSiDE is published two times a year by the
GAUSS Center for Supercomputing (HLRS, LRZ, JSC)

GCS
Gauss Centre for Supercomputing

Editorial

Welcome to this new issue of InSiDE, the journal on Innovative Supercomputing in Germany published by the Gauss Centre for Supercomputing (GCS). A lot has happened over the last months in German High Performance Computing. In June, an administrative agreement for the funding of the next generation of high performance computing systems in Germany was signed by the federal government and the state governments of the states of Baden-Wuerttemberg, Bavaria and North Rhine-Westphalia. We will report on the implications of this agreement for future systems at GCS in the coming issues. Today GCS is running three of the fastest systems in the world with the Cray XC40 "Hazel Hen" at HLRS claiming the title of vice world champion for the HPGMG benchmark.

This issue of InSiDE presents a new layout which brings a slightly modified organization of the content for the reader. We start with a section on the HPC landscape and educational issues—including scientific workshops. You will find the traditional section on applications which covers

a wide spectrum of fields using GCS systems. We highlight a paper on the world's largest turbulence simulation in this issue showing how GCS systems and centers help to support world class science.

The project section highlights the human brain project where JSC takes a leading role both in terms of high performance computing and in terms of modelling and brain research. Finally we have streamlined and shortened our section on centers and trainings since most information is anyway available online.

We hope that we have put together again a mix of information on high performance computing systems, applications, projects and HPC activities that our readers enjoy.

Prof. Arndt Bode
Prof. Thomas Lippert
Prof. Michael Resch

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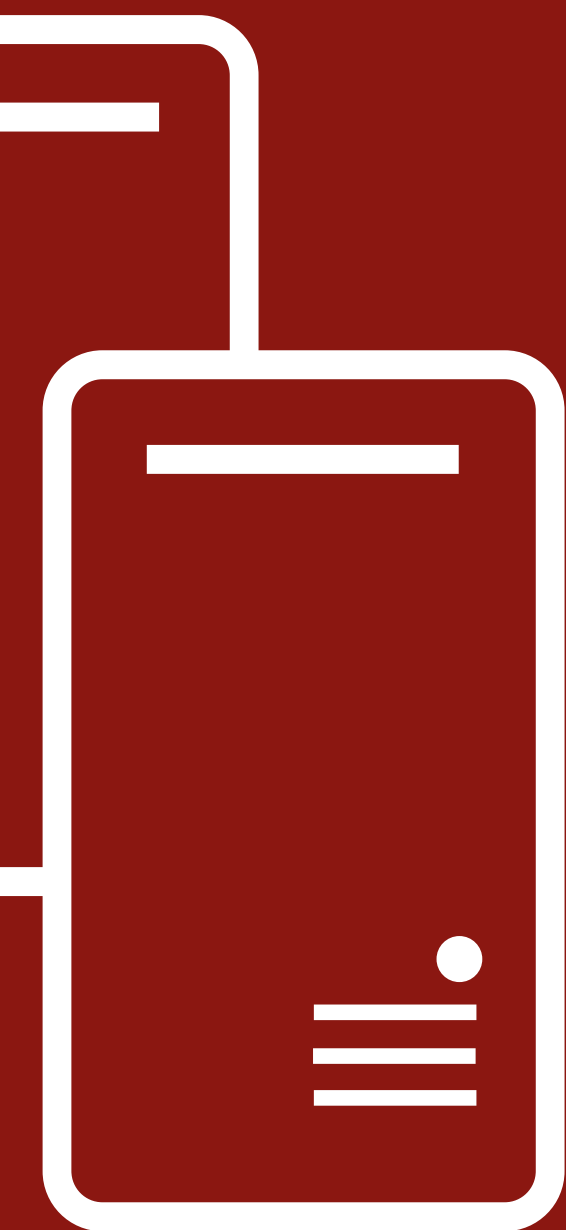
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HPC Landscape



Home & Education

In this section you will find general activities of GCS in the fields of HPC and education.

Gauss Centre for Supercomputing @ ISC'16 (June 19-23)

At ISC'16, the international supercomputing conference held in Frankfurt/Main (June 19–23), the 64 m² large booth of the Gauss Centre for Supercomputing (booth #1310) proved once again to be the pivotal platform for the international scientific and industrial HPC community.



The GCS booth (#1310) at ISC'16.

The open and enticing layout of the booth, designed to encourage the ISC attendees to stop by and interchange with the representatives of the GCS centres HLRS (High Performance Computing Center Stuttgart), JSC (Jülich Supercomputing Centre), and LRZ (Leibniz Supercomputing Centre, Garching/Munich) has again paid off. It attracted countless like-minded researchers, technology leaders, and scientists, amongst other visitors interested in HPC technologies and HPC activities.

The Virtual Reality (VR) presentation set up on the booth by the visualisation team of the HLRS revealed to be a true eye catcher for ISC attendees. The HLRS scientists had used a 3D tiled display in table configuration to interactively investigate data acquired from CT or MRI scans in combination with biomechanical simulations of bone implant compounds, blood flow simulations as well as anatomical structures and forensic data. One of the demonstrations displayed clinical CT-data of a trauma patient. A second demonstration displayed the 3D-image acquired from the torso of a crime victim who had been shot three times and killed. Visitors were able to observe the virtually recreated body structures from all different angles and follow the explanations by the HLRS scientists regarding the analysis and derived insights of the biomechanical simulation results or the reconstruction of the crime scenario.

Extremely well received were also the ISC exhibits arranged by the JSC team. Their in-house developed supercomputing applications and tools,



Uwe Wössner of HLRS gives the VR demonstration.



Wolfgang Frings of JSC explains LLview.

in particular LLview, the interactive monitoring software for supercomputers which demonstrated live the operation of various supercomputers worldwide, found an enormous level of interest. Video showcases of the **LRZ**, presenting SuperMUC user projects respectively activities related to energy efficient data centre management and operation, completed the presentations on the GCS booth which provided a comprehensive demonstration of the wide spectrum of challenging HPC activities the GCS is involved in, underlining GCS's role as a global leader in high performance computing.

GCS Award 2016

At ISC's Research Paper session, Prof. Michael M. Resch, Director of the HLRS, was very pleased to put the spotlight on a young and bright researcher of the University of Bologna. The paper Predictive Modeling for Job Power Consumption in HPC Systems, written and submitted by Mr. Andrea Borghesi (University of Bologna) and his team of five, had been selected by the International Award Committee as the most outstanding research paper submitted at this year's ISC and thus was honoured with the coveted GCS Award 2016. The paper focuses on methods to accurately predict the power consumption of typical supercomputer workloads and provides insight into how to implement and successfully execute power-saving techniques to real working environments. Prof. Resch as chairman of the award committee and Dr. Claus Axel Müller, Managing Director of GCS, handed the award certificate over to Mr. Borghesi, who had introduced his very interesting work to the attentively following large audience attending this ISC research paper session.



From left: Claus Axel Müller (GCS), Andrea Borghesi, Michael M. Resch (HLRS).



Stephanie Wollherr of LMU München presents her research project to the interested audience at ISC.

ISC Conference

In addition to its presentations on the exhibition floor of the ISC, GCS contributed to the HPC conference with numerous talks and presentations in various tutorials and sessions, workshops, and birds-of-a-feather meetings. One of the highlights, brought to the ISC attendees by GCS, was the special conference session Advanced Disaster Prediction and Mitigation, hosted by Prof. Arndt Bode of the LRZ.

Three users introduced their research projects, which they had carried out on the GCS HPC systems Hazel Hen, JUQUEEN, and SuperMUC and provided detailed insight into the challenges of their undertakings and presented their up to now achieved results:

- Safety in the Underground – Coupling CFD with Pedestrian Simulations
Prof. Dr. Armin Seyfried, Jülich Supercomputing Centre & University of Wuppertal

- Large-Scale Multi-Physics Earthquake Scenarios with the ADER-DG Method on Modern Supercomputers
Stephanie Wollherr, Ludwig-Maximilians-Universität München
- Advancing Numerical Weather Prediction & Downscaling Global Climate Models with Emphasis on Weather Extremes
Prof. Dr. Christoph Kottmeier, Karlsruhe Institute of Technology/KIT

Additionally, representatives of the GCS centres supported activities of GCS partners and/or related HPC initiatives, such as by the Partnership for Advanced Computing in Europe (PRACE), European Exascale Projects (DEEP/DEEP-ER, Mont-Blanc, EXDCI), the two European Centres of Excellence CoeGSS and POP, the Jülich-Aachen Research Alliance (JARA), the UNICORE Forum, and others.



The speakers at the GCS conference session, from left: Armin Seyfried, Christoph Kottmeier, and Stephanie Wollherr. Right: Session host Arndt Bode.



HPC system Hazel Hen of HLRS delivers a Linpack performance of 5.64 Petaflops.

TOP500, June 2016

While the Chinese supercomputer Sunway TaihuLight, the new #1 on the 47th edition of the TOP500 list revealed at ISC'16, surprised the global HPC community with its impressive Linpack performance of 93 Petaflops (Rmax), GCS is proud to emphasize that its supercomputing installations Hazel Hen (at HLRS), JUQUEEN (at JSC), and SuperMUC Phase 1 and Phase 2 (at LRZ) continue to represent significant positions in the TOP500. In the list, which enumerates the world's most powerful HPC systems world-wide, Hazel Hen is registered on position 9 (Linpack: 5.64 Petaflops) with which the HLRS supercomputer defended its ranking amongst the top-10 most powerful HPC systems world-wide.

Despite meanwhile being in its 5th year of operation, JSC's JUQUEEN holds an impressive 14th place with its Linpack performance of 5.01 Petaflops. The supercomputing installations at LRZ, SuperMUC Phase 1 on position #27 (Linpack: 2.90) and SuperMUC Phase 2 (#28, Linpack: 2.81), complement the solid and strong outcome of the GCS HPC systems in the current TOP500 rankings. Combined, the GCS continues to provide the by far most powerful HPC platform in all of Europe for research in science and industry. Apart from its world-class performance, the GCS infrastructure excels at its complementary system technologies and architectures to meet the most demanding needs of the individual fields of research.



Written by Regina Weigand
(GCS Public Relations)

Regina Weigand is the Public Relations representative of the Gauss Centre for Supercomputing. In this role, she is responsible for, among other things, organizing GCS's participation in the annually recurring ISC.

Contact: Regina Weigand, r.weigand@gauss-centre.eu

ISC'16 PhD forum And the winner is...

The ISC 2016 conference has organized for the first time the ISC PhD forum. This new event provided an excellent opportunity for PhD students to present their ongoing research to a wide audience of international HPC experts.

The event was conducted in a lively and inspiring setting: First, every student had to summarize their work in a lightning talk within a strict time limit of four minutes. Although there were several students in the early phase of their PhD studies, all participants did a very good job on that challenge. The second stage consisted of a 60 minute poster session in which the

students had the opportunity to present their work in more detail. Both events were very well attended and many lively discussions evolved at the posters. The 14 PhD forum presenters had been selected by an international committee led by Prof. Lorena Barba (George Washington University) out of 28 submissions. Considering oral and poster presentation as well as the research contributions, the committee finally selected Alfredo Parra Hinojosa (TU Munich) to receive the first ISC PhD forum award, which comprised an iPad and a book voucher (sponsored by Springer). His research focuses on tolerating hard and soft faults with the sparse



Impressions from the poster session



grid combination technique and is funded by the DFG SPPEXA priority program through the EXAHD project. Congratulations!

The DFG SPPEXA Priority program supported the event by providing travel funds for all candidates, thus enabling many students from outside Germany to present at the PhD forum.

Next year, ISC will host the PhD forum again. The committee led by Prof. Bill Gropp (University of Illinois at Urbana-Champaign) is looking forward to receiving many high-quality submissions.

Overview of PhD forum presentations:

http://isc-hpc.com/isc16_ap/sessiondetails.htm?tsession&o=309&a=select&ra=byday



Award Ceremony – from left to right: Thomas Meuer, Alfredo Parra Hinojosa, Lorena Barba

Written by Prof. Dr. Gerhard Wellein

(Department of Computer Science, Erlangen-Nürnberg University)

Contact: Gerhard Wellein, Gerhard.Wellein@rzr.eu-erlangen.de

Vice World Champion is located in Stuttgart



Supercomputer „Hazel Hen“ received top grades for its performance under real working conditions.

The supercomputer „Hazel Hen“, a Cray XC40 system located at HLRS, is the second best system in the world regarding its performance under real application conditions. This is a result of the High Performance Geometric multigrid (HPGMG) benchmark, which was published at the International Supercomputing Conference (ISC) in Frankfurt in 2016.

Hazel Hen exploits its strengths in real applications

The supercomputer surpassed much more expensive and larger systems in the HPGMG ranking. Only the system „Mira“, located at Argonne National Laboratory in the USA ($5.00e^{11}$ DOF/s), achieved better results than Hazel Hen ($4.95e^{11}$ DOF/s). The HLRS system could even be well ahead of systems which got better results in the Top500 world ranking.

Number 9 in Top500 list

As the fastest supercomputer in the EU, Hazel Hen currently ranks at the ninth place in the worldwide TOP500 List. Unlike this Linpack benchmark the HPGMG benchmark doesn't examine the theoretical performance of the system, but focuses on the benefits for users in practical application. The base of the HPGMG benchmark is a geometric multigrid solver, which is for example also used in fluid dynamics calculations.

"We are proud to have defended our position in the top 10 in the TOP500 list. But our excellent results in HPGMG benchmark, a test under real working conditions, is much more important. The benefits for our users are our top priority", says Prof. Michael Resch, Director of HLRS.

Written by Felicitas Knapp

(High-Performance Computing Center Stuttgart (HLRS), Germany)

Contact: Felicitas Knapp, knapp@hlrs.de



Prototyping next-generation supercomputing architectures: ISC'16 Workshop



Developing Next-gen HPC Architectures

Thu June 23, 2016

Marriott Hotel, Frankfurt / Germany

The DEEP-ER and Mont-Blanc projects organised an ISC'16 workshop on prototyping.

At this year's ISC'16, the DEEP-ER and Mont-Blanc projects, two European funded FP7 Exascale initiatives, co-organised a workshop on hardware prototyping for next-generation HPC architectures. The event took place on Thursday, June 23, 2016 at the Marriot Hotel in Frankfurt, Germany.

The evolution curve of the computational power of supercomputers is getting flat and after hitting the frequency wall, the HCP community is facing a critical point for Moore's law. For these reasons experimenting with novel architectures is a must. While the trend towards heterogeneous computing in the form of coprocessors, accelerators or on-chip helper cores is more evolutionary, revolutionary approaches like neuromorphic computing are in the limelight, as well. Their common goal is to increase performance while being energy efficient. Yet, all those concepts and ideas need to be demonstrated and verified with prototypes.

With strong involvement of the GCS members JSC and LRZ, the DEEP-ER and Mont-Blanc organisation team put together a compelling workshop programme featuring the aforementioned diverse range of approaches. Whereas the first session was devoted to ARM-based prototyping, the second session focused on Intel Xeon Phi architectures, e.g. the QPACE 1 and 2 projects carried out at Universität Regensburg. Special contributions to the workshop included a keynote by Prof Toshihiro Hanawa from the Tokyo University and Prof Steve Furber from the University of Manchester. Prof Hanawa added some international perspective to this European workshop and talked about research projects developing innovative interconnection prototypes using FPGA technology. The invited talk by Prof Furber detailed the SpiNNaker project, based on ARM cores and going into the direction of neuromorphic computing.

More information on the workshop is available on this website:

<http://www.deep-er.eu/press-corner/events/past-events/25-isc16-prototyping-workshop.html>

Compute Cloud Training at LRZ



On July 5, 2016, LRZ organised a training for their Compute Cloud. The purpose of the workshop was to introduce the service to beginners and to give an overview on the functionalities.

Next to a general introduction to the concept of Cloud Computing and details on the LRZ service, the training featured two sessions for hands-on training. In these sessions, best practices were covered to address the most common tasks and challenges for basic and advanced use cases in the Cloud.

The Compute Cloud is an additional HPC resource at Leibniz Supercomputing Centre which has been officially launched as a service in early 2015. The main purpose is to provide scientific customers with HPC resources needed on short notice. Hence, users are not required to issue an official application via a GAUSS or PRACE call. The Compute Cloud allows them to adjust the resources dynamically and very flexibly according to their needs and offers the possibility to create a personalised environment as it is an Infrastructure-as-a-Service (IaaS) solution based on the open source software OpenNebula.

The training material is accessible via this website: http://www.lrz.de/services/compute/cloud_en/training/2016/
More information on the service itself can be found here: http://www.lrz.de/services/compute/cloud_en/



First JARA-HPC Symposium

The first JARA-HPC Symposium took place in Aachen, Germany, from October 04–05, 2016. The symposium was jointly organized by the Forschungszentrum Jülich and RWTH Aachen University in the framework of the Jülich Aachen Research Alliance (JARA).

systems are increasingly used for data analytics and complex workflows. Successful application development requires collaboration between the domain scientists on one side, and computer science/HPC experts on the other.



The IT Center of RWTH Aachen University hosted the JARA-HPC Symposium 2016.

JARA-HPC is the High Performance Computing section of JARA. Its scientists combine the knowledge of massively parallel computing on supercomputers with the respective expert competences from different research fields.

JARA-HPC organized this symposium to motivate lively discussions on the various aspects of the development of HPC applications among experts. About 60 participants had the opportunity for an in-depth exchange with colleagues from different research fields who also make use of HPC systems in their scientific work.

Current HPC systems consist of complex configurations with a huge number of components, very likely heterogeneous, and typically with not enough memory. The hard- and software configuration can change dynamically due to fault recovery or power saving procedures. Deep software hierarchies of large, complex software components are needed to make efficient use of such systems. On the applications side, HPC

The program comprised a keynote by Victor Eijkhout of the Texas Advanced Computing Center (TACC), followed by two days of presentations on diverse topics in scientific computing. A topical focus was placed on Aeroacoustics and CFD in HPC during a mini-workshop on the second day. The symposium closed with a panel on software engineering in HPC.

Marc-Andre Hermanns, Bernd Mohr
(Jülich Supercomputing Centre (JSC), Germany)

Contact: Marc-Andre Hermanns,
m.a.hermanns@fz-juelich.de

Michaela Bleuel
General Manager, JARA-HPC, Germany

Big BlueGene Week at JSC on JUQUEEN

Capability computing is a major pillar of advances in computational science. Governed by the paradigm of solving otherwise intractable single scientific problems by means of extremely large parallel computing architectures, it is distinct and complementary to capacity computing. At the same time, contemporary HPC facilities aim at providing services for both these demands, which can compromise in particular the potential of capability computing. JSC thus decided to favour very large compute jobs on JUQUEEN, its IBM BlueGene/Q HPC system within a special event over a whole week. From June 14 to 20 JUQUEEN was dedicated exclusively to large-scale massively parallel computations.

The response to this offer was tremendous, with users taking the chance to execute some of their scientifically and computationally most demanding simulations in full parallelism on up to 458.752 compute cores. More than 77% of the available time was used for true full machine runs, and in total 22 users could complete 84 jobs, which amounts to about 70 Mio core-h. The availability of the system during the week was higher than 93%, demonstrating a remarkable level of reliability. The event served various scientific use cases in topics such as turbulent fluid dynamics, neuroscience, elementary particle physics, molecular dynamics and complex stencil code development. Modeling the propagation of polarized light through brain tissue by means of a massively parallel three-dimensional Maxwell solver to enhance the understanding of the structural organization of the human brain, and simulating the mixing of

species in a turbulent decaying flow as it occurs in various practical situations are examples for specific problems addressed.

JUQUEEN BigWeek – case study „turbulent flows“

The turbulent motion of fluid is still one of the unsolved problems of classical physics and its description remains challenging. The understanding of turbulent flows and turbulent mixing is of great interests for many applications. Prominent examples are the turbulent combustion of chemical reactants and the dynamics of the atmosphere or the oceans. As a continuum field phenomenon, turbulence is in principle infinite-dimensional and strongly non-local and

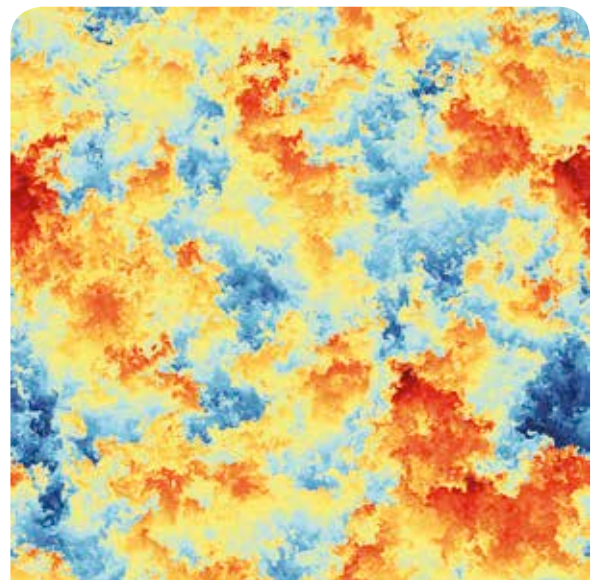


Fig. 1: Two-dimensional slice through the field of the passive scalar. Large coherent regions are separated by sharp highly convoluted boundaries. Resolving all relevant scales with high accuracy requires access to the complete 28 racks of the JUQUEEN supercomputer.



non-linear. The temporal and spatial evolution of a velocity field is described by the Navier-Stokes equations, which contain all necessary information to fully characterize the motion of turbulent flows. Although the Navier-Stokes equations are formally deterministic, turbulence dynamics are by no means the same.

Even for the simplest turbulent flows, an analytical solution of the Navier-Stokes equations is not known. Therefore, a solution of the Navier-Stokes equations can only be obtained by numerical methods. Direct numerical simulation (DNS) has become an indispensable tool in turbulence research. DNS solves the Navier-Stokes equations for all scales down to the smallest vortices and can be regarded as a numerical experiment.

The DNS of decaying homogeneous isotropic turbulence is a canonical case of significant interest. Performing DNS of decaying turbulence at high Reynolds numbers is challenging as two opposing constraints need to be satisfied: it is necessary to accurately resolve the smallest length scales by the numerical grid, while keeping the largest length scales small compared to the size of the numerical domain to reduce confinement effects. Based on the highly optimized simulation code psOpen/nb3dfft [1, 2] a direct numerical simulation (DNS) of decaying turbulence with more than 231 Billion grid points was

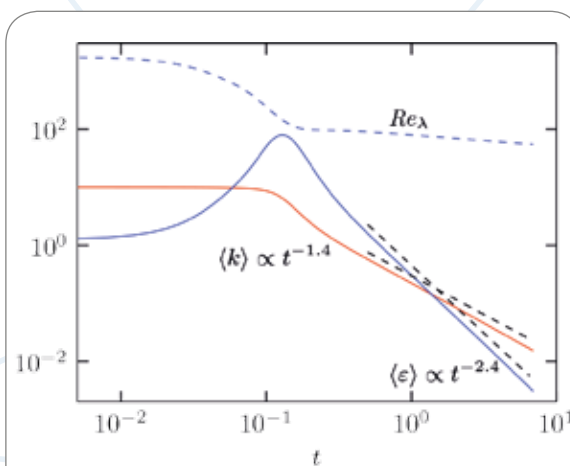


Fig. 2: Temporal evolution of the turbulent kinetic energy $\langle k \rangle$, dissipation $\langle \epsilon \rangle$, and Taylor length-scale based Reynolds number Re_λ . The indicated decay exponents are very close to the theoretical prediction. A high resolution of the direct numerical simulation (232 billion grid points) is essential to provide a well defined turbulent flow at $t = 1$, when turbulence becomes self-similar and suitable for further analysis.

carried out during the big-week. With access to the complete 28 racks of the JUQUEEN supercomputer it was possible to perform DNS of decaying turbulence in a thus far not reached accuracy and resolution. The high resolution is essential during the transition and the early decay phase.

This simulation contributes to a better understanding of turbulent flows and the self-similarity during decay.

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Line segments in homogeneous scalar turbulence. Physics of Fluids (1994-present) Vol. 27 Nr. 9 (2015) pp. 095102. AIP Publishing.
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Direct Numerical Simulation of Fluid Turbulence at Extreme Scale with psOpen. Advances in Parallel Computing Vol. 27 pp. 777-785 (2016). International Conference on Parallel Computing, ParCo 2015, Edinburgh, Scotland, UK.

Due to the positive response, JSC is considering to repeat this type of event and encourages all users with suitable codes and applications to join in and report on their experiences. All users interested in further information are invited to contact JSC via sc@fz-juelich.de.

International Workshop „Quantum Annealing and its Applications in Science and Industry“ [QuAASI'16]

The international workshop „Quantum Annealing and its Applications in Science and Industry (QuAASI'16)“ took place from 26 to 28 July 2016 in the Rotunda of the Jülich Supercomputing Centre. The goal of the two-day workshop, followed by a D-Wave Exploration Day, was to bring together researchers from different communities to discuss both the challenges in using quantum annealing to approach the solution of real-world problems and the requirements on optimization and design of existing and future quantum annealing hardware.

About 60 researchers from Germany, Switzerland, the Netherlands, the United Kingdom, the United States and Canada participated in the workshop. The history of quantum annealing

and the design of D-Wave's quantum processors, the implementation of various optimization problems and machine learning on D-Wave machines, the study of the behavior and performance of D-Wave quantum computers, the various approaches designed to extend the applicability of these devices to larger, more connected optimization problems, and related topics were highlighted in the talks. The D-Wave Exploration Day provided detailed insights into the hardware architecture. Programming techniques and tools available were demonstrated by remotely running examples on one of the D-Wave 2X™ quantum computers with more than 1000 qubits located at the headquarters of D-Wave Systems in Burnaby, Canada.





Discrete optimization and quantum annealing

Optimization challenges are ubiquitous. They affect the sciences and the whole of society directly and indirectly. They comprise, among others, flight and train scheduling, vehicle routing, power trading and scheduling, supply chain network optimization, planning and scheduling of production processes, organ allocation and acceptance optimization, cancer radiation treatment scheduling, and optimizing target interactions for drug design. Optimization also lies at the heart of machine learning, artificial intelligence, computer vision and data mining.

In many of these practical optimization problems the task is to find the best solution among a finite set of feasible solutions. Such problems are formulated as discrete optimization problems. A standard way for solving discrete optimization problems is to first construct an integer or mixed-integer programming model, involving discrete or both continuous and discrete variables, and then use a software package such as CPLEX to solve the constructed model.

The new strategy proposed is to use quantum annealing for solving those optimization problems which can be mapped to a QUBO, a quadratic unconstrained binary optimization problem. Quantum annealing is a new technique, inspired by the classical simulated annealing techniques which are based on temperature fluctuations, for finding the global minimum of a quadratic function of binary variables by exploiting quantum fluctuations. Its main potential

targets are combinatorial optimization problems featuring a discrete search space with many local minima. Many challenging optimization problems playing a role in scientific research and in industrial applications naturally occur as or can be mapped by clever modeling strategies to QUBOs.

D-Wave Systems

D-Wave Systems, founded in 1999, is the first company that has commercialized quantum annealers to carry out quantum computations. Their quantum annealers are programmable artificial spin systems manufactured as integrated circuits of superconducting qubits. Qubits or quantum bits are the elementary building blocks of a quantum computer, similar to the bits in a digital computer. The latest D-Wave quantum computers, D-Wave 2X™ systems, operate with more than 1000 qubits and over 3000 couplers connecting the qubits for information exchange. The D-Wave 2X™ niobium quantum processor, a complex superconducting integrated circuit containing more than 128,000 Josephson junctions, is cooled to 15 mK and shielded from external magnetic fields, vibrations and external radiofrequency fields of any form. A D-Wave 2X™ system requires less than 25 kW of power, most of which is consumed by the refrigeration system and the front-end servers. Currently, D-Wave Systems is testing their next generation of quantum computers having more than 2000 qubits. These new systems are scheduled for release in mid 2017.



D-Wave quantum processors are capable of solving QUBOs by mapping binary variables to qubits and correlations between variables to couplings between qubits. During a “quantum computation”, the system of interacting qubits evolves according to a quantum adiabatic annealing process. At the end of this process the qubits are read out to get the optimal or near optimal solution of the optimization problem.

Current D-Wave quantum processors have a so-called Chimera graph architecture, thereby

connecting a given qubit with at most six other qubits. Solving optimization problems on such an architecture requires the embedding of the problems on the Chimera graph. This obviously limits the range of optimization problems that potentially can be solved on such a machine, but nevertheless, some very hard real-world optimization problems might be among them. Hence, exploring the potential of quantum annealing on this operational prototypic hardware for some real world problems is a challenge that should be taken up.

Written by Prof. Kristel Michielsen , Prof. Thomas Lippert
(Jülich Supercomputing Centre (JSC), Germany),

Prof. Wolfgang Marquardt
(Chairman of the Board of Directors, Forschungszentrum Jülich)

Contact: Kristel Michielsen, k.michielsen@fz-juelich.de



Fourth Extreme Scale Workshop at the Leibniz Supercomputing Centre

The fourth „Extreme Scale“ workshop on SuperMUC was conducted from February 29, 2016 until March 3, 2016 at LRZ with the goal of the optimization of existing and new Peta-scale applications. 13 projects participated in the workshop with 7 new projects who participated the first time. 11 Projects succeeded in full scaling on all the nodes of SuperMUC Phase I.

As in the workshops before, the scientists were able to perform scale-out tests on SuperMUC, this time on the whole Phase I Partition, which consists of 9216 Nodes featuring 2 Intel Xeon E5-2680 “Sandy Bridge” Processors with a total of 147456 cores and a total memory of 131 TB. During the Extreme Scale workshop a total of 14.1 Mio CPUh were available to the participants which could be used for short debug and test jobs during the day and larger production runs with a maximum of 6 hours runtime during the night.

For the first time, the “Leibniz Extreme Scale Award” for the best scaling behavior of a program on SuperMUC Phase I was awarded. The winner of the award was the program VERTEX which showed linear strong scaling on the whole SuperMUC Phase I. The award was presented by Prof. Bode (Chair of the Board of Directors of the LRZ) to the team leader of VERTEX, Dr. Andreas Marek.

The participating projects of the fourth “Extreme Scale” workshop were:

1. INDEXA (CFD), TU München (M. Kronbichler)
2. MPAS (Climate Simulation), KIT (D. Heinzeller)
3. Inhouse (Material Science), TU Dresden (F. Ortmann)
4. HemeLB (Life Science, Bloodflow Simulation), UCL (P. Coveney)
5. KPM (Chemistry), FAU Erlangen (M. Kreutzer)
6. SWIFT (Astro), University of Durham (M. Schaller)
7. LISO (CFD), TU Darmstadt (S. Kraheberger)
8. ILDBC (Lattice Boltzmann) FAU Erlangen (M. Wittmann)
9. Walberla (Lattice Boltzmann), FAU Erlangen (Ch. Godenschwager)
10. GPI (Parallelization Framework), Fraunhofer, (M. Kühn)
11. GADGET (Astro), LMU München (K. Dolag)
12. VERTEX (Astro), LMU München (T. Melson)
13. PSC (Plasma), LMU München (K. Bamberg)

In the following the results of two participating projects are discussed further:

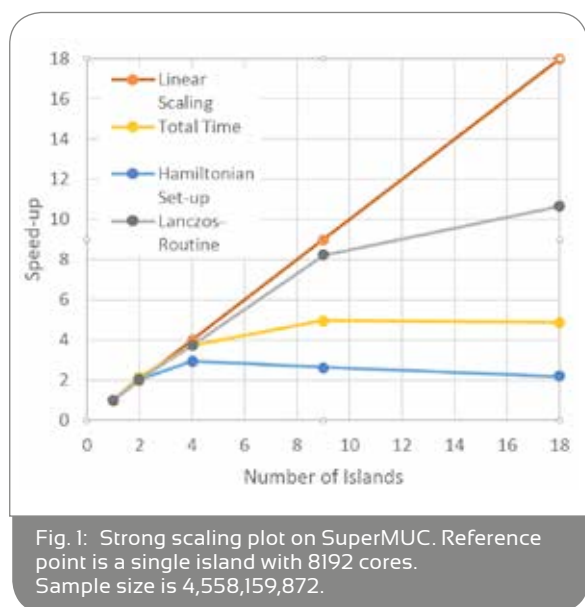
Linear-Scaling Transport Approach for Innovative Electronic Materials (F. Ortmann, TU Dresden)

Topological insulators are a new state of quantum matter, which exist in two and three dimensions and can be realized in certain materials and compounds. We use time-propagation Kubo methodology implemented in a highly efficient and MPI parallel real-space code. The order-N scaling with sample size (N) of the implemented algorithm

potentially allows to tackle macroscopic 3D samples and study realistic structures, thus providing unprecedented insight into the transport physics of novel exciting material classes.

Scaling of the Code

We demonstrate here that the dominating part of the code which is the Lanczos routine for matrix-vector multiplication scales very well beyond 32,768 cores on SuperMUC. For this intensive part, we measure a speed-up of 8.2 on 73,728 cores (9 islands) compared to a single island (grey line in figure 1). This corresponds to 91% efficiency.



When increasing the number of processes by another factor of 2 for the full phase I of SuperMUC (18 islands), we observe only a speedup of 1.3 for this last step. This leads to a significant drop in total efficiency to 59% (speedup of 10.7

compared to 1 island). Further analysis of this effect indicates that the domain size which is handled by a single MPI process has dropped down to only 30,912 sites (orbitals) when running on the full machine. Therefore, the work load that is performed on the processes without communication (internal part of matrix-vector multiplication) is strongly reduced (strong scaling approach) such that communication starts to become much more relevant.

Another important observation from our runs concerns another part in the code which, at the scale of extreme scaling, becomes apparent in figure 1. Here we identify mainly the random-number generation of the initial random-phase state and of the potential in the Hamiltonian, which takes 70 sec and 264 sec, respectively for the 18-islands run. Here we identify a bottleneck in the scaling which can be removed in subsequent work by using a parallel generator.

Performance analysis

With likwid we measured branching rate, flops and memory consumption of the intensive computation part doing the matrix-vector multiplications (Lanczos recursion). Thanks to a hint by LRZ staff Fabio Baruffa, we found out, that the main loop can be optimized, since renaming of variables and unnecessary branching is occurring. By restructuring the loop, we were able to increase the MFLOPS value in the loop from 867 to 1097. At the same time, we observed a reduction of the corresponding memory usage per MFLOP (from 1.87 MB to 0.94 MB). Further analysis and optimization is ongoing.



Using allinea, we did a comprehensive analysis of memory usage, MPI communication and pure computation time. We found out, that for large sample sizes per core, which amounts to a bigger work load for each core, the communication can be neglected in terms of the total time. The code is then computation (memory) bound. Most time is spent in the main matrix–vector loop. In this loop, 80% of the computation time is due to memory access. The performance can thereby be enhanced by making the loop more compatible to vectorization, which is current work in progress in collaboration with LRZ experts. By lowering the sample size per core, corresponding to a ‘strong scaling’ to higher number of tasks, the MPI communication increases from 2% up to 15%, explaining the scaling behavior at large scales. This effect occurs due to the delay happening at MPI_receive.

Reverse Time Migration with GPI-2

(M. Kühn, Fraunhofer ITWM, Kaiserslautern)

Reverse Time Migration (RTM) is a seismic imaging method delivering high quality results for oil and gas exploration. Solving the full wave equation it tracks very well the steep dips and complex overburdens. It is applicable for wide azimuth data sets as well as anisotropic velocity models (TTI). The zero lag correlation of a forward modeled acoustic source signal (shot) and the backward modeled receiver signals delivers a high quality partial image (figure 1). Although a typical data set consists of ten thousands of independent shots, the quick processing of a few decisive shots is intriguing e.g. for the interactive modeling of salt domes.

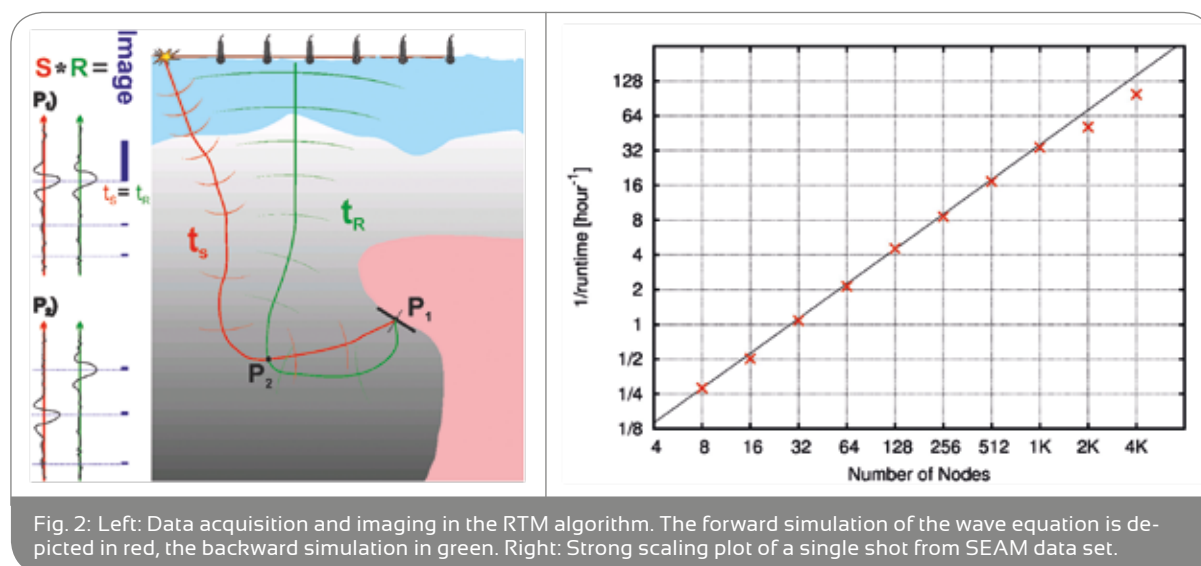


Fig. 2: Left: Data acquisition and imaging in the RTM algorithm. The forward simulation of the wave equation is depicted in red, the backward simulation in green. Right: Strong scaling plot of a single shot from SEAM data set.

Our RTM implementation (FRTM) models the wave equation using a Finite Differences (FD) scheme on a regular grid. The parallelization approach for each shot is a static domain decomposition on a regular grid with halo exchanges. The latter are executed fully asynchronously in a data dependency driven scheme. This scheme replaces completely the barriers that would typically be applied between the time steps in standard implementations. It allows superior strong scaling by relaxation of the synchronization between the compute nodes. Our communication library GPI-2 is the appropriate tool to implement this communication pattern efficiently [1].

Our benchmark calculates a single shot at 15Hz of the well established synthetic SEAM benchmark [2]. The velocity is modeled as Tilted Transverse Isotropic (TTI), the simulation domain has 800x915x1291 voxels and the wave equation is discretized with an 8th order stencil in space and 2nd order in time. The strong scaling plot in figure 1 shows almost perfect scaling up to 1024 nodes and still well scaling properties up to 4K nodes (72% efficiency at 4K nodes). At 4K compute nodes we have a run time of 2 milliseconds for each simulated time step which corresponds to an average total network bandwidth of approximately 8 terabyte per second. The maximum floating point performance (SP) is about 310 TFlop/s.

Beyond 1K nodes the domain decomposition produces very small subdomains consisting of boundary elements only. This situation tightens the coupling between subdomains and reduces the overlap of communication by computation. This explains well the drop in parallel efficiency observed in the scaling plot. However, even under these unfavorable circumstances our approach is able to scale further to a higher absolute performance.

References

- [1] **GPI-2:**
<http://www.gpi-site.com>
- [2] **SEAM Benchmark:**
<http://www.seg.org/resources/research/seam>

Written by Ferdinand Jamitzky, Helmut Brühle, M. Kühn & F. Ortmann
(Leibniz Supercomputing Centre)

Contact: Ferdinand Jamitzky, jamitzky@lrz.de



“Intel MIC Programming” & “HPC for Water Related Hazards” Workshops @ LRZ



Fig. 1: Participants of the “Intel MIC Programming Workshop” at LRZ, June 27–29, 2016. The main speakers in the first row are holding Intel Xeon Phi coprocessors.

To foster the Czech-German collaboration in high performance computing, the Leibniz Supercomputing Centre (LRZ), the Department of Informatics of TUM and the National Supercomputing Centre of the Czech Republic, IT4Innovations, recently joined forces and established the Czech-Bavarian Competence Centre for Supercomputing Applications (CzeBaCCA).

IT4Innovations at Ostrava is hosting the Salomon supercomputer, the largest Intel Xeon Phi based system currently operating in Europe. Besides their joint research program around simulation

software and tools for Salomon, one of the main objectives of the new Competence Centre is to organise a series of scientific workshops and Intel MIC (Many Integrated Core) architecture specific trainings.

The first series of workshops took place in Ostrava in February 2016 and combined a two-day “Intel MIC Programming Workshop” with a one-day scientific workshop “SeisMIC – Seismic Simulation on Current and Future Supercomputers” (see InSiDE Vol. 14 No. 1 p. 76f).



IT4Innovations
national
supercomputing
center



Fig. 2: Participants of the scientific workshop “High Performance Computing for Water Related Hazards” at LRZ, June 29–July 1, 2016.

The second series of workshops took place at LRZ in Garching in June 2016 and combined a three-day “Intel MIC Programming Workshop” (June 27–29, 2016) with a three-day scientific workshop on “High Performance Computing for Water Related Hazards” (June 29–July 1, 2016). To create synergy effects between the different communities, both events shared a plenum session about Intel MIC experience on June 29.

The Intel MIC Programming Workshop attracted 50 participants from the Czech Republic, Finland, Germany, Italy, Spain and UK (see figure 1). The first two days provided an introduction about the Intel Knights Corner architecture and various Intel Xeon Phi programming models. The talks by LRZ staff members were interleaved with many hands-on sessions. The hands-on sessions were done on the SuperMIC system at LRZ, which was exclusively reserved for the workshop. On the last day Dr.-Ing. Jan Eitzinger from the Regional Computing Centre in Erlangen (RRZE) presented advanced MIC programming techniques such as SIMD or assembly programming. Mr. Andrey Semin from

Intel presented the newest version of the Intel Xeon Phi Knights Landing architecture, which has been launched on the International Supercomputing Conference (ISC) in Frankfurt just one week before the workshop. In a plenum session 7 invited speakers from Intel, RRZE, IPP, IT4Innovations, TUM and LRZ talked about experiences and best practices using Intel Xeon Phi based systems like e.g. Salomon @ Czech Republic, HELIOS @ Japan or SuperMIC @ LRZ. A guided tour of the Weißenstephan brewery, the oldest still-operating brewery in the world (see figure 3), and a self-paid dinner at the brewery restaurant, has been organised as social event.

The Intel MIC Programming Workshop was followed by a three-day scientific workshop about “High Performance Computing for Water Related Hazards” with 44 participants from the Czech Republic, Finland, Germany, Hungary, Italy, Netherlands, Norway, UK and USA (see figure 2). The focus of this workshop was on the simulation of environmental catastrophes caused by water. The researchers discussed various aspects of



water related natural disasters: online prediction systems for floods, rain-induced flooding, simulation of storm surges and tsunamis, rise of the sea level by melting glaciers and similar events. A special focus was on demands and desired features of (future) simulation software, parallelisation for current and novel HPC platforms, as well as establishing scalable simulation workflows on supercomputing environments. A special session on "Flood Simulation in Bavaria" with invited speakers from the research areas hydrology, regional climatology, earth and environmental sciences concluded the workshop. With the recent floods in Bavaria the workshop gained unexpected local importance.

The next series of workshops will take place at IT4Innovations in early 2017. Planned is an Intel MIC workshop concentrating on simulations on the Salomon machine combined with a scientific workshop on "HPC for Atmospheric Models and Air-Related Environmental Issues".

Acknowledgements

The Czech-Bavarian Competence Centre for Supercomputing Applications is funded by the Federal Ministry of Education and Research. The



Fig. 3: Participants enjoying the guided tour of the Weihenstephan brewery during the social event.

Intel MIC programming workshop was financially also supported by the PRACE-4IP project funded by the European Commission's Horizon 2020 research and innovation programme (2014-2020) under grant agreement 653838.

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- <https://www.lrz.de/forschung/projekte/forschung-hpc/CzeBaCCA/>
- <http://www.lrz.de/services/compute/courses/>
- <http://www.training.prace-ri.eu/>

Written by Michael Bader,

(Technical University of Munich (TUM), Germany)

Momme Allalen, Fabio Baruffa, Arndt Bode, Anton Frank, Volker Weinberg,

(Leibniz Supercomputing Centre (LRZ), Germany)

Ondřej Jakl, Branislav Jansík, Martin Palkovic, Vít Vondrák

(IT4Innovations, Czech Republic)

Contact: Volker Weinberg, Volker.Weinberg@lrz.de

21st VI-HPS Tuning Workshop at LRZ

On 18-22 April 2016 the Leibniz Supercomputing Centre hosted the 21st VI-HPS Tuning Workshop in a very fruitful cooperation with the Jülich Supercomputing Centre (JSC) and the VI-HPS consortium. This series of tuning workshops gives an overview of the VI-HPS performance analysis and tuning tools suite, explains the functionality of individual tools and how to use them effectively, and offers hands-on experience and expert assistance using these tools on participants' own applications.

The Virtual Institute High-Productivity Supercomputing (VI-HPS) combines the expertise of twelve partner institutions spread around the globe, each with a strong record of high-performance computing research. Its partners have long experience in the development and application of HPC programming tools and host well-known tool projects that are contributing leading-edge technology to this partnership. Most of these tools are open source and freely available to the HPC user communities.

The 5-day workshop attracted over 35 international participants. Talks were given by 15 lecturers from 9 VI-HPS member institution—a record in the long history of VI-HPS tuning workshops which was initiated in 2008.

The following 14 HPC tools were covered during the workshop:

- Score-P instrumentation and measurement
- Scalasca automated trace analysis
- Vampir interactive trace analysis
- Periscope/PTF automated performance analysis and optimisation
- Extra-P automated performance modeling
- Paraver/Extrae/Dimemas trace analysis and performance prediction
- [k]cachegrind cache utilisation analysis
- MAQAO performance analysis & optimisation
- MAP+PR profiling and performance reports
- mpiP lightweight MPI profiling
- Open|SpeedShop profiling and tracing toolset
- MUST runtime error detection for MPI
- ARCHER runtime error detection for OpenMP
- STAT stack trace analysis

The participants especially appreciated the opportunity to optimise their own code during many hands-on sessions with direct help by the instructors, who were in most cases also the developers of the tools. Hands-on sessions were done on the symmetric multiprocessing (SMP) system SGI UltraViolet at LRZ, which was exclusively reserved for the workshop. Also, the organisational efforts of the VI-HPS consortium were greatly acknowledged by the participants.



Fig. 1: Participants of the "21st VI-HPS Tuning Workshop" hosted by LRZ in front of the Weihenstephan Brewery during the social event.

A social event consisted of a guided tour of the Weihenstephan Brewery, the oldest still-operating brewery in the world (see figure 1), followed by a self-paid dinner at the brewery restaurant which encouraged intensive participant and instructor networking in a relaxed environment.

Slides of the workshop are available at:

<http://www.vi-hps.org/training/tws/tw21.html>

The workshop was a PRACE Advanced Training Centre (PATC) event financially supported by the PRACE-4IP project funded by the European Commission's Horizon 2020 research and innovation programme (2014-2020) under grant agreement 653838.

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<http://www.training.prace-ri.eu/>



Written by Anupam Karmakar, Volker Weinberg,

(Leibniz Supercomputing Centre (LRZ), Germany)

Brian Wylie

(Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich, Germany)

Contact: Volker Weinberg, Volker.Weinberg@lrz.de

Fiber optics study in regard of animation and VFX companies

The ASAPnet study was dealing with the problem of the lack of an affordable glass fiber network for animation and VFX studios in the region of Stuttgart. In the focus of the study was furthermore an improvement of the access to the computational power of the High Performance Computing Center Stuttgart. The various sections of the topic, such as the short project times of the animation industry but also the obstacle of the software integration were comprehensively processed and solutions proposed. The Media Solution Center BW (MSC, www.msc-bw.de) project of HLRS was not only involved in the preparation of the study, but is also part of those solutions.

Initial impulse

In 2014 the majority of the frames for the "Maya the Bee" movie were rendered at HLRS. At that time, the large amounts of data had to be transported on hard drives via public transport to the HLRS for the rendering process. Which is especially alarming as Stuttgart is one of Germany's leading cities, when it comes to animation and visual effects. Since the described procedure, which found its way into the local press under the term "sneaker network", not exactly matches the political aim of digitalisation, the Economic Development Corporation for the Region of Stuttgart (Wirtschaftsförderung

Region Stuttgart) in cooperation with the media and film society Baden-Württemberg GmbH (Medien- und Filmgesellschaft, MFG) initiated a study in order to analyze the problem in detail. The SICOS BW GmbH was involved as a partner, in this context also as a representer for HLRS and as an expert for technology transfer towards small and medium enterprises.

The map (figure 1) gives an overview of the geographical distribution of the involved and participating institutions and companies:

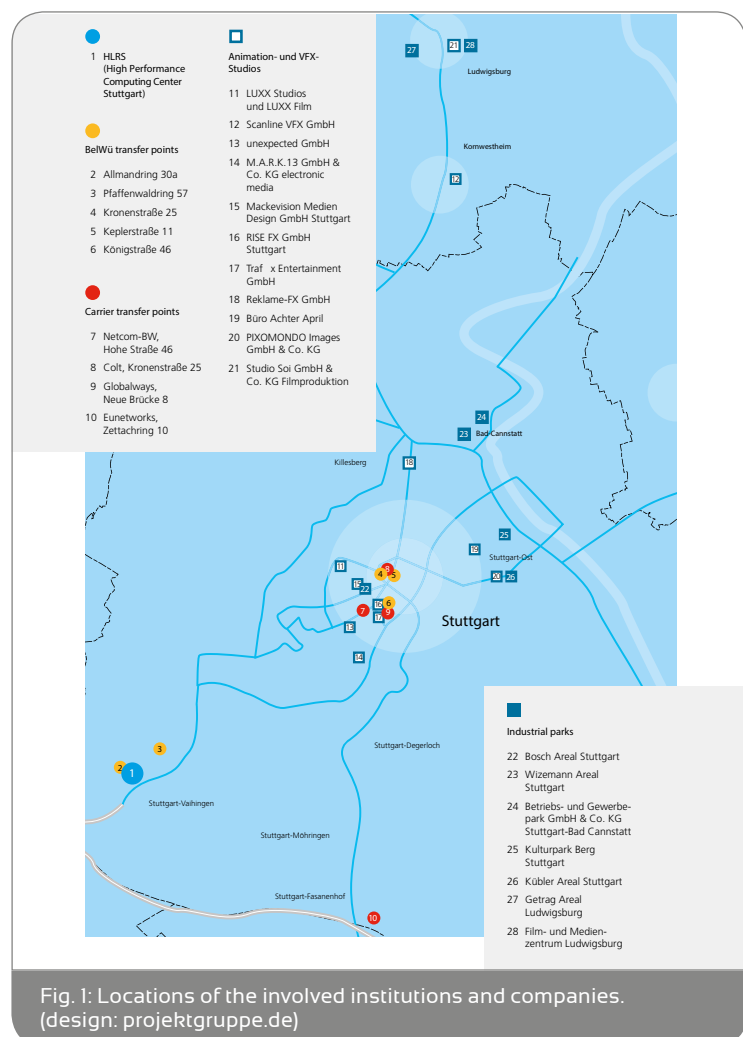
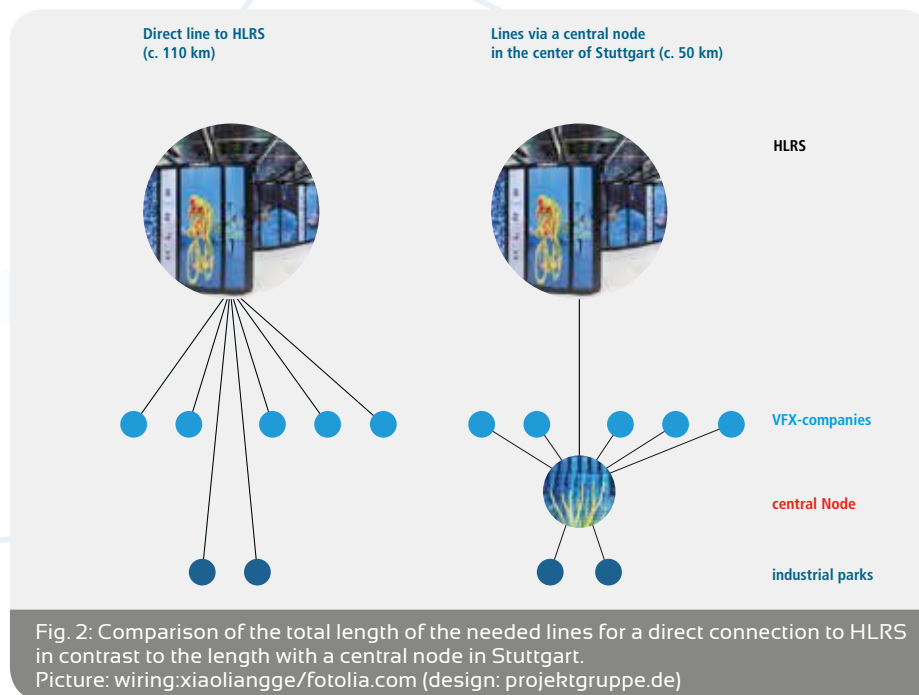


Fig. 1: Locations of the involved institutions and companies. (design: projektgruppe.de)



Course of action

Through individual talks with the participating animation and VFX studios their operation manner and the need for a faster data connection were interrogated and analysed. It has shown, that almost all of the companies are interested in an expansion of their computing capacities. However, as their work is tremendously project-based, the detailed planning for a fiber optic cable infrastructure ideally including a connection to HLRS, is already beyond capacity. Apart from obvious obstacles like the mentioned time consuming planning for a fiber connection, the issues with regard of the rental situation, the negotiations with the telecommunication providers and in many cases also the expensive earthwork operations, there is another immense challenge for this specific industry: if you want to have a fiber connection and be able to use external render capacities, it also needs an adjustment of the usually very complex and unique software pipeline. A new partner for the animation and VFX studios, who is willing to join them in developing technical innovations, is the Media Solution Center BW (MSC): a cooperation project of the HLRS, the media university Stuttgart, the Filmakademie Baden-Württemberg and the ZKM in Karlsruhe. It is the declared aim to give the companies access to HLRS, but not

only for classical rendering. The MSC rather intends to also give the possibility of trying out new approaches and to support future-oriented working habits.

Fiber optics suggestions

In regard of fiber optics the ASAPnet study has explicit recommendations: Interested animation and VFX companies should form a demand pool. As a group it is more likely to get reasonable quotes for the so-called dark fiber, which is an unlit fiber for individual and especially practically unlimited use.

The idea is that the lines of the single companies converge at a central node in the center of Stuttgart, where multiple telecommunication providers are present. The thereby increased competition within the market situations allows the achievement of better prices.

Another advantage of a central node is the reduction of the total length of cableway to HLRS. Such shortening would also have the benefit of being cost-saving, since the bulk of the costs for a fiber optic cable connection is the laying costs (figure 2).



From left to right: Dr. Andreas Wierse (CEO SICOS BW GmbH), Prof. Dr. Michael M. Resch (Director HLRS), Kurt Jaeger (Author of the ASAPnet study, Dr.-Ing. Nepustil & Co. GmbH), Prof. Carl Bergengruen (CEO Medien- und Filmgesellschaft Baden-Württemberg GmbH), Dr. Walter Rogg (CEO Wirtschaftsförderung Region Stuttgart GmbH)

According to the study, the proposed model could be realised with a 10,000 Euro one-time investment and 1,000 Euro per month operating costs per studio.

The results of the study were presented at HLRS in front of invited guests and the press. The representatives of the involved institutions agree:

if the gathered recommendations get realized, a significant improvement of the fiber optic infrastructure can be achieved from which also sectors besides animation can benefit tremendously.

The whole study can be read here:
<http://www.wrs.region-stuttgart.de/asapnet>
(german version)



Written by Annekatriin Baumann

(MSC BW project coordinator, HLRS)

After finishing her Bachelor in Audiovisual Media Annekatriin Baumann specialised with a Master in Electronic Media—both at Stuttgart Media University. As project coordinator of the Media Solution Center she continues her work at the intersection of technology and creative content. She was actively involved in the development of the ASAPnet study.

Contact: Annekatriin Baumann, baumann@hlrs.de



Symposium on Theoretical Chemistry at Ruhr-Universität Bochum:

Chemistry in Solution



From September 26-29 2016, the 52nd Symposium on Theoretical Chemistry (STC) took place at the Ruhr-Universität Bochum organized by the Center for Theoretical Chemistry (Prof. Dr. Dominik Marx) and the DFG Cluster of Excellence RESOLV (Ruhr Explores Solvation). The STC is an annual international meeting of scientists from all areas of Theoretical Chemistry. This year's focus was on Solvation Science.

The majority of chemical reactions take place in a liquid-state environment. Solvents—water being the most prominent—are used to solvate molecular species, ranging from industrial reagents to biological molecules in living cells. Solvents also wet surfaces, such as lipid membranes or metal electrodes, thus, creating extended inhomogeneities and, thereby, interfaces. It is,

therefore, not astonishing that research into liquids, solutions and their interfaces has a long-standing tradition in Theoretical Chemistry. The aim of STC 2016 in Bochum dedicated to the featured topic *Chemistry in Solution* has thus been to advocate that a lot of progress in Theoretical Chemistry can be achieved by a fruitful combination of the wide range of available modern methods. About 400 participants discussed new developments and research results that have been presented in 13 high-level invited lectures given by leading international experts in the field. They covered research into chemistry in liquid-state environments bringing together many different perspectives, from advanced electronic structure calculations to sophisticated computer simulation methods, but also technical challenges and possible

solutions in the application of these methods on modern architectures towards exascale computing have been discussed. In addition, numerous contributed talks and posters addressed all fields of Theoretical Chemistry.

A particular highlight of each STC is the ceremony of the Hans G.-A. Hellmann award, the most prestigious prize for young researchers in the field of theoretical chemistry that have an outstanding scientific record but not yet received a full professorship. This year, the Hellmann prize has been awarded to Dr. Ralf Tonner (Universität Marburg) for his contributions to the

understanding of chemical bonding and reactivity at surfaces using concepts from chemistry and physics. Furthermore, for the first time the new Erich-Hückel Prize of the Gesellschaft Deutscher Chemiker (GDCh) for Outstanding Achievements in the Field of Theoretical Chemistry has been awarded to Professor Werner Kutzelnigg (Emeritus at Ruhr-Universität Bochum) for his groundbreaking work on the nature of chemical bonding, on the description of electron correlation and magnetic properties, and for his contributions to relativistic quantum chemistry.



Written by Michael Römelts

(Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum)

Dr. Michael Römelts leads an Otto-Hahn research group at the Lehrstuhl für Theoretische Chemie of the Ruhr-Universität Bochum and the Max-Planck Institut für Kohlenforschung in Mülheim an der Ruhr. The main focus of his research group is the development and application of electronic structure methods with the aim to yield an accurate description of physical and chemical properties of complex molecular systems.

Contact: Michael Römelts, michael.roemelt@theochem.ruhr-uni-bochum.de



and Jörg Behler

(Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum)

PD Dr. Jörg Behler is a Heisenberg fellow at the Lehrstuhl für Theoretische Chemie and a member of the cluster of excellence RESOLV at the Ruhr-Universität Bochum. The research of his group is focused on the development of accurate interatomic potentials using machine learning techniques and their application to chemical problems at interfaces and in materials science.

Contact: Jörg Behler, joerg.behler@theochem.ruhr-uni-bochum.de



TranSim: bringing philosophy and computer simulations together

Someone could ask, with genuine surprise: “what has philosophy to do with computer simulations?”. Depending on whom we ask, the answer would be a relatively direct “quite more than you expect”. Before fleshing out any more elaborate answer, it is important to delimit what it is being asked. It is not so unusual to find that answers to this question are taken as also asking “what is philosophy, and what is it good for?” and “why should anybody, being a non-philosopher, care about it?”.

The question (what is philosophy—what is it good for) aims at justifying a field of knowledge, and it is definitely not the purpose of our initial question. Nevertheless, an answer to the second question could help to understand the connection between philosophy and computer simulation (first question) and it would give us an idea of why should anybody care about philosophy (third question).

Let us begin with some common opinions about what philosophy is—and what it is good for (more on this point, see Kaminski, Andreas (2016): Art. Philosophie, in: Richter, Philipp (Hg.): Professionell Ethik und Philosophie unterrichten. Ein Arbeitsbuch, Kohlhammer: Stuttgart, S. 275–279.)

A first position: Philosophy as the practice of conceptual clarification

Philosophy is a discipline hard to grasp, and even more to define (as many others). But among its interests, we can mention clarifying concepts, exposing (false) assumptions, challenging ways

of understanding our world and surroundings and, last but not least, defiance our most solid beliefs. So, couldn't we say: this is what philosophy is, and what it is good for. Some philosophers are quite convinced that this characterizes philosophy. But the problem is that every discipline is eager to clarify its concepts. From this point of view, the practice of a philosopher would not be any different from a scientist. And worse, philosophy would not have a legitimate area. Scientists would do a better job in clarifying their concepts than philosophers. *Why should a philosopher be in a better position to understand neutrons or Navier Stokes equations?*

A second position: Philosophy as Weltanschauung

For some people, philosophy might appear as a Weltanschauung, a fundamental belief about the world as whole. From this point of view, the history of philosophy appears to be at the best a cabinet of bold and interesting opinions (Plato's opinion about that all of this means is x, Kant's that it means y), in principle undecidable and therefore up to one's personal beliefs. Many questions can be cleared up and answered by the empirical sciences, and the remaining part seems to be what philosophy is about. This would explain why there seems to be not a similar progress in philosophy as in science, why it has no empirical methods—and especially why modern sciences liberated themselves from philosophy. *And worse, this would make philosophy a very private opinion, not quite understandable, teachable and knowable.*

A different approach: philosophy as the study of notion of reflection

Let us have a second and closer look. Philosophy examines notions like truth, justification, justice, self, and so on. Let us imagine, we would like to overcome philosophy by starting to study the structure of these notions empirically. We start an empirical study of truth. Two problems emerge. First, by an empirical study we would at best discover how people use the notion of truth. Therefore, we could discover an average usage of the notion. But what if the people we observe are using the notion in the wrong way? Second, *we already require an understanding of truth in order to do our empirical study*. Why? Because, we have to distinguish between true and false statements within our study. This thought experiment gives us a hint of what philosophy is about. *It is the examination of notions that we require for living and for doing science, and which are not or at least not thoroughly explorable empirically*. Philosophers call these notions of reflection (Kant, Hegel). For instance, truth, justice, and self are notions which we presuppose in our everyday life, and they have structures which are not investigable just by observing or asking people. Therefore, the history of philosophy is a history of different models (compare the correspondence, coherence, pragmatic, and other models for truth), as other models they have advantages and limits.

Let us note that these three approaches are a general overview about philosophy, but by no means exhaust all the different ways in which philosophers relate to philosophy. Now, when it comes to our original question “what has philosophy to do with computer simulations?”, we can put *the third approach to work*. Computer simulation transforms the way we try gain and justify knowledge, to predict the future, it changes the way we handle uncertainty and make decisions. Knowledge, justification, future, uncertainty, decision making are (at least) partly notions of reflection. Philosophy aims to analyze and to understand how this method affects these notions.

Computer simulations and philosophy

This might give us an insight on how philosophy, science, and computer simulation are connected. First, computer simulation studies and philosophy are both model-driven ways of thinking. Second, computer simulation studies involve notions like knowledge, justification, truth, and value, among others. Third, computer simulations change the way to gain and to justify knowledge, to understand nature, to make decisions under uncertainty, to involve values in science, and so forth.



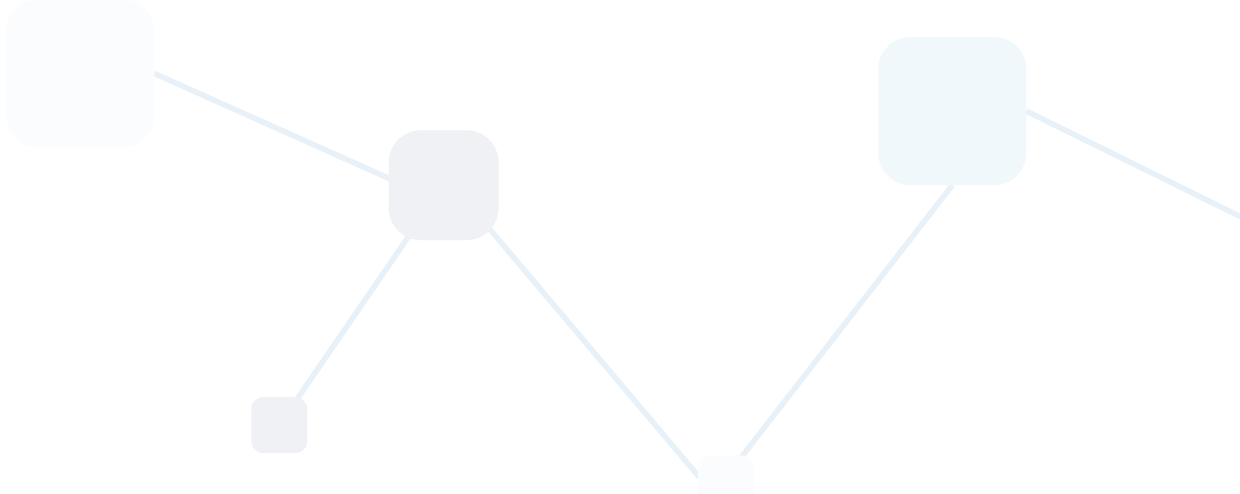
The department Philosophy of Science and Technology of Computer Simulations

In 2014, Prof. Michael Resch and Dr. Andreas Kaminski created the department Philosophy of Science and Technology of Computer Simulations at the HLRS – University of Stuttgart. The idea was to understand how computer simulations change science, engineering, and society. Therefore, the departments move the technical dimension of computer simulation to the fore (computer simulation has been studied by philosophers of science, but less by philosophers of technology). In close collaboration with engineers, physicists, mathematicians, and others, several research areas had been identified.

The research project: Transforming Society – Transforming Simulation (TranSim)

The next year, the project Transforming Society – Transforming Simulation (TranSim) was created by Michael Resch and Andreas Kaminski. It obtained funding for four PhD students and one Post-Doc position. At the beginning of this year, all five positions were filled out. Here is a brief introduction of the six projects currently operating in the department of philosophy (the four PhD, two projects under the Post-Doc position) and their relation between philosophy and computer simulations.





Project 1. Possibilities and limitations of simulating

The first project examined the validity of the theory of science simulations. In its current development, simulations are considered “computer experiments”. That is, computer simulations are understood as a kind of advanced laboratory where the results are easier, quicker, cheaper, and less risky to generate. Unlike the classical experiment, however, the virtual reality of the experiment is completely dependent on the modeling. Only what is part of the model plays a role. An independent nature does not exist in this case. Hence, the task of determining the boundaries of the validity of simulation results.

Project 2. The normativity of simulations

The second project addresses an essential step of modeling: selections. Models have to be selective. And selection presupposes a criterion of what is seen as relevant to the area to be simulated, and what it is not. The assumption is that values play an important role in that process. Economic, scientific, technical, and moral values orientate modelers on what is relevant and what it is not. This implicative use of values is to be examined in this project.

Project 3. Visualization of computer simulations

The imaging techniques in neuroscience have triggered a wide debate on the validity of their results. Analogously, computer simulations result in visualizations that make their outcomes

(more) understandable and comprehensible. To avoid similar objections as neuro images faced, visualization of computer simulations should be examined in this project. Are visualizations comparable to pictures or to a special kind of model? And how do scientists use visualizations? What is their function? Is it to represent an object, a process, or to make the simulation models adjustable?

Project 4. Simulations as basis for political decisions

The results of computer simulations have proved to be heavily used for input in policy-making. Examples in the climate change come first to mind (e.g., the capture and storage of CO₂), but one can find more examples in sociology, economics, and the like. Such studies involve the transfer of knowledge, which typically is marked by different expectations and relevance patterns. This project investigates how computer simulations influence policy-making decisions, which relevant aspects of the simulations play a more prominent role, and how communication of results is generally performed. The project also aims at evaluating recommendations for improved communication, and assessing problematic expectations of simulations. This project holds close links to projects 1, 2 and 3, especially on issues related to the possibilities and limitations of simulation, value perspectives, and forms of visualization.



Project 5. Changes in the working world through simulation

In the industrial world (most prominently, although not limited to, the automotive and aerospace industry), computer simulations have proved their central importance beyond doubt. They simplify, accelerate, and drive the general progress of technological developments. It would not be an exaggeration to say that computer simulations have substantially and sustainably changed engineering practice. The core objective of this project is to explore the relationship between heuristic systems (e.g., those that analyze a space of possible solutions to a problem), and computer simulations.

Project 6. Changes in science by simulation

For a long time, computer simulations were conceived simply as fast (and, to certain extent, reliable) ways to solve very complex scientific models. The kind of models that humans would not be able to solve in a lifetime, if at all. But that was it. Computer simulations were more or less considered as number crunching machines. This project aims at confronting this classic picture with the use of computer simulations in science. Computer simulations are influencing not only our way of doing science and engineering (as it is discussed in project 5), but also in the ways we describe the world in these fields. In simpler worlds, computer simulations seem to be changing scientific thinking. This is the main aim of this project.



Written by Andreas Kaminski

(Head of the department of philosophy, HLRS Stuttgart)

Andreas Kaminski is the head of the department dedicated to the philosophy of simulations at HLRS. He is co-editor of *Jahrbuch Technikphilosophie* and the spokesperson for the DFG-Network for the history of psychometrics. His research interests include epistemic opacity in computer simulation and machine learning algorithms, antinomies of trust. Publications amongst others: *Technik als Erwartung: Grundzüge einer allgemeinen Technikphilosophie*, Bielefeld 2010; *Zur Philosophie informeller Technisierung*, Darmstadt 2014.

Contact: Andreas Kaminski, kaminski@hlrs.de



and Juan M. Durán

(Department of philosophy, HLRS Stuttgart)

Juan M. Durán research focuses on the philosophy of computer simulations from the perspective of philosophy of science and STS studies. Regarding the former, his work addresses scientific explanation, scientific models, and scientific experimentation. As for the latter, he examines the importance of computer simulations, values, and science in a democratic society. He is currently under contract with Springer for a book on computer simulations in science and engineering.

Contact: Juan M. Durán, duan@hlrs.de





Applications

In this section you will find the most worth mentioning applications of external users on GCS computers.

The world's largest turbulence simulations

Introduction

Understanding turbulence is critical for a wide range of terrestrial and astrophysical applications. For example, turbulence on earth is responsible for the transport of pollutants in the atmosphere and determines the movement of weather patterns. But turbulence plays a central role in astrophysics as well. For instance, the turbulent motions of gas and dust particles in protostellar disks enables the formation of planets. Moreover, virtually all modern theories of star formation rest on the statistics of turbulence [5].

Especially the theoretical assumptions about turbulence behind star formation theories allow the prediction of star formation rates in the Milky Way and in distant galaxies [2]. Interstellar turbulence shapes the structure of molecular clouds and is a key process in the formation of filaments which are the building blocks of star-forming clouds. The key ingredient for all these models is the so-called sonic scale. The sonic scale marks the transition from supersonic to subsonic turbulence and produces a break in the turbulence power spectrum from $E \propto k^{-2}$ to $E \propto k^{-5/3}$.

While the power-law slopes of -2 and -5/3 for the supersonic and subsonic parts of the spectrum have been measured independently, there is no simulation currently capable of bridging the gap between both regimes. This is because previous simulations did not have enough resolution to separate the injection scale, the sonic scale and the dissipation scale.

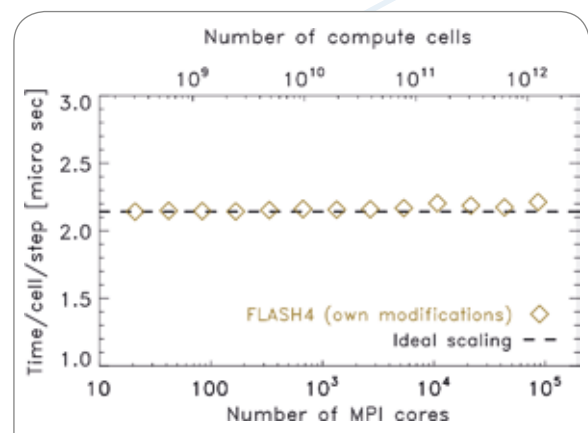


Fig. 1: Weak scaling of the customized version of the FLASH code, used during the SuperMUC scale-out workshop on Phase 2 in 2015. The diamonds indicate the scaling tests of the FLASH code, while ideal scaling is represented by the dashed line.

The aim of the project presented in this contribution is to run the first simulation that is sufficiently resolved to measure the exact position of the sonic scale and the transition region from supersonic to subsonic turbulence. A simulation with the unprecedented resolution of $10,000^3$ grid cells will be needed for resolving the transition scale.

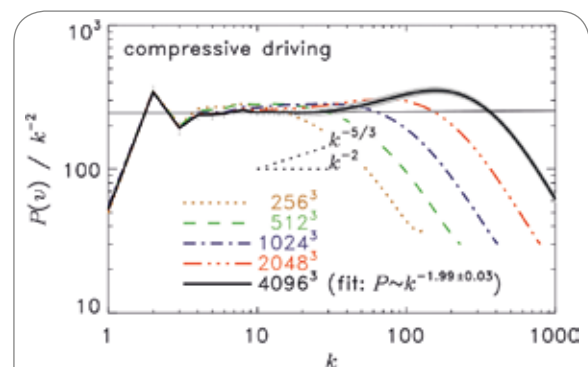


Fig. 2: Power spectrum from highly-compressible, supersonic turbulence simulations (compressive driving), demonstrating a k^{-2} scaling [1].



Results

In the framework of a GAUSS Large Scale Project, an allocation exceeding 40 million core-h has been granted to this project on SuperMUC. The application used for this project is FLASH, a public, modular grid-based hydrodynamical code for the simulation of astrophysical flows [3]. The parallelisation is based entirely on MPI. In the framework of the SuperMUC Phase 2 scale-out, the current code version (FLASH4) has been optimised to reduce the memory and MPI communication requirements. In particular, non-critical operations are now performed in single precision, without causing any significant impact on the accuracy of the results. In this way, the code runs with a factor of 4.1 less memory and 3.6 times faster than the version used for the previous large-scale project at LRZ [1], and scales remarkably well up to the full machine on SuperMUC Phase 2 (see figure 1).

Our current $10,048^3$ simulation has been nearly completed at the time of writing, and data processing is in progress. Some early impression of the forthcoming results can be seen from the highlights of the work of [1], based on the previous large-scale project on turbulence simulations (up to $4,096^3$ grid cells), selected as the SAO/ NASA ADS paper of the year 2013.

Highly-compressible supersonic turbulence is complex, if compared to the subsonic, incompressible regime, because the gas density can vary by several orders of magnitude. Using three-dimensional simulations, we have determined the power spectrum in this regime (see figure 2), and found $E \propto k^{-2}$, confirming earlier indications obtained with much lower resolution [4]. The resolution study in figure 2 shows that we would not have been able to identify this scaling at any lower resolution than 4096^3 cells. Extremely high resolution and compute power are absolutely necessary for the science done here.

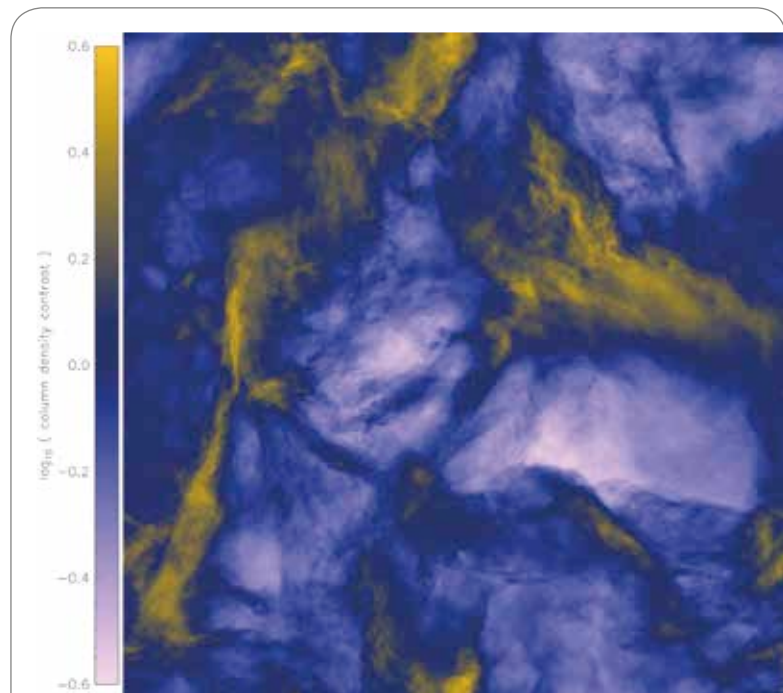


Fig. 3: Column gas density projection in our simulation of supersonic turbulence with a grid resolution of 10048^3 cells (Federrath et al., in preparation).

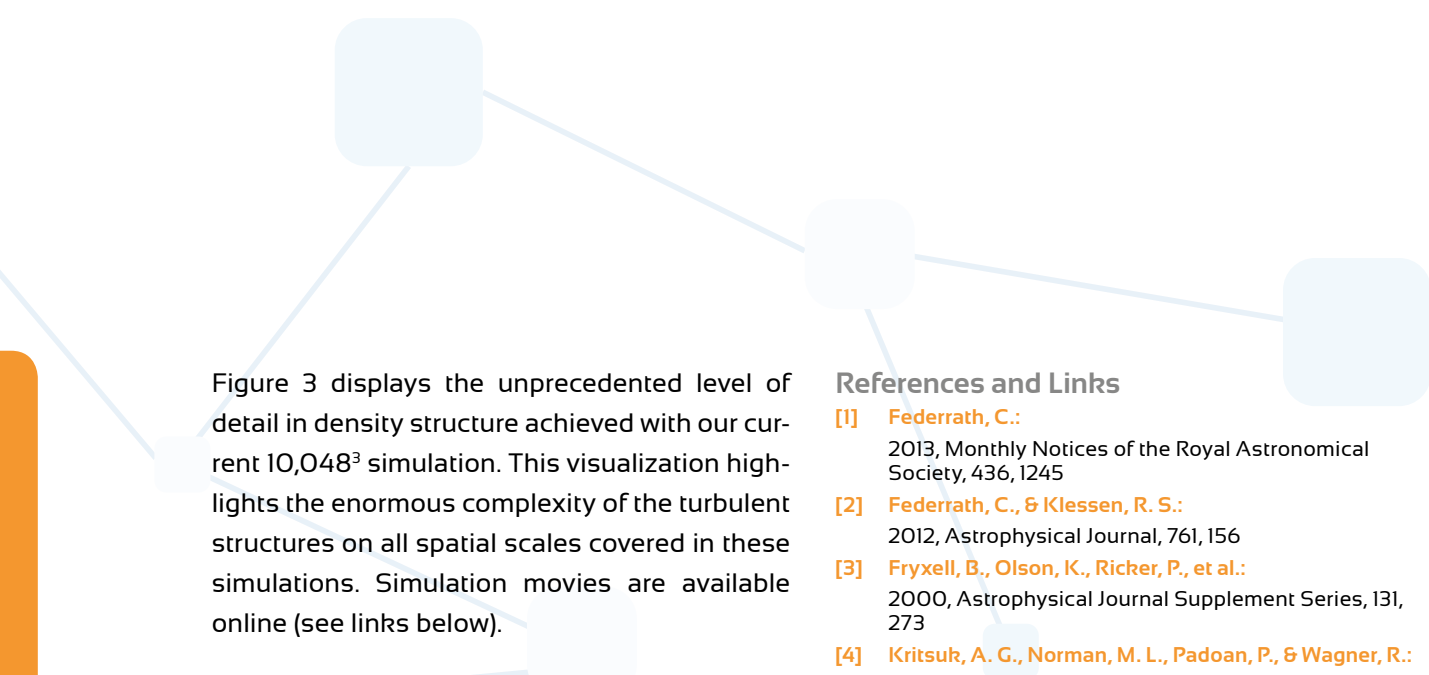


Figure 3 displays the unprecedented level of detail in density structure achieved with our current $10,048^3$ simulation. This visualization highlights the enormous complexity of the turbulent structures on all spatial scales covered in these simulations. Simulation movies are available online (see links below).

Future Work

Turbulence has a wide range of applications in science and engineering, including the amplification of magnetic fields, star and planet formation, mixing of pollutants in the atmosphere, fuel ignition in engines, and many more. Generating the huge dataset of turbulence presented here, we have begun to reach the technical limits of what is feasible on any supercomputer in the world to date. We are currently pushing the boundaries even further by running the world's first turbulence simulation with $10,048^3$ grid cells on SuperMUC. We hope to unravel the statistics of supersonic and subsonic, magnetized turbulence in the near future, with cutting-edge supercomputing systems provided by the LRZ.

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Written by Christoph Federrath¹, Ralf S. Klessen^{2,3}, Luigi Iapichino⁴, Nicolay J. Hammer⁴

¹ Research School of Astronomy and Astrophysics, Australian National University

² Zentrum für Astronomie der Universität Heidelberg, Institut für Theoretische Astrophysik

³ Universität Heidelberg, Interdisziplinäres Zentrum für Wissenschaftliches Rechnen

⁴ Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften

Contact: Christoph Federrath, christoph.federrath@anu.edu.au



CFD based low-order modeling of the nonlinear flame dynamics and of swirl fluctuations

Introduction

Despite the development of power plants using renewable energy sources, gas turbines will play an important role in future energy production. They offer operational flexibility and at the same time low emission of greenhouse gases. These are important properties to serve as backup solution in the age of renewable energy sources, which is essential to maintain net stability and a reliable energy supply.

Thermoacoustic oscillations limit the development of gas turbines aimed to lower emission of pollutant and a higher operational flexibility. The basic mechanism behind thermoacoustic oscillations is as follows: Small initial fluctuation of the velocity, say, yield fluctuation of the global heat release rate of the flame. This unsteady heat release rate acts as a volume source, which in turn creates acoustic waves. These waves are reflected at the boundaries of the burner back to the flame and perturb the flame, again. This feedback can get unstable and yield very large oscillations. If the machine is not turned down, these oscillations can cause significant damage.

The occurrence of those instabilities in a gas turbine depend on the interaction of all parts of the engine. However, due to limited computational power it is by no means possible to simulate a whole gas turbine within a single LES (Large Eddy Simulation). Low order network models are the state of art approach for estimating these instabilities. First, a low-order model of each component in a gas turbine is determined.

Then the low order models are interconnected in order to predict the global heat release rate of the flame. Entirely acoustic elements without reactive flows can be modeled with a linearized version of the Navier-Stokes equations. However, a low-order model for the flame cannot be found on this way.

Therefore, in the present project the so called CFD/SI approach is investigated [3]: The flame is simulated with a LES. These simulations are expensive and necessitate the use of Super-MUC. In order to deduce low-order models efficiently from the LES, the LES is perturbed with a broadband excitation signal. The resulting fluctuation of a reference velocity and of the global heat release rate are measured. The time series collected are post-processed with system identification methods in order to determine the low-order models.

This method has already been proofed to be both accurate and efficient. In the scope of the present project two new aspects are investigated: (1) It is investigated how non-linear low order models can be deduced. (2) The impact of swirl waves on the flame dynamics is investigated. For this purpose, two different swirl burners are investigated, one having axial swirler (BRS burner) and the other radial swirler (FVV burner) shown in figure 1 and 2, respectively.



Fig. 1: Heat release rate shown in BRS burner.

Results and Methods

The object-oriented C++ Software package OpenFOAM [4] is used to perform the LES simulations. OpenFOAM employs an implicit finite volume scheme with well-known PISO and SIMPLE algorithms. The solver is based on the standard solver reactingFOAM.

The turbulence is modeled with Smagorinsky sub-grid scale LES model. Global 2-step chemistry is used to model Methane-Air combustion. The Thickened Flame Model is implemented for decreasing the mesh resolution requirement by artificially thickening the flame. The low Mach number assumption is used in order avoid acoustic wave reflection at boundaries. Adaptive Mesh Refinement capability is added to the solver for refining the mesh only in flame region and therefore saving computational time.

The BRS burner rig is used for code benchmarking. Experiments and numerical results using AVBP [3] are available in literature. In figure 3, the Flame Transfer Function calculated by means of experiment is compared against numerical approach (LES-SI) by different solvers AVBP

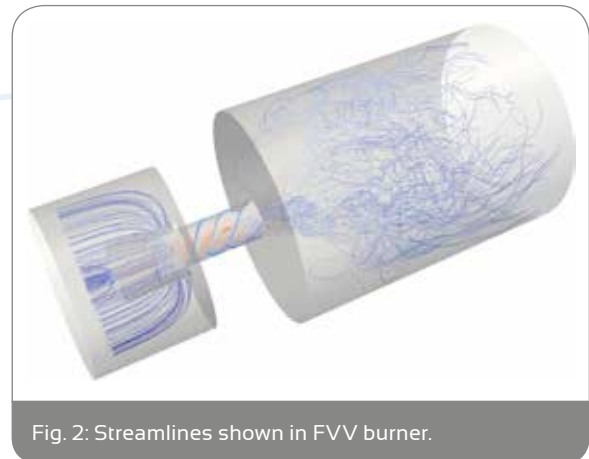


Fig. 2: Streamlines shown in FVV burner.

and OpenFOAM. A good agreement with experiment is achieved with OpenFOAM simulations.

In order to compute a single Flame Transfer Function for BRS burner, time series around 0.35 seconds are required. This can be achieved in 120000 CPU hours with 840 processors.

On-going Research / Outlook

For the nonlinear system identification we created long time series with broadband, high amplitude excitation. Due to the resulting large movement of the flame these simulations were numerically demanding. At the moment the focus is on post-processing the time series obtained in order to investigate the capability of the nonlinear system identification. Here, the objective is to investigate how well methods that have been validated for laminar flames [6] can be used to model thermoacoustic oscillations of turbulent flames. As the focus of this work is now on post-processing the CFD data the SuperMuc is not required anymore for this part of the work.

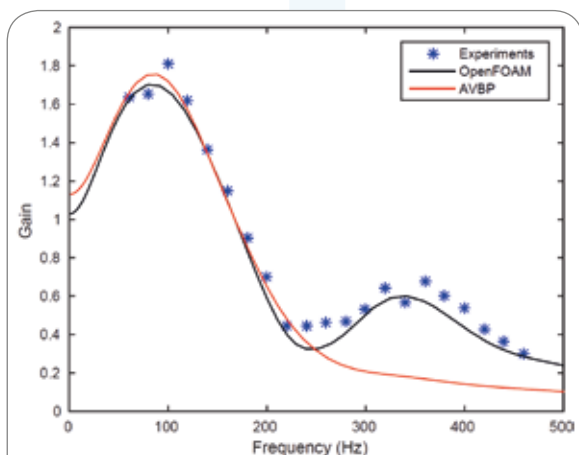


Fig. 3: Comparison of Flame Transfer Functions from experiment and numerical simulations by OpenFOAM and AVBP.

With the SuperMuc our current focus is on the investigation of the swirl flames. Here, a model for the influence has been developed by the authors of the present project [7]. This model is to be validated against a turbulent swirl flame. Extensive numerical studies with the SuperMuc will be necessary.

One proposal continuing the work done within this project has just been submitted. The idea is to use the CFD/SI approach to deduce low-order models for the combustion noise. This is of high

industrial interest, as such model combined with a thermoacoustic network models allows to predict the noise emitted by the engine.

In future it is planned to investigate the uncertainty of the prediction in more detail. Here, physical parameters as the wall temperature and the turbulence model as well as numerical parameters as the discretization scheme or the mesh are to be investigated. These study will require are huge computational and thus, necessitate the use of SuperMUC.

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Written by Christian Lang, Wolfgang Polifke, Stefan Jaensch and Alp Albayrak

(Technische Universität München, Fakultät für Maschinenwesen, Professur für Thermofluidynamik)

Contact: Christian Lang, lang@tfm.tum.de

Improving scalability for the CFD software package MGLET

The code MGLET has been designed for the numerical simulation of complex turbulent flows. MGLET uses a Finite Volume method to solve the incompressible Navier-Stokes equations. It uses a Cartesian grid with staggered arrangement of the variables that enables an efficient formulation of the spatial approximations. An explicit third order low-storage Runge-Kutta method is used for time integration. The pressure is computed within the framework of fractional step or Chorin's projection method, respectively. Therefore, at every Runge-Kutta substep, a linear system of equations, a Poisson-equation, has to be solved. Geometrically complex surfaces are represented by an Immersed Boundary Method.

The code is currently being used by several research groups. At the Fachgebiet Hydromechanik of the Technische Universität München, geometrically complex turbulent flows, flow in porous media and fibre suspensions have been investigated using MGLET. The groups of Prof. Helge Andersson and Prof. Bjørnar Pettersen (both NTNU Trondheim) use the code to predict and analyse bluff-body flows primarily using DNS and the Immersed Boundary Method. At the Institute for Atmospheric Physics (DLR Oberpfaffenhofen), aircraft wake vortices are investigated including their interaction with atmospheric boundary layers and ground effects. These applications demonstrate the power and flexibility of the code.

MGLET has always been used on high performance computing hardware. There is a trend towards higher Reynolds numbers, more

complex flow configurations and the inclusion of micro-structural effects such as particles or fibres. The simulation so far that has used the largest number of degrees of freedom is the one simulating a fully turbulent channel flow of a fibre suspension [1]. This simulation is the only one using a full micro-mechanical model for the fibres' orientation distribution function without closure published so far.

MGLET is parallelized by a domain decomposition method using MPI as a framework. This implementation scaled well to about 2000 processes on SuperMUC, but the performance is strongly dependent on the algorithms and models used. It has been observed that above approximately 2000 processes the scaling behaviour was poor, especially for the fourth order solver. Additionally the memory requirement per core of MGLET scales linearly with the number of processes. This is one of the design-bottlenecks in the current implementation of MGLET. Finally the current input/output mechanism is done by only one rank, collecting/distributing data from/to the other ranks, which does not scale.

This article presents the results of the performance evaluation and scalability improvements that are done in the frame of an effort funded by KONWIHR (Bavarian Competence Network for Technical and Scientific HPC).



Analysis of the performance issues

With the aid of MPI tracing tools, we quickly discovered that there were significant problems in the communication of the ghost cell values at

between others the transfer rate is above 2 GB/second. Another interesting effect is that the transfer rate does not seem to be symmetric. In figure 1 this is for example seen between process

291 and 296, where process 291 sends data to process 296 with a rate of 2.1 GB/second, and the opposite, process 296 sends data to process 291 at only 17.3 MB/second.

Results

After discovering this huge bottleneck, we redesigned this part of the code completely, and the effect was a dramatic increase in performance. We still use plain non-blocking MPI_Isend and MPI_Irecv to do the communication, however, we ensure a consistent calling order and always do all calls to MPI_Irecv before we do any

calls to MPI_Isend. This resulted in a dramatic performance improvement.

In addition to improving the ghost-cell exchange algorithm, we also reduced the amount of ghost-cell exchanges, collective communication and some obvious and low-hanging memory improvements.

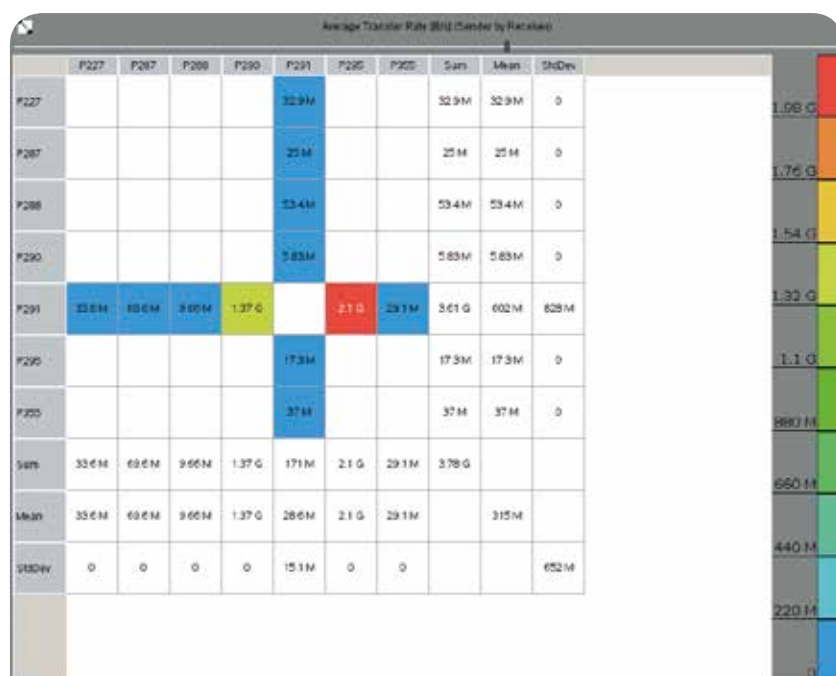


Fig. 1: Screenshot from the Intel Trace Analyzer tool showing the transfer rate between seven processes in a 1024-process computation. Sender is at the vertical axis, receiver is the horizontal.

the boundaries of the computational grids. The exchange of these ghost cell values is the core of the domain decomposition method, and is very frequently performed, so any problems in these routines will cause major performance degradation.

Without presenting too much details, figure 1 shows the most important symptom of the problem: the average transfer rate between some processes are as low as 10 MB/second, while

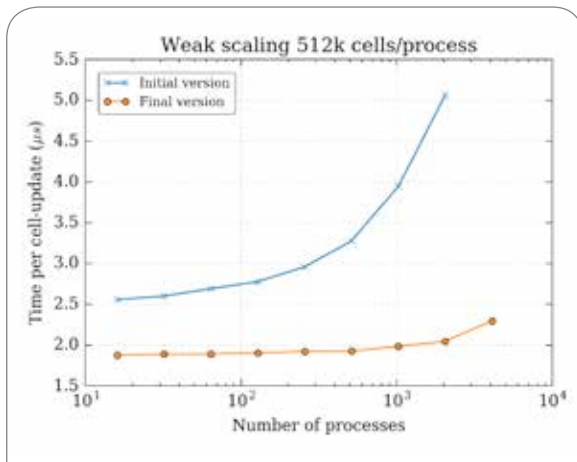


Fig. 2: Performance (lower is better) for a weak scaling test before any improvements (initial version) and after all improvements (final version).

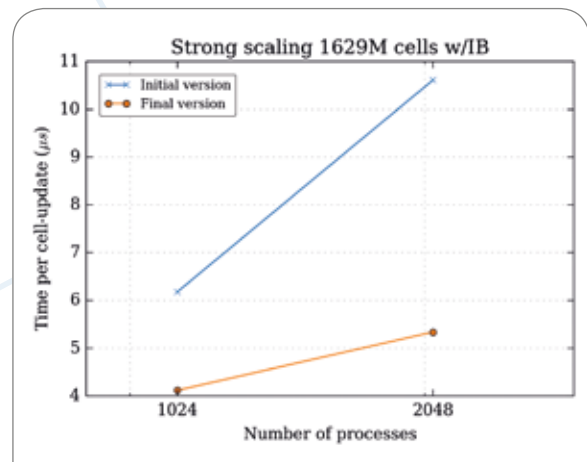


Fig. 3: Performance (lower is better) for a large, strong scaling test before any improvements (initial version) and after all improvements (final version).

To measure the performance improvements, we have used several benchmarks, both synthetic benchmarks (artificial and simplified flow problems) and real-life cases from the users of MGLET. All tests are performed at SuperMUC phase 1 nodes.

Our first benchmark, shown in figure 2, is a synthetic flow case we use to quickly test MGLET. It is a very simple case, without any bodies present in the flow, no statistical sampling and no IO, thus only testing the core of the flow solver. This case shows a huge improvement in performance, in the entire range from one compute node (16 processes) to 256 compute nodes (4096 processes). Even though the scaling in the region beyond 1024 processes is not perfect, this might not be a problem in practice when additional workloads that do not depend on communication is added, such as statistical sampling, immersed boundaries and IO work.

The second testcase we show here in this article is a large testcase with 1.6 billion grid cells. It is a real-world case from Fachgebiet Hydromechanik at TU München and simulates the flow around a wall-mounted cylinder at a Reynolds number of $Re=78000$ by Large Eddy Simulation [2], see figure 4. As figure 3 shows, the run-time of this case is reduced by 50% during this project. In practice this means that we can compute a case of this size with only half the amount of CPU hours as before this project. It also allows us to increase the problem sizes significantly beyond this point, which opens new and interesting research fields.

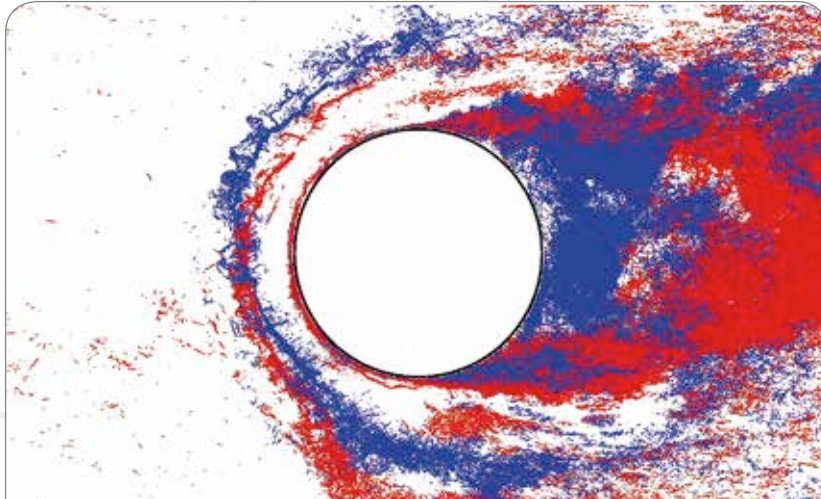


Fig. 4: Flow around a wall mounted cylinder at $Re=78000$. Isosurfaces of the second invariants of the velocity gradient tensor render vortical structures at two different time instants. The flow is coming from left and in front of the cylinder a so-called horseshoe vortex forms. The two instances clearly render the complex dynamics of this vortex.

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Written by H. Strandenes^{1,2}, M. Manhart², M. Allalen³, I. Pasichnyk⁴, W. Schanderl²

- (1) Department of Marine Technology, Norwegian University of Science and Technology
- (2) Hydromechanics Working Group, Technical University of Munich
- (3) Leibniz Supercomputing Centre
- (4) IBM Deutschland

Contact: M. Allalen, allalen@lrz.de

High Performance Computing for Welding Analysis

As an integral part of the PRACE SHAPE project “HPC Welding” [1], the parallel solvers of LS-DYNA were used by Ingenieurbüro Tobias Loose to perform a welding analysis on the Cray XC40 “Hazel Hen” at the High Performance Computing Center Stuttgart (HLRS).

A variety of test cases relevant for industrial applications have been set up with DynaWeld, a welding and heat treatment pre-processor for LS-DYNA, and run on different numbers of compute cores. The explicit mechanical solver was tested on up to 4080 cores with significant scaling. As far as we know, it was the first time that a welding simulation with the LS-DYNA explicit solver was executed on 4080 cores.

Welding simulation

Welding structure simulation is a highly sophisticated finite element (FE) application [2]. It requires a fine mesh discretisation in the weld area so that, in combination with large assemblies and long process times, welding simulation models are very time consuming during the solver run.

HPC with massively parallel processors (MPP) can provide a solution to this issue. In crash applications and forming analysis, it is known that the commercial finite element code LS-DYNA, using the explicit solution algorithm, provides good performance on HPC

systems. However, at the authors’ knowledge, performance benchmarking of LS-DYNA for welding simulations have never been performed prior to this study. This project has analysed the feasibility of welding analysis with parallelised LS-DYNA solvers and its performance.

In this project a Cray-specific LS-DYNA mpp double precision (I8R8) version has been used. The version used, named as revision 103287, was compiled by Cray using the Intel Fortran Compiler 13.1 with SSE2 enabled. The Extreme Scalability Mode (ESM) was used.

In addition, the commercial pre-processor DynaWeld [3, 4] is used to set up the welding simulation models for the solver.

Welding tasks

The welding technique covers a very wide range of weld types, process types, clamping and assembly concepts and assembly dimensions.

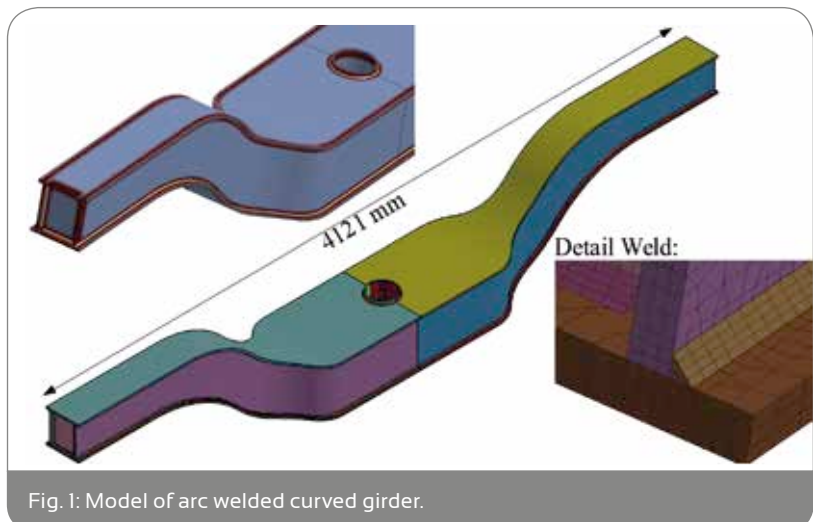


Fig. 1: Model of arc welded curved girder.

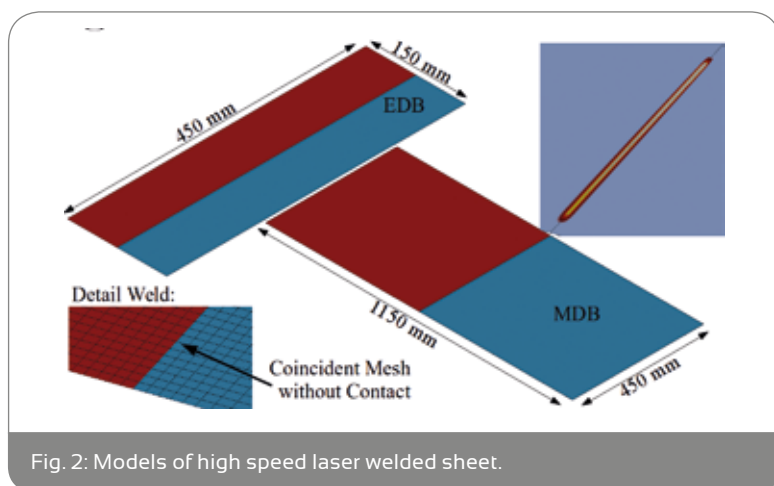


Fig. 2: Models of high speed laser welded sheet.

For example: arc weld, laser weld, slow processes, high speed processes, thin sheets, thick plates, single welds, multi-layered welds, unclamped assemblies, fully clamped assemblies, prestress and predeformations. This shall illustrate that there is not only one „welding structure analysis“ but a wide range of modelling techniques to cover all variants of welding. In consequence, welding simulation cannot be checked in general for HPC, but every variant of modelling type has to be checked separately.

This project considers several representative modelling variants for welding structure with the aim to cover a range as wide as possible. Figure 1, for example, shows a model of a gas metal arc welded curved

girder. This model covers a complex and large industrial case with many welds. A high speed laser welded thin sheet was the test case for the explicit analysis of the project (figure 2). This case was modelled with 200,000 shell elements (EDB) and 1 million shell elements (MDB).

Results of the project

The results of the test cases with explicit analysis provided the following results: The scaling behaviour in the double-logarithmic scale is linear with nearly constant gradient up to 4080 cores (figure 3). Above 96 cores the model MDB with 1 million elements provides a better scaling than the model EDB with 200 000 elements due to the fact that the number of elements per core domain is larger in this case. Regarding the parallel efficiency (the ratio of speedup and number of cores), the larger

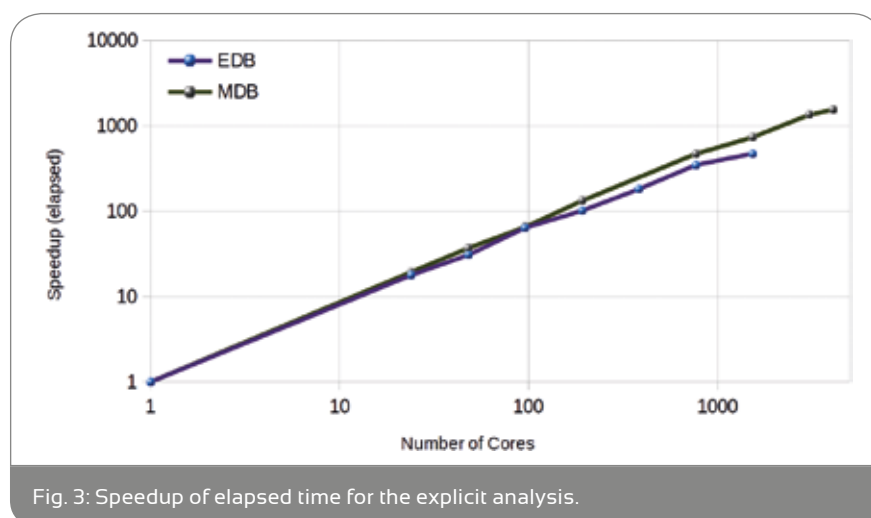


Fig. 3: Speedup of elapsed time for the explicit analysis.

model has a ratio of 0.45 at 768 cores, and at the highest number of cores (4080) a ratio of 0.4.

As a result of the project in general, recommendations for the number of cores in order to obtain the optimal performance are provided and the expected speedup is given. Both the number of the cores and the speedup depend on the model type.

The overall effort for welding analysis on HPC is now much better known with the help of this SHAPE project [1], leading to the ability of a more accurate cost estimate of welding consulting jobs. This project provides a good basis for further investigations in high performance computing for welding structure analysis.

Acknowledgements

This work was financially supported by the PRACE project funded in part by the EU's Horizon 2020 research and innovation programme (2014-2020) under grant agreement 653838.

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Written by Tobias Loose

(Ingenieurbüro Tobias Loose)

Tobias Loose is civil engineer and international welding engineer. After his PhD on welding simulation and buckling analysis at university Karlsruhe he founded his own company, the first engineering office for welding and heat treatment simulation in Germany, in 2007. Loose develops special methods for this kind of manufacturing simulations. In 2015, he started the development of DynaWeld, a preprocessor with focus on industrial application of welding and heat treatment simulation models. Contact: Tobias Loose, loose@tl-ing.de

Co-Authors: Martin Bernreuther, Bärbel Große-Wöhrmann, Jörg Hertzner (Hochleistungsrechenzentrum Stuttgart) and Uli Göhner (DYNAmore Gesellschaft für FEM Ingenieurdienstleistungen mbh)



Large eddy simulation of pulverized coal and biomass combustion

Introduction

Pulverized coal and biomass combustion (PCBC) is currently among the major sources of energy supply and is expected to play an important role in future energy supply. However, coal combustion releases large amounts of carbon dioxide. Future power plants are required to be efficient and low-polluting, which could be achieved by carbon capture and storage or co-firing coal with biomass.

While experimental studies provide valuable and fundamental understanding of the processes of pulverized coal and biomass combustion, they cannot provide all information due to limited optical access and other issues related to the harsh combustion environment. Simulations, such as large eddy simulations (LES), can complement experimental findings by providing large data sets that can be analyzed in great detail. However, numerical methods and modeling approaches need to be developed further to facilitate a comprehensive investigation of the physics of PCBC. Our work is on developing such models and methods for PCBC. In particular, methods to treat particle conversion and the gas phase combustion are developed.

Results and Methods

The code used for all simulations is the in-house finite volume (FV) Fortran code PsiPhi. The code solves the implicitly filtered Navier-Stokes equations in the low Mach number limit. Continuity is enforced by a pressure-correction scheme and projection method using a Gauß-Seidel solver with successive over-relaxation. The code is

parallelized by MPI with non-blocking communication and scaling is demonstrated for up to 128,000 cores. Cartesian, equidistant grids are used, which allow for an efficient usage of a large numbers of cells. A third order Runge-Kutta scheme is used for time-advancement.

Coal and biomass particles are treated as Lagrangian parcels. Their parallelization relies on the same domain decomposition as the gas phase treated by the FV method. Coupling between particles and gas phase is facilitated by tri-linear interpolation schemes. The discrete ordinates method is used to solve for the radiative heat transfer. The code is compiled with Intel Fortran and both IBM and Intel MPI is used. The code has been sped up by improving parallelization and algorithms by us and our collaborators during the projects on SuperMUC.

The overall CPU-hours used in project pr84mu were around 21 million and 10 million in project PRACE 2013081677. Typical, coarse grids consisted of ~500,000 cells and fine grids consisted of up to ~1,700,000,000 cells. Numerical particles were typically around 40,000,000. Coarse runs were conducted with ~1000 cores, whereas fine runs were conducted with ~15,000 cores. To reduce the issue of very long initialization times, results from coarse grids were used to initialize runs on finer grids. The largest run conducted, 16384 cores, generated one restart file per core with the total size of four terabytes. Data relevant for post processing was combined to a hdf5-file of around one terabyte. The overall WORK storage required was 31 terabytes.

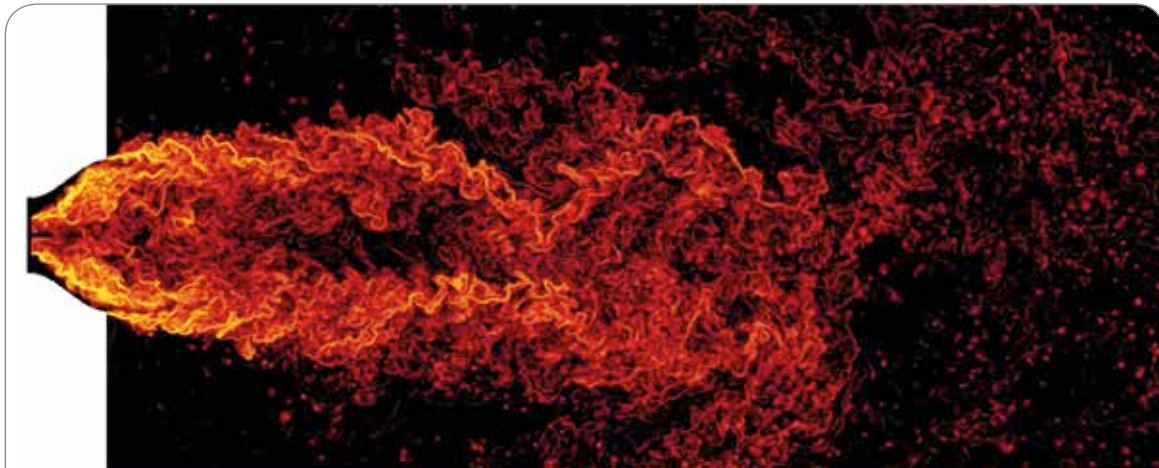


Fig. 1: Logarithmic scalar dissipation rate of the sum of volatile and char-off gas mixture fractions in a section of around 1.5 x 3 m of the flamelet LES of the IFRF semi-industrial furnace.

Large-scale coal and biomass flames in furnaces that have been studied in detail experimentally—the IST and the BYU furnace—were used as reference cases. The classical coal and biomass conversion models, originally developed in cooperation with Imperial College were tested, as well as improved models and strategies. The first step of particle conversion, pyrolysis, is too complex to be explicitly modeled in LES. In cooperation with TUB Freiberg, a pre-processing strategy was developed to optimize the parameters of a simple empirical model based on the predictions of advanced pyrolysis models [1]. The massively parallel simulations provided a good description of scalar and velocity fields, confirmed by the good agreement with experiments. Flame stabilization, flame structure and particle burnout are strongly affected by the fuel properties and the fluid dynamics, and LES is able to provide insights to the phenomena occurring in this type of application that are currently not available through

experimental means. Single particles were tracked over time and instantaneous ensembles were collected to obtain a better understanding of the conditions that coal particles are subjected to [2]. The effect of conversion modeling, particularly the empirical devolatilization model and the mode of char combustion model, on the flame lift-off and flame length of a co-fired flame was also investigated [3].

A part of the project was to incorporate the flamelet model, which is particularly popular in gaseous turbulent combustion computations, to the LES of coal combustion. The test case used for the flamelet LES is a semi-industrial scale furnace with a thermal power of approximately 2.5 MW. The first flamelet table used to describe the chemical state of the reacting gas phase was based on two mixture fractions for volatile and char-off gases as well as on enthalpy and variance. The flamelet table was generated before the simulation, and chemical



state variables looked up from the table based on the four parameters obtained during the simulation. First simulations provided good results and could demonstrate the suitability of the flamelet model for such simulations [4]. A further improvement was achieved by including scalar dissipation rate as a look-up variable [5]. Scalar dissipation rate is an important parameter in the flamelet model and can be understood as an inverse mixing time-scale. The large simulations show very good results compared to the experiment and reveal a wealth of information that is yet to be analyzed. A key feature of such furnace simulations is depicted in figure 1, where the logarithmic scalar dissipation rate of the sum of the two mixture fractions is presented, showing regions of intense mixing

in the volatile flame close to the inlet but also in the shear layers between flue gases and fresh combustion air at the edges of the quartz outlet. Figure 2 shows the temperature field of approximately the first half of the furnace. Individual coal parcels are illustrated in figure 3 along with the circumferential gas velocity for a coarser simulation of the same furnace.

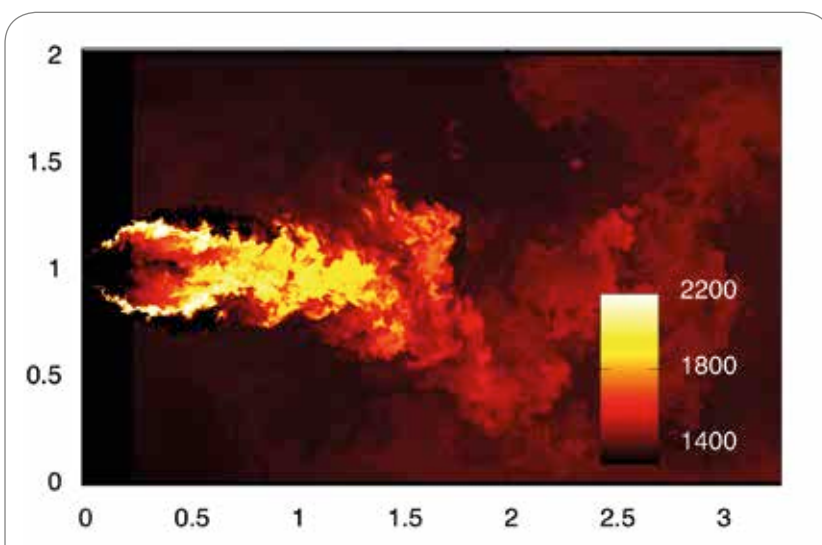


Fig. 2: Temperature distribution in a part of the computational domain of the flamelet LES of the IFRF semi-industrial coal furnace. Axis labels are given in meters.

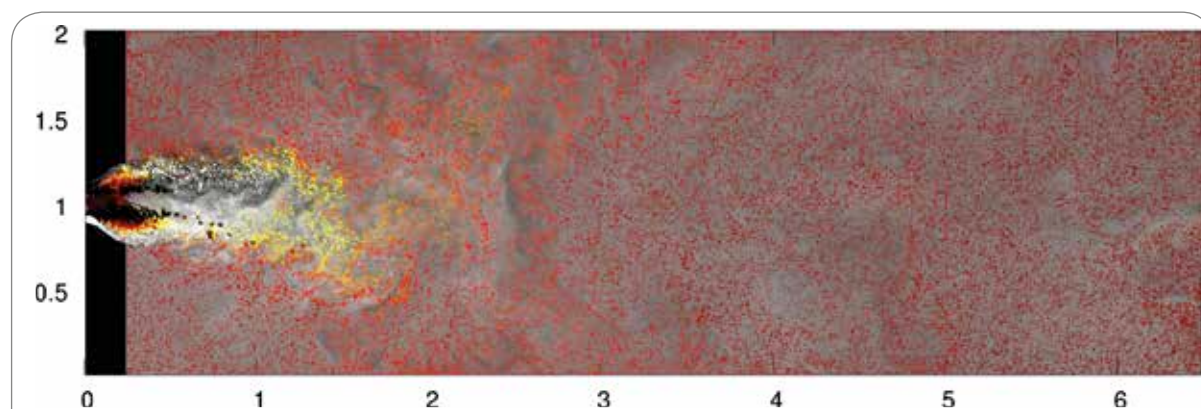


Fig. 3: Coal parcels colored by their temperature (glow color scale) and gas phase circumferential velocity (gray color scale) of the flamelet LES of the IFRF semi-industrial coal furnace. Axis labels are given in meters.

On-going Research / Outlook

PCBC LES require large computations, which can only be conducted with HPC on systems like SuperMUC. Further work will be directed to improving the developed methods, such as investigating a more elaborate flamelet model, which is currently developed within a DFG project with collaborators from University of Stuttgart and TU Freiberg. This is part of a follow-up project currently conducted on SuperMUC. Furthermore, the interaction between coal and biomass particles will be extensively investigated to understand the role of each fuel in co-fired flames, which is critical to understand for the next generation of more efficient and clean boilers.

"SuperMUC Next Generation" will enable to simulate test cases even closer to industrial applications. But also to run laboratory scale configurations at higher resolution to resolve physics down to the scales of turbulence and particle-turbulence interaction, which provides valuable understanding of the physics of turbulent coal conversion.

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Written by Andreas Kempf, Miriam Rabacal and Martin Rieth

(University of Duisburg-Essen, Instituto Superior Técnico (University of Lisbon))

Contact: Martin Rieth, martin.rieth@uni-due.de



From the radioactive decays of mesons to the interactions of quarks and gluons

The determination of a fundamental constant of Nature

The ALPHA Collaboration has computed one of the most elusive fundamental parameters of Nature: the strong coupling. It governs the interactions of quarks and gluons. At high energies, such as the ones reached at the Large Hadron Collider (LHC) at CERN, many processes can be computed in terms of a Taylor series in this coupling. A precise input value for these series is thus essential to make full use of the accelerator. We have simulated the fundamental theory of strong interactions called Quantum Chromodynamics (QCD) over a large range of energy scales in order to extract the coupling at LHC energies.

Fundamental constants of Nature and the Standard Model

Over the last few decades, particle physicists have explored the fundamental forces down to distance scales of $\approx 10^{-18}\text{m}$. It was found that the experimental observations are described to very high accuracy by a theory which is known as the Standard Model of particle physics.

The Standard Model describes the interactions of the fundamental constituents of matter through electromagnetic, weak and strong forces in terms of three different quantum gauge theories. It does so in terms of a few fundamental constants of Nature. Its success is not only a consequence of the mathematical simplicity of its basic equations. It is also due to the fact that the forces they describe are relatively weak at the typical energy transfers in particle physics scattering experiments of about

10–100 GeV.¹ The strengths of the interactions are characterized by coupling constants. When the forces are weak, the predictions of the theory can be worked out in terms of an expansion in powers of these coupling constants, a procedure known as perturbation theory. For instance, in Quantum Electrodynamics (QED), the quantum gauge theory describing the interactions between electrons and photons, the coupling constant is the well-known fine structure constant $\alpha \approx 1/137$. Its small size guarantees that only a few terms in the power series are sufficient in order to predict physical quantities with high precision.

In the gauge theory for the strong force, called QCD, quarks and gluons assume the rôle of electrons and photons in QED. Quarks are the constituents of the more familiar proton and neutron. QCD's coupling constant is called α_s . As a consequence of Quantum Physics, all coupling "constants" in the Standard Model depend on the energy transfer μ in the interaction process. In this sense they are not really constant, rather they "run" with the energy scale. At $\mu \approx 100$ GeV the strong coupling is about $\alpha_s \approx 0.11$. Although this is much larger than the fine structure constant of QED, perturbation theory still works well and essential aspects of processes of high energy scattering can be computed accurately.

¹ In particle physics it is customary to use "natural units" where the speed of light, c and Planck's constant, $\hbar$ are set to one and energies as well as masses are given in GeV. As an orientation note that $m_{\text{proton}} \approx 1$ GeV, where $1 \text{ GeV}/c^2 = 1.602 \cdot 10^{-7} \text{ J}$.

An example is the probability of two-jet events in proton-proton scattering, cf. figure 1.

leave direct tracks in experiments. Examples are shown in figure 1 and in figure 2.

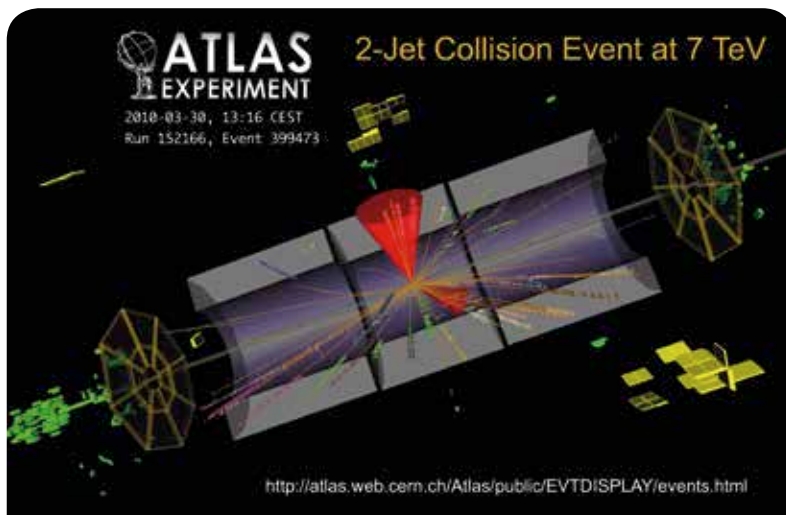


Fig. 1: Proton-proton scattering with 7 TeV center of mass energy at the Large Hadron Collider (LHC) yields a so-called two-jet event. It is characterized by large amounts of energy visible in tracks of hadrons within two distinct (red) cones. The probability for such an event to occur and specific properties of such events are computable in a power series expansion in α_s and a jet can thus be traced back to being caused by a quark. Still, due to confinement no direct track of a quark is visible. A comparison of computations based on the Standard Model with the jet rates observed in the experiment allows us to test our understanding of the fundamental forces.

Challenges

We are then faced with the task of connecting the analytically accessible realm of QCD at high energies (jets, figure 1) with the properties of protons, π -mesons, K-mesons and other hadrons observed at low energies (for example figure 2). For the latter analytic methods such as perturbation theory fail completely.

Instead, computer “simulations” of QCD formulated on a discrete lattice of space-time points allow for a non-perturbative treatment of the theory in the low-energy regime. The lattice-discretized formulation of QCD contains more information

than the Feynman rules of perturbation theory and also low-energy quantities like hadron masses and matrix elements related to decays are computable. This requires the numerical evaluation of the lattice path integral by numerical methods. As usual when numerical approximations on grids come into play, one must study sequences of progressively finer discretizations and take the lattice constant to zero by an extrapolation. In addition, computers demand the restriction of space-time to a finite region which is an approximation that has to be controlled as well.

However, as the energy scale μ decreases below 100 GeV, the value of α_s increases. At μ below 1 GeV, it becomes so large that perturbation theory cannot be relied upon anymore at all. In fact, this energy region is intrinsically non-perturbative, which means that the perturbative expressions even fail to give a qualitatively correct description. The qualitative change is due to the striking property of “confinement”: despite being the fundamental constituents of QCD, quarks and gluons are confined inside protons, neutrons, π -mesons and many other particles, all known as hadrons. Only hadrons are produced in experiments and

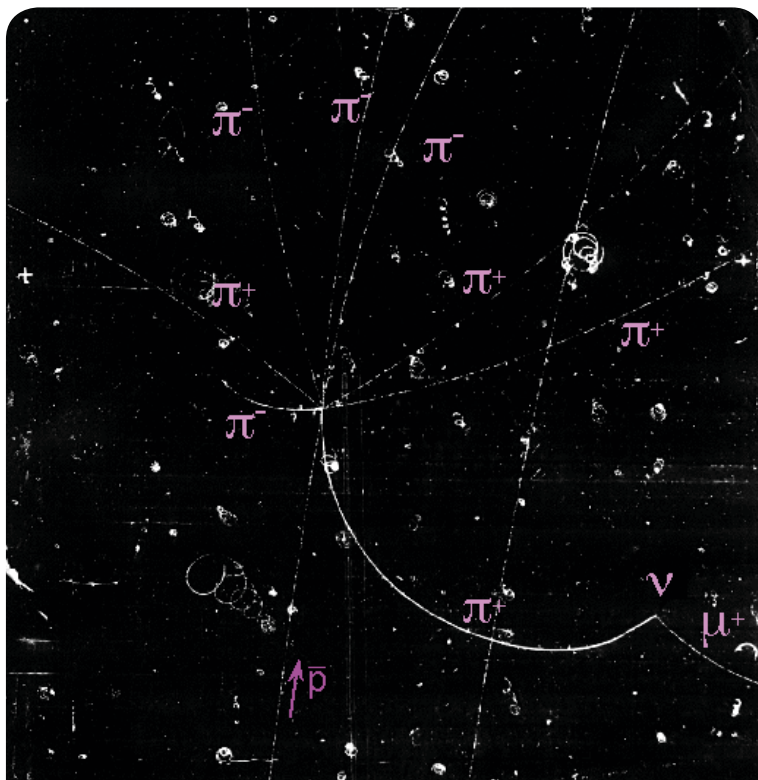


Fig. 2: An incoming anti-proton collides with a proton at rest and annihilates into various π -mesons. In the lower-right corner one of the π -mesons decays into a lepton and an invisible neutrino. The decay-constant characterising these decays plays a central rôle in our computation. This illustrated bubble chamber photo is taken from http://particleadventure.org/all_decay.html

In such simulations it is natural to use a few hadron masses as input to tune the free parameters in lattice QCD in order to predict the rest afterwards.

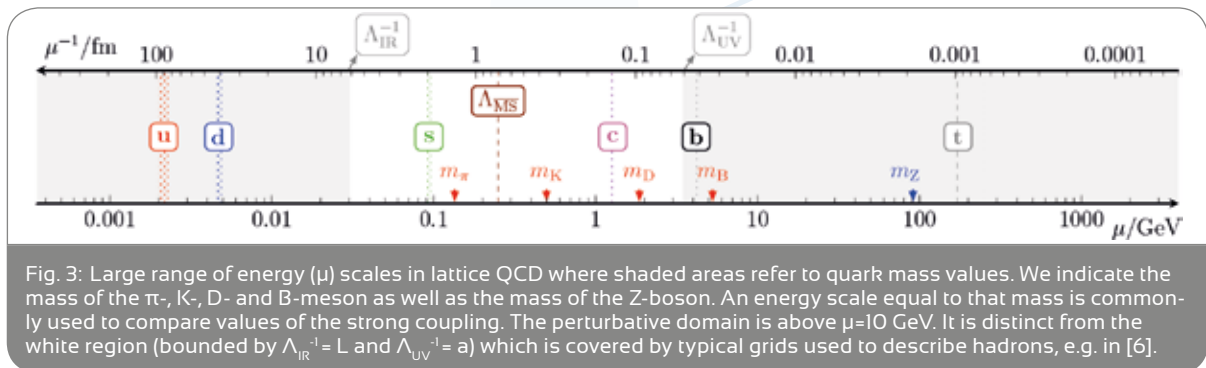
We are faced with a multi-scale problem: on the one hand we want to probe the short distance/high energy properties of the theory. On the other hand, we need to make contact to the observable hadrons at much lower energy scales. This is a challenge for the computational

approach using a grid discretization. The short distance investigation needs much finer grids than the long range part where, however, the overall size of the simulated space-time must be rather large. Accommodating all scales on a single lattice is not feasible. The ALPHA collaboration has developed a recursive finite size scaling technique and demonstrated that it works in simpler lattice theories.

Finite size scaling

The crucial idea of this method is to consider a sequence of sizes for the finite space-time box containing QCD ("femto universe") [1]. The smallest system is chosen such that due to Heisenberg's uncertainty relation it corresponds to high energy where perturbative QCD applies. Within perturbative QCD it is then connected to high energy scattering in an infinite volume.

Furthermore, successive boxes differ by scale factors of two (cf. figure 4) and are related to each other by taking the continuum limit. Eventually one arrives at a box sufficiently large for hadrons to fit in. In this way the multi-scale problem is circumvented and a physical scale ratio is implemented that grows exponentially with the number of steps. In terms of figure 3, one starts



in a situation where the white window is on the right, and then moves it recursively to the left, until the one suitable for hadrons is reached. This method does not compromise with the multiple scales by handling them on single lattices and is thus amenable to systematic improvement and error control. Its application to QCD is now far advanced [2–6].

New precision for the strong coupling

In particular, we have now computed the energy dependence for two different non-perturbative definitions of the QCD coupling. They are called “Schrödinger functional” and “Gradient Flow”. Like all sensible definitions of the coupling, they coincide at the lowest order of the perturbative expansion, but differ by higher powers and non-perturbative physics. In figure 5 we show the β -function, which is the logarithmic derivative of the coupling $g=\sqrt{4\pi\alpha_s}$ with respect to the energy scale. It is now known with unprecedented precision in the whole region up to $\alpha_s=1$ or $L\approx 1$ fm. The difference to perturbation theory (dashed line) is considerable.

Furthermore, we have connected the finite volume coupling of $L\approx 1$ fm, to the decay rate of π - and K-mesons which is known from low energy experiments, cf. figure 2. Decays of these mesons are radioactive decays into, e.g. a μ -lepton and a neutrino which happen only due to the weak interaction of the Standard Model. At the fundamental level radioactive decays proceed by a quark of one species annihilating with an antiquark of another species, producing a very short-lived W-boson which then decays into a lepton and a neutrino. Roughly speaking, the decay rate is then given in terms of the probability of the quark and antiquark to be at the same point in the meson. In precise terms, the decay rate is encoded in the “decay constant” of the meson which is a QCD property. Reverting this, the decay constant is known from the experimentally measured decay rate. We then use this particular quantity as input to connect our computer experiments to the real world since it is computable with high precision, including all systematics, from our lattice simulations. Other inputs that enter are the masses of the π - and K-meson.

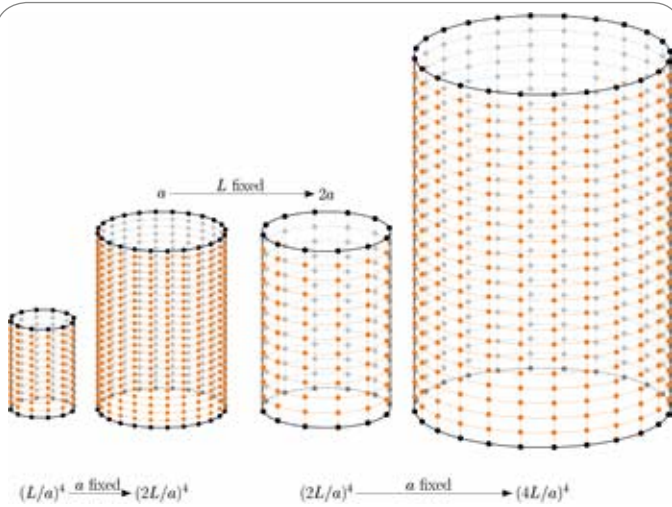


Fig. 4: Illustration of the Finite size scaling method [1]. At fixed lattice spacing a one simulates both a lattice with L/a points and $2L/a$ points in each dimension to obtain the change of $g^2(L) \rightarrow g^2(2L)$. One may then increase a and thus continue to larger and larger L . Repeating the whole procedure with a different L/a but same L allows to remove the discretization errors by taking the continuum limit (not shown). We depict a cylinder because boundary conditions are periodic in the three spatial dimensions and Dirichlet in the time direction.

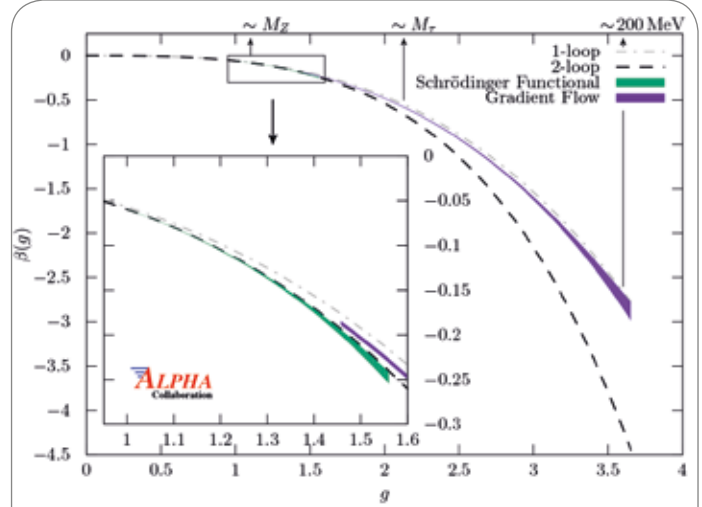


Fig. 5: $\beta(g) = \mu \partial_\mu g$ in the SF-scheme (green) [4] and in the GF scheme (purple), where $g = \sqrt{4\pi\alpha_s}$

Computational Aspects

The finite size scaling analysis illustrated in figure 5 required a couple of hundred different simulations on space-time volumes with up to $32 \times 32 \times 32 \times 32$ points. Some of these simulations could be done with local resources but most of them were run on the Crays at the HLRN. The largest computational effort went into the connection of the femto universe to the meson decay constants, where very large volumes are required. These challenging simulations were done together with our colleagues in the Coordinated Lattice Simulations consortium (CLS)[6]. It took a small series of PRACE-projects and Gauss-projects on BG/Q in Jülich and SuperMUC in Munich to make the simulations more and more realistic, concerning the lattice spacing and the masses of the light quarks. The largest lattices with $64^3 \times 192$ lattice points were simulated on 65536 cores. The field-configurations generated in these simulations will be used in the future to study other interesting aspects of QCD. Besides our projects at the Gauss Center, it was essential for us to be able to also run a large number of smaller scale simulations at the HLRN in Berlin.

Result

The final result of our computations, just released at the annual lattice field theory symposium [7], is

$$\alpha_s(m_Z) = 0.1179 \pm 0.0010 + 0.0002.$$

It is in agreement and more precise than the current world average of a number of different determinations. Most importantly, our computation in the three-flavor theory is at a new level of rigor, using perturbation theory only when α_s is small, but still keeping excellent non-perturbative precision.

We have included only the three lighter of the six quarks in our simulations. The heavier ones have been added perturbatively. The power series describing these additions are very well behaved and we have estimated the small, second uncertainty in the value given above. It will be an interesting and worthwhile project to remove any doubt of this use of perturbation theory by including the next heavier quark in the simulations.

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Mattia Dalla Brida^a, Mattia Bruno^{a,g}, Patrick Fritzsche^b, Tomasz Korzec^c, Alberto Ramos^d, Stefan Schaefer^a, Stefan Sint^e, Rainer Sommer^{a,f}

^a John von Neumann Institute for Computing (NIC), DESY, Platanenallee 6, 15738 Zeuthen, Germany

^b Instituto de Física Teórica UAM/CSIC, Universidad Autónoma de Madrid, C/ Nicolás Cabrera 13-15, Cantoblanco, Madrid 28049, Spain

^c Department of Physics, Bergische Universität Wuppertal, Gaußstr. 20, 42119 Wuppertal, Germany

^d CERN, Theory Division, Geneva, Switzerland

^e School of Mathematics, Trinity College Dublin, Dublin 2, Ireland

^f Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

^g Physics Department, Brookhaven National Laboratory, Upton, NY 11973, USA



Electron-injection techniques in plasma-wakefield accelerators for driving free-electron lasers

Plasma wakefields can sustain electric fields on the order of 100 GV/m for the acceleration of electrons up to GeV energies in a distance of only few centimetres. Control over the process of injection of electron beams that witness these high accelerating gradients is of utmost importance for applications that require excellent beam quality as e.g. needed for free-electron lasers (FELs) in photon science. Utilising plasma wakes, it is envisaged that miniaturised FELs may be constructed, dramatically increasing the proliferation of this technology with revolutionary consequences for applications in biology, medicine, material science and physics.

Plasma wakefield acceleration is a quickly developing novel-acceleration technology, allowing for a substantial increase of the average gradient in particle accelerators when compared to current state-of-the-art facilities. When focused into a plasma, an ultra-short laser pulse (laser-wakefield acceleration, LWFA [1]) or a relativistic particle beam (beam-driven plasma acceleration, PWFA [2,3]) repels electrons from its vicinity and forms waves in electron density which are following the driver with a phase velocity close to the

speed of light. This allows to create a cavity with simultaneous accelerating and focusing properties for charged particle beams. Inside such a plasma-accelerator module, gradients on the order of 100 GV/m can be sustained without being limited by material breakdown,

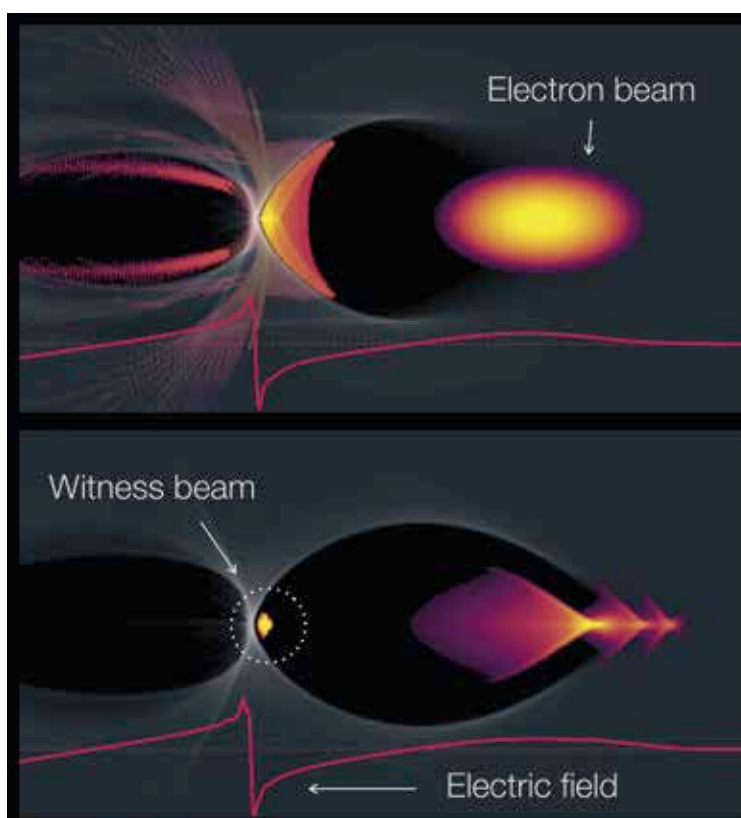


Fig. 1: OSIRIS 3D PIC simulation of a 1 GeV electron beam traversing a uniform plasma of $\sim 10^{18}$ electrons per cm^3 . A short electron bunch is injected at the back of the accelerating plasma cavity, by means of the wakefield-induced ionisation injection method [8]. The injected bunch features high peak current and low normalised emittance, and it is being accelerated at a rate of more than 100 GV/m. After just 3 cm of acceleration, its electron energy becomes three times the initial electron energy of the driver.

outperforming conventional radio-frequency schemes by orders of magnitude. Plasma-based accelerators offer a unique opportunity for the production of high-brightness beams for applications, such as FELs. In the future, plasma accelerators may allow for miniaturised FELs [4, 5] with order-of-magnitude smaller cost and footprint than available today.

The FLASHForward project at DESY [6] is a pioneering plasma wakefield acceleration experiment that aims to produce, in a few centimetres of plasma, beams with energy of order GeV that are of a quality sufficient to demonstrate FEL gain. To achieve this goal, FLASHForward will utilise the electron beams produced in the FLASH accelerator as drivers for the generation

of strong wakefields in a novel hydrogen plasma cell at a density of around 10^{17} cm^{-3} . The length of the accelerating cavity at these plasma conditions is on the order of 100 microns, and therefore, only ultra-short beams can be created and accelerated inside these structures.

One of the challenging tasks of the FLASHForward project is to study and design injection techniques for the generation of high-brightness witness beams, suitable for application in FELs. Owing to the highly nonlinear nature of the dynamics in plasma-wakefield accelerators, analytical treatment only allows for an approximate description. Thus, efficient numerical modelling is required in order to obtain a full description of the relevant physics. The particle-in-cell (PIC) method allows for a precise rendering of the complex

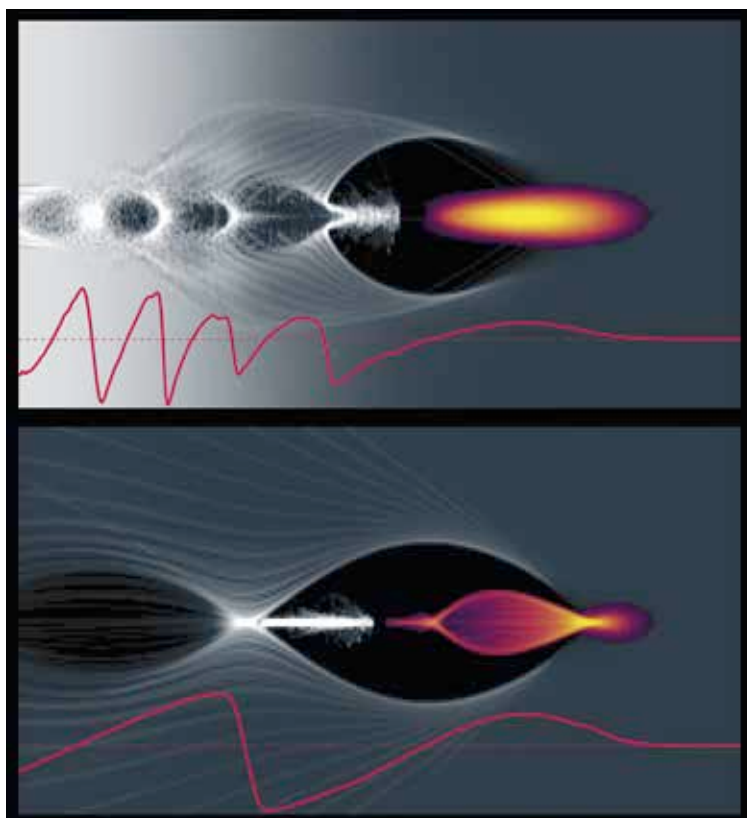


Fig. 2: OSIRIS 3D PIC simulation of a 1 GeV electron beam propagating through a plasma density transition. Due to a rapid expansion of the plasma wavelength during the down-ramp, electrons from the crest of the plasma wave can be trapped in the accelerating cavity. The injected bunch features low emittance and a suitable duration for FEL generation. The average accelerating field is $\sim 10 \text{ GV/m}$ in this example.



dynamics with available computational costs. The electromagnetic fields of the system are discretised on a three-dimensional spatial grid (the cells), while the individual particles of the involved plasma or beam species (electrons, ions etc.) are represented by numerical particles. The computational load is distributed over a large number of processors, which simultaneously solve the underlying equations in different spatial regions of the system. The parallelization and distribution of the work among hundreds to tens of thousands of processing units and their efficient communication in supercomputers allows for high-fidelity numerical modelling of all relevant phenomena in plasma-based acceleration.

By employing the PIC code OSIRIS [7] on the high-end supercomputer JUQUEEN at the Jülich Supercomputing Centre (JSC), we have been able to propose and study several novel injection techniques for the generation of high-quality beams in the plasma wake driven by FLASH-like electron beams in three spatial dimensions (3D). The simulation results shown in figure 1 illustrate the newly proposed wakefield-induced ionisation injection technique [8]. The wakefields at the rear end of the plasma cavity are capable of ionising electrons from a well-localised neutral helium gas region coexisting

with the hydrogen plasma. Once the beam and the plasma wake have crossed the helium region, the ionised electrons are trapped and are forming a high-quality electron beam which is being accelerated by a field magnitude of more than 100 GV/m. After injection and acceleration over a distance of about 3 cm (compared to required ~100 m in conventional accelerators), the generated beam features three times higher per-electron-energy than the initial driver, and a brightness 10 times higher than the initial one. A simulation result depicting the injection of electrons in plasma-density transitions [9] is shown in figure 2. Due to a rapid elongation of the plasma wave during the down-ramp, electrons at the crest of the plasma wave can be trapped in the accelerating region of the cavity.

Control over the process of injection of electron beams in plasma wakefield accelerators is of utmost importance for the generation of high-quality electron beams. Therefore, our research project aims at exploring and analysing a number of regimes and methods for high-brightness-beam production from plasma-based accelerators with the intention to identify the most promising plasma-wakefield-accelerator design to power the next-generation of miniaturised X-ray FELs.

Acknowledgements

We thank the OSIRIS consortium (IST/UCLA) for access to the OSIRIS code. Special thanks for support go to J. Vieira and R. Fonseca. Furthermore, we acknowledge the grant of computing time by the Jülich Supercomputing Centre on JUQUEEN under Project No. HHH23 and the use of the High-Performance Cluster (Maxwell) at DESY. This work was funded by the Humboldt Professorship of B. Foster, the Helmholtz Virtual Institute VH-VI-503, and the ARD program.

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Written by A. Martinez de la Ossa^{1,2}, T. J. Mehrling^{2,3} and J. Osterhoff¹

¹ Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany.

² Institut für Experimentalphysik, Universität Hamburg, Germany.

³ Instituto Superior Técnico, Universidade de Lisboa, Portugal.



Alberto Martinez de la Ossa

Alberto Martinez de la Ossa is the Principal Investigator of the project for supercomputing “Electron-injection techniques in plasma-wakefield accelerators for driving Free-Electron Lasers”, that received the Mention of Excellence by the John von Neumann-Institut für Computing (NIC) in 2016.”

Contact: Alberto Martinez de la Ossa, alberto.martinez.de.la.ossa@desy.de



Realistic modeling of semiconductor properties by first principles calculations

Motivation

For the development of new communication and computing technologies conceptually new materials and device architectures are needed. One pathway of increasing the efficiency of e.g. integrated transistor circuits is to implement photonic functionality to the devices. With the HLRS project "GaPSi" we contribute to the developments in designing and producing optically active compound semiconductor materials that can be integrated into conventional silicon-based (Si) technology.

Critical challenges are posed by the growth of nanoscale thin films of different III/V materials (i.e. elements from groups 13 and 15 of the periodic system) due to stability and kinetic effects. We analyze the reactivity of precursor chemicals used during growth as well as the final materials' properties with accurate, parameter-free calculations of the atomic and electronic structure. Chemical reactivity and other elementary processes determine whether a certain material combination can be realized as intended for implementing new phenomena into computer chips or sensors communicating via light instead of electrons.

Computations

We apply ab initio method without experimental input parameters, namely density functional theory and wave function based quantum chemical methods in static and dynamic simulations to describe the physical properties and reaction mechanisms relevant to semiconductor epitaxy

via chemical vapor deposition. To achieve the necessary accuracy, firstly, a large number of reaction trajectories is often needed. The configurational space of an adsorbate close to a substrate can be highly complex and decomposition or surface diffusion dynamics depend strongly on a meaningful sampling of possible pathways.

Secondly, for calculating optical properties—e.g. band structures—of multinary compound semiconductor materials, large unit cells and tight sampling of reciprocal space are needed. These requirements can only be met with large computational resources and the capability of running several trajectories in parallel. The HLRS delivers optimal platforms to pursue our research and perform up-to-date calculations on a diverse range of questions in chemistry and materials science.

Results

In recent years the reactivity of precursor molecules that carry III/V elements to the semiconductor substrate for functionalization has been in our focus. We examined decomposition mechanisms of gas phase and adsorbate species [1-3]. Efficient elimination of carbohydrate side groups is important as to minimize defect contamination of the materials produced. Furthermore, crystal nucleation mechanisms are both of fundamental scientific interest and determine the material's quality and interface structure. One aspect under investigation are the thermodynamic properties of the hydrogen

passivation layer on Si substrates [4]. The coverage-dependent electronic and vibrational properties require large supercells as shown in figure 1. We applied different models (ab initio thermodynamics, interpolated and explicit phonon dispersion relations, Einstein model) for the evaluation of the equilibrium temperatures that allow activation of the H/Si(001) surface with respect to hydrogen desorption. Gallium phosphide (GaP) can be grown lattice-matched onto activated Si and represents a possible nucleation layer for further functionalization.

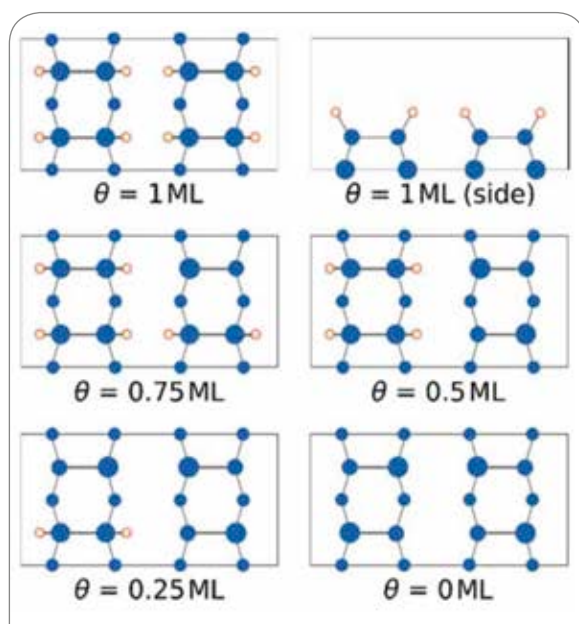


Fig. 1: Supercells of the Si(001) surface with different hydrogen coverages. Figure from [4].

We have also studied chemical growth processes related to GaP growth on H/Si(001) (precursor chemisorption in early nucleation) [5] and the resulting morphology and properties of the GaP-Si interface grown [6]. In close cooperation with chemical vapour deposition experiments, transmission electron microscopy analysis and kinetic Monte Carlo modeling of growth processes, we found that kinetic aspects enable the atomic structure to intermix within a region of eight atomic layers across the interface. On the other hand, thermodynamic stabilities determine pyramidal shapes to occur at the interface (figure 2) as was concluded from our first principles calculations applying large supercells.

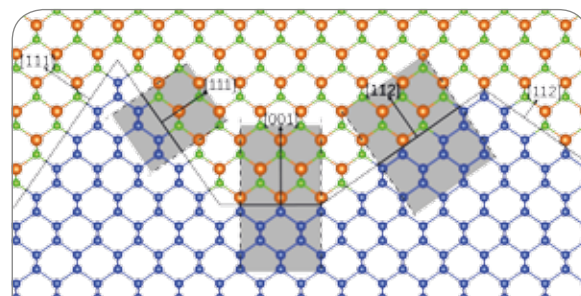


Fig. 2: Schematic of the GaP-Si interface morphology. The supercell models of different interface orientations used for the ab initio stability determination are indicated by shaded areas. Figure from [6].



Further, we have investigated strain and chemical influences on the band gaps of the optically active semiconductor alloys Ga(NAsP) and dilute Ga(AsBi). Those can be used in device superstructures based on Si substrates with a GaP nucleation layer. Figure 3 shows the charge density of the valence band with two different local configurations of the Bi atoms in the GaAs lattice of dilute Ga(AsBi). The material's band gap largely depends on this local configuration which we could rationalize by solid state chemical bonding models [7].

All of our studies are compared to experimental measurements on samples grown under commercially relevant conditions. The results are thus both directly related to larger-scale production of novel semiconductor materials as well as they have proven to be helpful in discovering new features, properties, or optimizing the growth conditions applied. Realistic models for ab initio calculations require large computational resources and reliable collaboration between theoretical and experimental scientists.

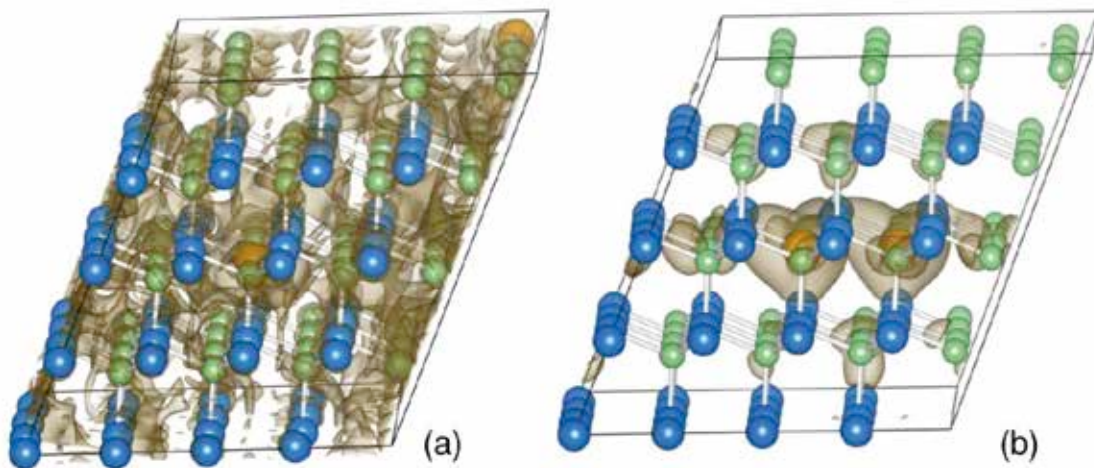


Fig. 3: Heavy hole valence band of Ga(AsBi) in a) a [111] chain and b) cluster arrangement of the dilute Bi atoms. Charge density integrated over the Brillouin zone at 10% of the maximum. Figure from [7].

Acknowledgements

The authors acknowledge gratefully the HLRS for providing computing facilities and IT support, the DFG via the graduate college 1782 and the Beilstein Institute for financial support.

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Andreas Stegmüller

Andreas Stegmüller studied chemistry at Frankfurt University and graduated an MPhil research course with Graeme M. Day on computational crystal structure prediction at the University of Cambridge. He pursued computational chemistry with more accurate methodology describing chemical reactions and electronic properties related to semiconductor growth and interface formation in a PhD with Ralf Tonner at Marburg University. As a postdoc he is now part of a DFG-funded research programme on functional materials.



Ralf Tonner

Ralf Tonner finished his doctoral studies at the University of Marburg under the supervision of Prof. Gernot Frenking in 2007 with the first computational studies of chemical bonding and reactivity of a new state of carbon (carbones). Supported by the Humboldt foundation and the German Academic Exchange Service, he conducted independent research on amino acid interaction with oxide surfaces mentored by Prof. Peter Schwerdtfeger in Auckland/New Zealand until 2010.

Contact: Ralf Tonner, tonner@chemie.uni-marburg.de

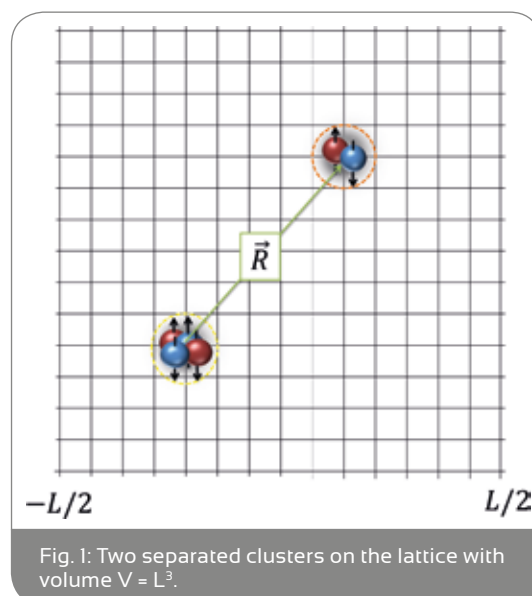


Towards the holy grail of nuclear astrophysics with JUQUEEN

Processes involving alpha particles (${}^4\text{He}$ nuclei) and alpha-like nuclei comprise a major part of stellar nucleosynthesis and mechanisms for thermonuclear supernovae. In an effort towards understanding alpha processes from first principles, we have performed the first *ab initio* calculation of the process of alpha-alpha scattering [1]. As our tool, we have used lattice effective field theory to describe the low-energy interactions of nucleons. To reduce the eight-body system to an effective two-cluster system, we have applied a technique called the adiabatic projection method. We find good agreement between lattice results and experimental phase shifts for S-wave and D-wave scattering. The computational scaling of the A_1 -body + A_2 -body problem is roughly $(A_1 + A_2)^2$, mild enough to make first principles calculations of alpha processes possible. This should be contrasted with existing methods that either scale factorially or exponentially with the number of nucleons involved. In particular, an *ab initio* computation of the so-called “holy grail of nuclear astrophysics” [2], the reaction $\alpha + {}^{12}\text{C} \rightarrow {}^{16}\text{O} + \gamma$, at stellar energies is now in reach.

The basic framework is the method of nuclear lattice simulations, that had its breakthrough by allowing for the first *ab initio* calculation of the so-called Hoyle state in the spectrum of ${}^{12}\text{C}$ [3]. This combination of the modern approach to the nuclear force problem based on an effective field theory with high-performance computing methods defines a completely new method to exactly solve the nuclear A -body problem (with A the number of nucleons, that is protons and

neutrons, in a nucleus). The first ingredient of this method is a systematic and precise effective field theory description of the forces between two and three nucleons, that has been worked out in the last decade by various groups worldwide. To go beyond atomic number four, one has to devise a method to exactly solve the A -body problem. Such a method is given by nuclear lattice simulations. Space-time is discretized with spatial length L_s and temporal length L_t , and nucleons are placed on the lattice sites. The minimal length on the lattice, the so-called lattice spacing a , entails a maximum momentum, $p_{\text{max}} = \pi / a$. On this lattice, the interactions between the nucleons are represented through auxiliary fields, that are integrated over. Such a lattice representation is ideally suited for parallel computing. Given this framework, the structure and spectrum of ${}^{12}\text{C}$ [4] and ${}^{16}\text{O}$ [5] as well as the ground state energies of all alpha-type



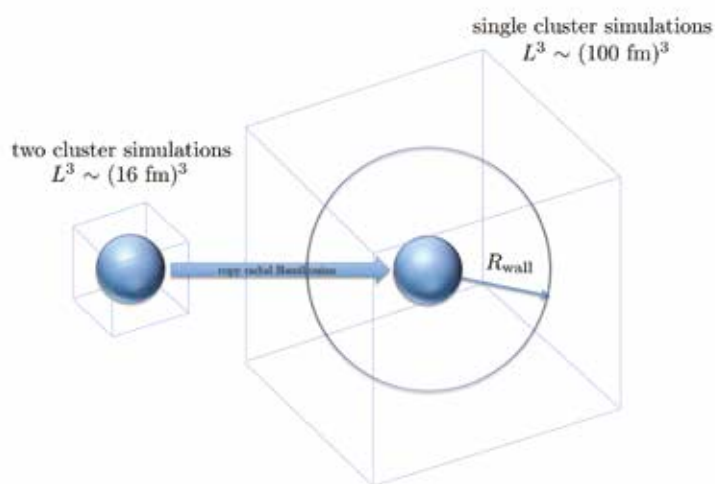


Fig. 2: Graphical representation of the cluster-cluster scattering process. The strong interactions are dealt with in the small volume $L^3 \simeq (16 \text{ fm})^3$, while the long-range Coulomb interaction is exactly computed by matching to Coulomb wave functions in the large volume $L^3 \simeq (100 \text{ fm})^3$.

nuclei up to ^{28}Si have been calculated within a 1% accuracy [6], based on the same microscopic Hamiltonian.

To calculate scattering processes on such a space-time lattice, our calculation proceeds in two steps. First, using exactly the same microscopic Hamiltonian as in the earlier nuclear structure calculations, allows one to construct an *ab initio* cluster Hamiltonian. This step is depicted in figure 1, where two clusters at large separation R are shown. Within the clusters, the full microscopic dynamic (strong and electromagnetic interactions) is included, such as polarization and deformation effects or the Pauli exclusion principle. As the separation R becomes very large, we can describe the system in terms of an effective cluster Hamiltonian (the free lattice Hamiltonian for two clusters) plus infinite-range interactions (like the Coulomb interaction). In the second step, we can then compute the two-cluster scattering phase shifts

or reaction amplitudes using this adiabatic Hamiltonian. Here, one has to account for the strong and short-range Coulomb interactions between the protons and the neutrons in the clusters as well the long-range Coulomb interactions between the protons. While the first set of interactions can be accurately computed in a small volume $L^3 \simeq (16 \text{ fm})^3$, the latter one requires matching to Coulomb wave functions in a much larger volume, typically $L^3 \simeq (100 \text{ fm})^3$, where the Coulomb boundary conditions are imposed on a spherical wall. This method allows to extract the scattering phase shifts and is visualized in figure 2.

We work with the microscopic Hamiltonian at next-to-next-to-leading order (NNLO) in the chiral expansion of the nuclear forces on a coarse lattice with a lattice spacing $a \simeq 2 \text{ fm}$. All appearing parameters, the so-called low-energy constants, have been fixed before in the systems with two, three and four nucleons. We thus can make *parameter-free* predictions of the low-energy α - α phase shifts. These are shown for the S- and the D-wave in comparison to the existing data in figure 3 and figure 4, respectively, at next-to-leading order (NLO) and at NNLO. The error bars are computed using a jackknife analysis of the stochastic errors of the Monte Carlo data. For the S-wave, we note that the calculated ^8Be ground state is bound at NNLO, though only a small fraction of an MeV away from threshold. In the D-wave, the 2^+ resonance energy and width are in fairly good agreement with the experimental results. We plan to revisit these $^4\text{He}+^4\text{He}$ calculations again in the



future with different lattice spacings and going one order higher to next-to-next-to-next-to-leading order. These phase shifts provide useful benchmarks to assess systematic errors in calculations of higher-body nuclear systems and our calculation further demonstrates that an *ab initio* calculation of the holy grail of nuclear astrophysics is in reach.

I thank my collaborators Serdar Elhatisari, Evgeny Epelbaum, Hermann Krebs, Timo Lähde, Dean Lee, Thomas Luu and Gautam Rupak for a superb collaboration and the JSC for providing the computational resources.

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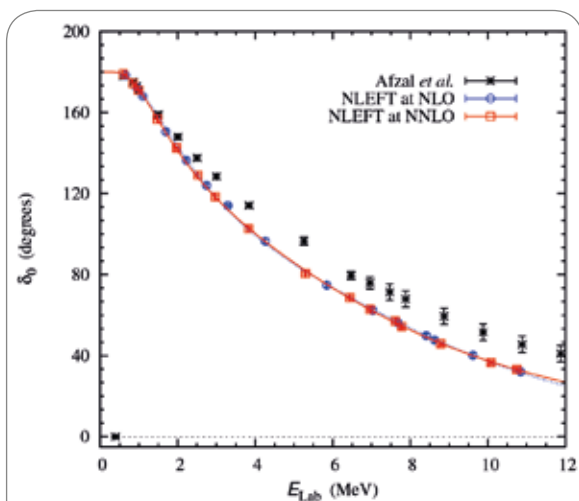


Fig. 3: S-wave phase shifts at NLO and NNLO and comparison with experimental data.

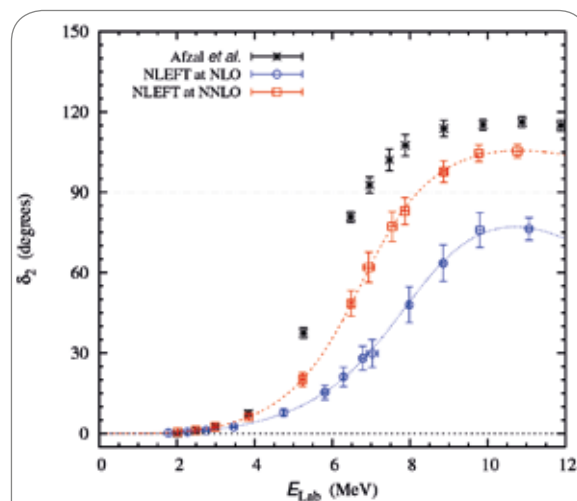


Fig. 4: D-wave phase shifts at NLO and NNLO and comparison with experimental data.



Written by Ulf-G. Meißner

(Universität Bonn & Forschungszentrum Jülich)

The author studied physics, astronomy and philosophy at Bochum and Stony Brook (USA) where he obtained his PhD. From 1997 to 2002 he was group leader at the IKP (FZ Jülich) and C3 Professor at Bonn University. Since 2003, he holds the chair in Theoretical Nuclear Physics at Bonn and is also director at IKP and IAS at Jülich. His work on the strong interactions using Effective Field Theories was recently acknowledged through the Lise Meitner Prize of the European Physical Society.
Contact: Ulf-G. Meißner, meissner@hiskp.uni-bonn.de

Magneticum Pathfinder: The simulation of the evolution of the universe in an unmatched precision

Introduction

Within modern cosmology, the Big Bang marks the beginning of the universe and the creation of matter, space and time about 13.8 billion years ago. Since then, the visible structures of the cosmos have developed: billions of galaxies which bind gas, dust, stars and planets with gravity and host supermassive black holes in their centres. But how could these visible structures have formed from the universe's initial conditions?

To answer these questions, theoretical astrophysicists carry out large cosmological simulations. They transform our knowledge about the physical processes which drive the formation of our universe, into models, as well as, they simulate the resulting evolution of our universe across a large range of spacial scales and over billions of years. To be comparable to ongoing and future cosmological surveys, such theoretical models have to cover very large volumes,

especially to host the rarest, most massive galaxy clusters expected to be the lighthouses of structure formation detectable already at early times (e.g. at high redshifts). While the Universe makes its transition from dark matter dominated to dark energy dominated (i.e. accelerated expansion), the objects which form within it make their transition from young, dynamically active and star formation driven systems to more relaxed and equilibrated systems observed at late time (e.g. low redshifts). Especially here theoretical models in form of complex, hydrodynamical cosmological simulations are needed to disentangle the internal evolution of clusters of galaxies with respect to the evolution of the cosmological background. Such simulations will be essential to interpret the outstanding discoveries expected from current and forthcoming astronomical surveys and instruments like PLANCK, SPT, DES and eROSITA.

Resolution [$N_{\text{Particles}}$]	Medium	High	Ultra high	Extremely high
Box 0 [$2688 \text{ Mpc}/h^3$]	2 x 4536 ³			
Box 1 [$896 \text{ Mpc}/h^3$]	2 x 1536 ³			
Box 2b [$640 \text{ Mpc}/h^3$]		2 x 2880 ³		
Box 2 [$352 \text{ Mpc}/h^3$]	2 x 594 ³	2 x 1584 ³		
Box 3 [$128 \text{ Mpc}/h^3$]	2 x 576 ³	2 x 576 ³	2 x 1536 ³	
Box 4 [$48 \text{ Mpc}/h^3$]	2 x 81 ³	2 x 576 ³	2 x 576 ³	
Box 5 [$18 \text{ Mpc}/h^3$]		2 x 81 ³	2 x 216 ³	2 x 576 ³

Table 1: Overall Magneticum Pathfinder simulation set listed by box size (volume) and resolution (number of particles). The gray shaded simulations where performed within previous simulation campaigns, whereas the two largest simulations emphasized by the orange shaded entries, are added by this project.



In cooperation with experts of the Excellence Cluster Universe's data centre C2PAP and of LRZ, the world's most elaborated cosmological simulation of the evolution of our universe was accomplished. The most comprehensive simulation within the *Magneticum* Pathfinder project pursues the development of a record number of 180 billion tiny spatial elements—each representing the detailed properties of the universe and containing about 500 bytes of information—in a previously unreachable spatial length scale of 12.5 billion light years (see table 1).

Results and Challenges

To perform such simulations, we incorporated a variety of physical processes in the calculations, among them three are considered particularly important for the development of the visible universe: first, the condensation of matter into stars, second, their further evolution when the surrounding matter is heated by stellar winds and supernova explosions and enriched with

chemical elements, and third, the feedback of super-massive black holes that eject enormous amounts of energy into the universe.

For the first time, these numerous characteristics of the simulations performed (see figure 1 and 2) make it possible to compare cosmological simulations in detail with large-scale astronomical surveys. Astronomical surveys from space telescopes like Planck or Hubble observe a large segment of the visible universe while sophisticated simulations so far could only model very small parts of the universe, making a direct comparison virtually impossible. Thus, *Magneticum* Pathfinder marks the beginning of a new era in computer-based cosmology.

This achievement is preceded by more than ten years of research and development accompanied through support by HPC centers, especially experts from the Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities. One of the biggest challenges for such a complex problem is to find the right balance between optimizing the simulation code and the development of the astrophysical modeling. While the code permanently needs to be adjusted to changing technologies and new hardware, the underlying models need to be improved by including better or additional descriptions of the physical processes that form our visible universe.

To perform these largest simulations of the *Magneticum* Pathfinder project took about two years, including initial preparation and testing

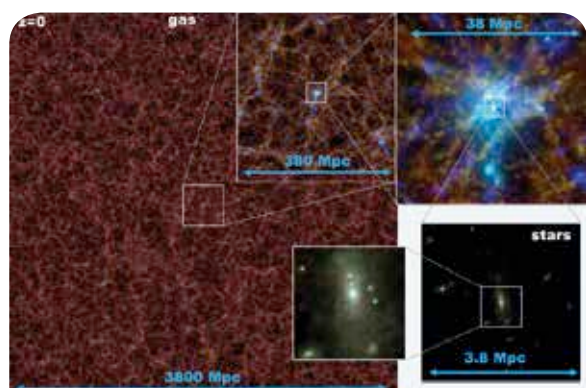


Fig. 1: Visualization of the large scale distribution of the gas and stellar component within Box0 at the end of the simulation, zooming onto the most massive galaxy cluster, where individual galaxies gets visible, see *Magneticum* web page [1].

works. The research group was supported by the physicists of the data centre C2PAP which is operated by the Excellence Cluster Universe and located at the LRZ. Within the framework of several one-week workshops, the *Magneticum* Pathfinder team got the opportunity to use the LRZ's entire highest-performance super-computer SuperMUC for its simulation.

Overall, the *Magneticum* Pathfinder simulation of BoxO utilized all 86,016 computing cores and the complete usable main memory—about 155 out of a total of 194 terabytes—of the expansion stage “Phase 2” of the SuperMUC which was put into operation last year. The entire simulation required 25 million CPU hours and generated 320 terabytes of scientific data.

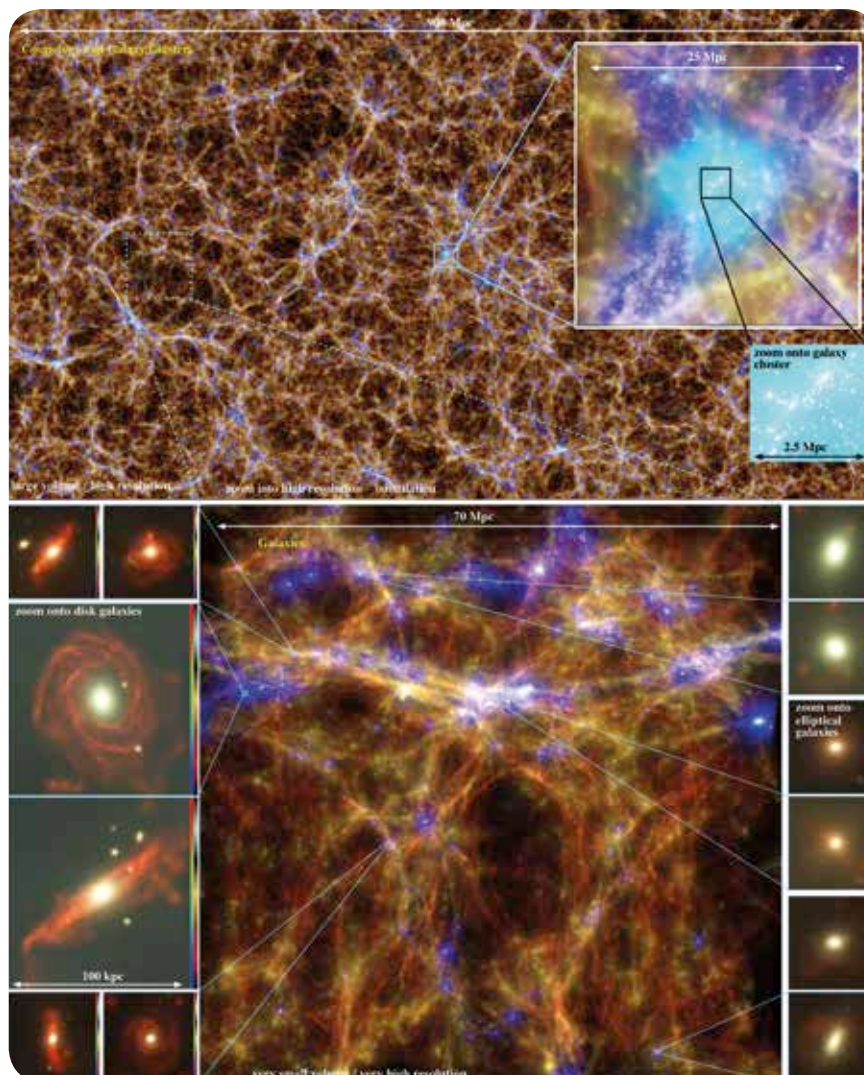


Fig. 2: The shown region of Box2b/hr spans a total size of ~900 Mpc. Shown is the gas which fills the space between the galaxies (color coded according to its temperature from cold/brown to hot/light blue) together with the galaxies and stars forming in the simulation (colored in white). The zoom onto the galaxy clusters reveals the ability of this simulation to resolve up to thousands of individual member galaxies within massive clusters, each resolved with hundreds up to even ten thousands of stellar particles. In the smaller simulation volumes, as the example of Box4/ubr shows, the resolution is finally large enough that the morphology of galaxies can be resolved within the simulations, reproducing the two observed, fundamental galaxy types in our universe, elliptical and spiral galaxies.



On-going Research / Outlook

The *Magneticum* research collaboration will continue to analyze the large amount of data produced within this project, see for example [2], [3], [4], [5] and [6]. Furthermore, these data will be made available for interested researchers worldwide via the public web service C2PAP-CosmoSim [7,8], which is currently in the testing phase. The Munich-based astrophysicists are already engaged in further projects: Among others, Klaus Dolag is currently collaborating with scientists from the Planck collaboration to compare observations of the Planck satellite with the results of the *Magneticum* simulations.

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Written by Klaus Dolag

(Universitäts-Sternwarte München, Fakultät für Physik der Ludwig-Maximilians-Universität)

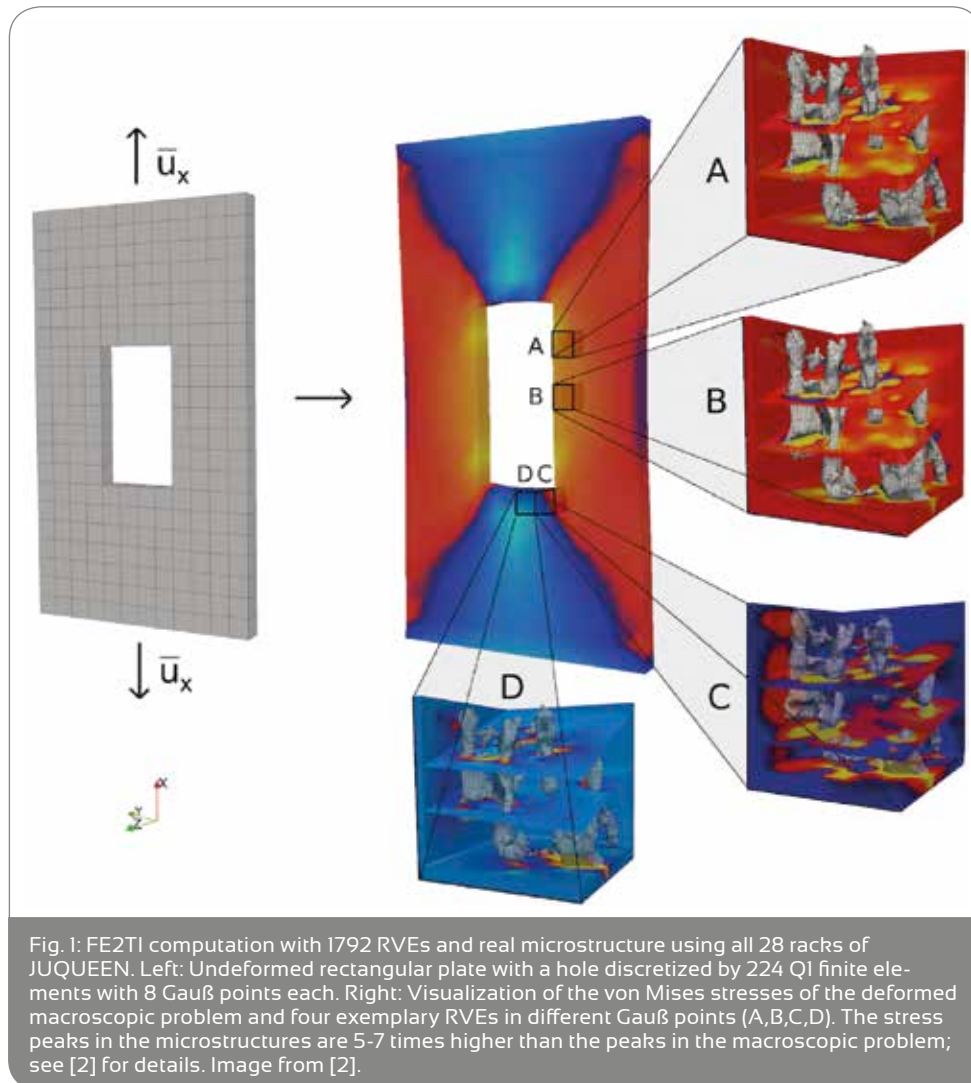
and Nicolay J. Hammer

(Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften)

Contact: Nicolay J. Hammer, hammer@lrz.de

EXASTEEL

From Micro to Macro Properties



Steel Materials

It has been said that the story of materials is the story of civilization. However, it is clear that, throughout the history of civilization, from the iron age to modern days, iron and steel have been among the most versatile materials known by humanity. Through processing, the mechanical properties of steel can be controlled over

a very wide range. These properties can range from extremely hard but brittle to ductile and formable. Indeed, many production and tempering processes have been invented throughout history to influence the strength, toughness, hardness, elasticity, and plasticity parameters of steel materials.

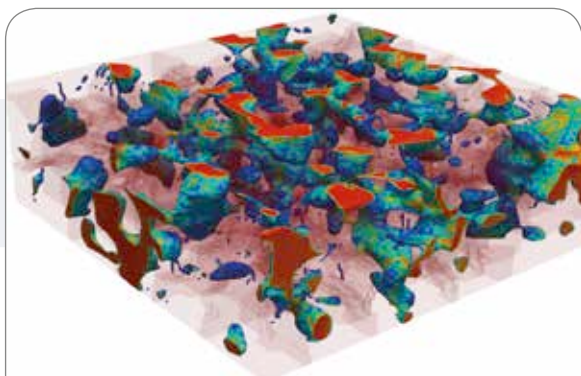


Fig. 2: Reconstructed steel microstructure from EBSD tomography. Courtesy of Jörg Schröder, Universität Duisburg-Essen.

At the core of the adaptability of steel to its particular application is its microstructure. Modern steel materials combine a still higher strength and better ductility with a lower weight. This is achieved through a special polycrystalline grain structure at the microscale: Dual phase (DP) steels consist at the microscopic level of a (softer) polycrystalline ferritic matrix phase and (harder) martensitic inclusions. The resulting microstructure leads to a complicated overall material behavior characterized by finite elastoplasticity combined with isotropic and kinematic hardening; see figure 2.

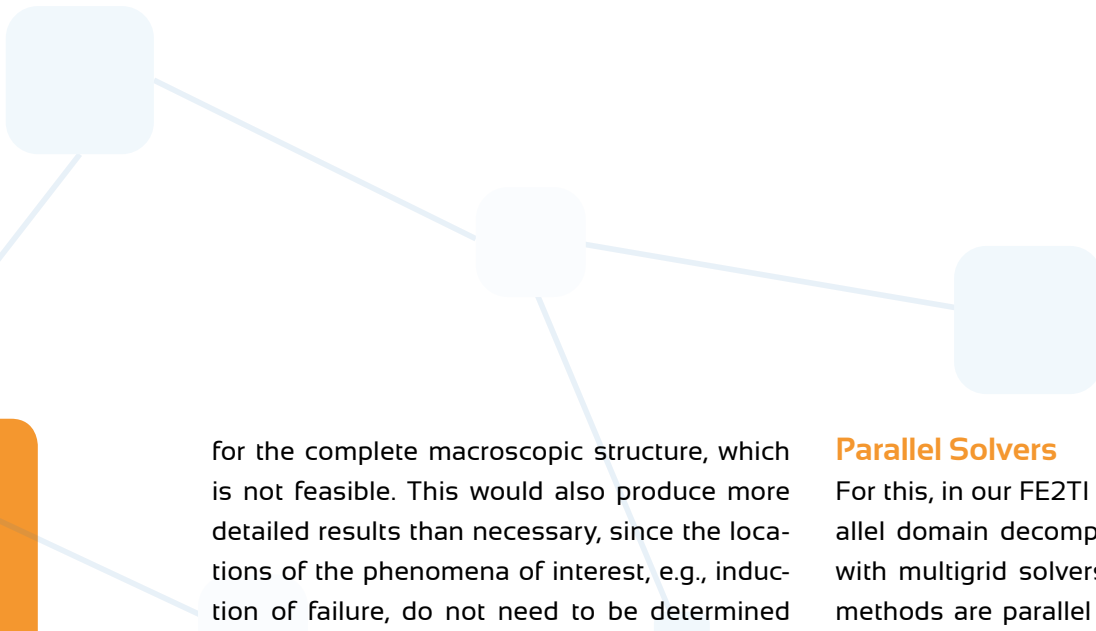
SPPEXA

In the DFG priority program SPP 1648 Software for Exascale Computing (SPPEXA), in the project “EXASTEEL – From Micro to Macro Properties”, we are developing a massively parallel simulation environment for computational material science. The focus are microheterogeneous materials such as modern high-strength steels. By combining robust and highly scalable nonlinear solver algorithms with the well-established

computational homogenization method FE^2 (on the algorithmic side) and including highly nonlinear material models such as crystal plasticity on the microscale (on the modeling side), we are developing an algorithmic tool serving as part of a virtual laboratory for material testing. Once completed, this will allow for the predictive numerical simulation of modern steel materials in a form not possible without massively parallel computers. The project EXASTEEL has brought together experts from computational mathematics (Axel Klawonn, Universität zu Köln; Oliver Rheinbach, TU Bergakademie Freiberg), experts from material science (Daniel Balzani, TU Dresden; Jörg Schröder, Universität Duisburg-Essen), and from computer science, experts in performance engineering (Gerhard Wellein, Universität Erlangen-Nürnberg) and in general purpose direct sparse solvers (Olaf Schenk, Universität Lugano).

Homogenization

For advanced high strength steels, the thermo-mechanical fields fluctuate at the microscale at length scales differing from the ones at the macroscale by 4 to 6 orders of magnitude. A reasonable FE-discretization down to the microscale would thus require 10^3 - 10^9 finite elements for a three-dimensional cube with the volume of $1 \mu m^3$. Extrapolating this to a metal sheet with an area of $1 m^2$ and a thickness of $1 mm$ would lead to 10^{18} - 10^{24} finite elements. This is an enormously large implicit finite element problem even for the largest current supercomputers. Moreover, a brute force simulation would require full knowledge of the microscale



for the complete macroscopic structure, which is not feasible. This would also produce more detailed results than necessary, since the locations of the phenomena of interest, e.g., induction of failure, do not need to be determined up to a level below micrometers. Therefore, a scale-bridging (homogenization) procedure is clearly the more desirable choice.

In our project, a computational homogenization method is applied, which, on the one hand, takes into account the microstructure on a representative volume element (RVE), but which applies a radically smaller number of degrees of freedom on the macro scale. The FE^2 computational homogenization method uses two levels of finite element problems coupled through the macroscopic Gauss points: The macroscopic problem, which is discretized by (relatively coarse) finite elements (FE), and the microscopic problem on the RVEs, where the microstructure is resolved by a fine finite element mesh. Then, in each Gauss point of the macroscopic FE problem, a microscopic RVE problem is solved; see figure 1.

The FE^2 computational scale bridging method helps us to reduce the problem size, compared with the full resolution of the microscale, by a factor of 10^3 - 10^6 . The resulting three-dimensional, heterogeneous, nonlinear structural mechanics problems on the RVEs can still be expected to exceed 10^9 - 10^{12} degrees of freedom. Therefore state-of-the-art parallel implicit solver algorithms are also needed in our project.

Parallel Solvers

For this, in our FE2TI software, we build on parallel domain decomposition solvers combined with multigrid solvers. Domain decomposition methods are parallel divide and conquer algorithms for the solution of implicit problems. They rely on a geometrical decomposition of the original problems into parallel problems defined on subdomains. For nonlinear problems, the problem is typically first linearized by Newton's method and then decomposed into parallel (linear) problems on the subdomains. In recent nonlinear domain decomposition methods [1], the order of these operations is reversed, i.e., the nonlinear problem is decomposed into parallel nonlinear problems to improve concurrency. We combine parallel nonlinear FETI-DP (Finite Element Tearing and Interconnecting) domain decomposition methods with parallel sparse direct solvers and Algebraic Multigrid (AMG) methods to obtain a robust and scalable family of solvers. We apply parallel AMG methods, because they are able to construct a multilevel hierarchy from an assembled sparse operator without knowledge of an underlying grid.

Parallel Multiscale Simulations using 6 Million FETI-DP Subdomains

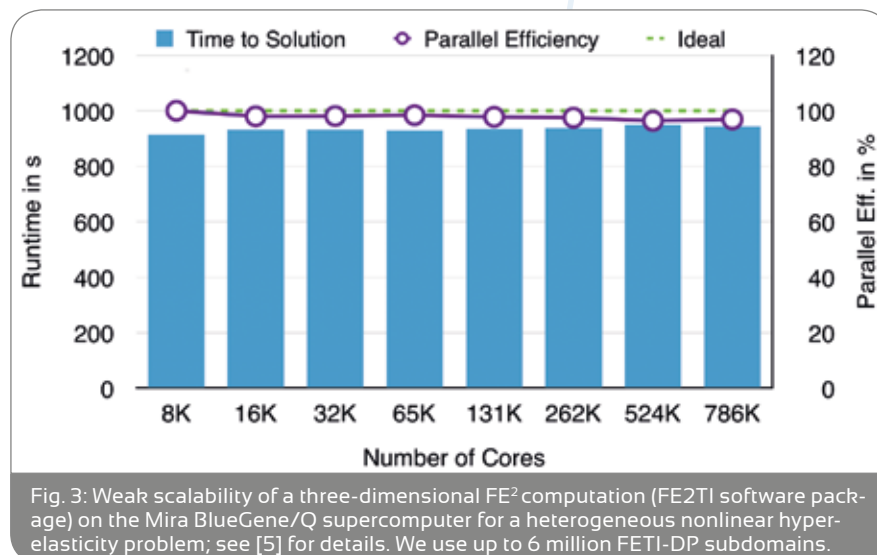
In figure 3, we present weak scalability of our multiscale simulation environment to the complete Mira supercomputer at Argonne National Laboratory (786 432 cores and 1.5 million MPI ranks) using our FE2TI software package, for nonlinear hyperelasticity, discretized with 10-noded tetrahedral finite elements. Mira is a 49 152 node 10-petaflops Blue Gene/Q system



at Argonne National Laboratory (USA) with a total number of 786 432 processor cores and is ranked No. 6 in the current TOP500 list (June 2016, www.top500.org). Mira uses a Power BQC 16C 1.6GHz processor with 16 cores and 16 GB memory per node.

Solver Scalability

Note that our solvers on their own, i.e., even without the FE² method, can scale to the largest current supercomputers: In figure 4, the scalability of our nonlinear FETI-DP domain decomposition method to the complete Mira supercomputer



In our example, in figure 3, the FE² multiscale approach allows to reduce the problem size from 5×10^{15} degrees of freedom to 2×10^{10} degrees of freedom, i.e., by more than 5 orders of magnitude. The resulting problem is then solved on up to 786 432 BlueGene/Q cores using parallel FETI-DP/AMG methods. For the largest problem, we use a total 1 572 864 MPI ranks and a total of more than 6 million FETI-DP subdomains.

with 786 432 processor cores is shown. Here, the largest problem has 62.9 billion unknowns; for more details, see [1,2]. The parallel Algebraic Multigrid (AMG) solver is also highly scalable and can efficiently make use of more than half a million parallel processes. We have considered recent AMG variants tailored for systems of PDEs and adapted especially to elasticity problems [4]. For this, we have cooperated with the authors of Boomer-AMG (Lawrence Livermore National Laboratory). Here, in H-AMG-LN, the BoomerAMG preconditioner uses a special

interpolation which exactly interpolates the rigid body modes. In figure 5, we compare the different approaches U-AMG, H-AMG, H-AMG-LN. The most recent H-AMG-LN approach, tailored

for linear elasticity, clearly performs best. These experiments were carried out on the JUQUEEN BG/Q at Jülich Supercomputing Centre (JSC).

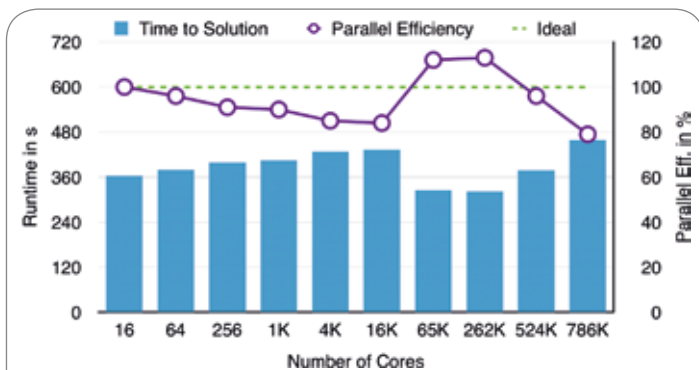


Fig. 4: Weak scalability of a nonlinear FETI-DP domain decomposition solver on the Mira BlueGene/Q supercomputer for a heterogeneous nonlinear hyperelasticity problem; see [2] for details.

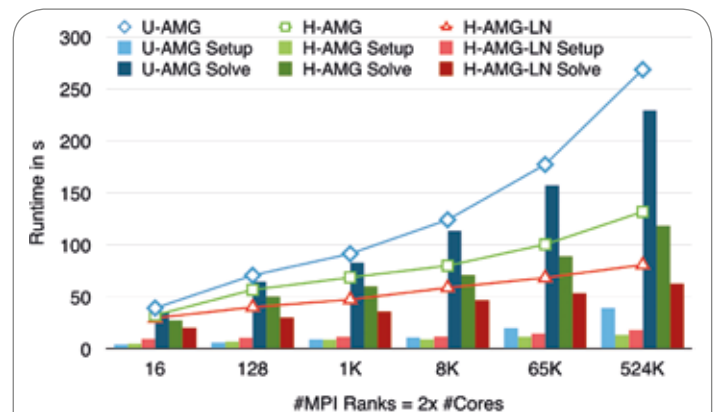


Fig. 5: Weak parallel scalability of an Algebraic Multigrid Method (AMG) adapted for linear elasticity problems on the JUQUEEN BG/Q at Jülich Supercomputing Centre (JSC); see [4] for details.

Acknowledgement

This work was supported by the German Research Foundation (DFG) through the Priority Programme 1648 “Software for Exascale Computing” (SPPEXA). This research used resources, i.e., Mira, of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357. The authors gratefully acknowledge the Gauss Centre for

Supercomputing (GCS) for providing computing time through the John von Neumann Institute for Computing (NIC) on the GCS share of the supercomputer JUQUEEN at Jülich Supercomputing Centre (JSC). The authors also gratefully acknowledge the use of JUQUEEN during the Workshop on “Extreme Scaling on JUQUEEN” (Jülich, 02/05/2015 - 02/06/2015).



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Written by Axel Klawonn, University of Cologne

Axel Klawonn is Professor of Applied Mathematics at University of Cologne, Germany. His research is focused on numerical methods for partial differential equations and high performance parallel scientific computing with applications in material science, continuum mechanics, and the life sciences.

Contact: Axel Klawonn, axel.klawonn@uni-koeln.de



and Martin Lanser, University of Cologne

Martin Lanser is Akademischer Rat at the Mathematical Institute of the University of Cologne, Germany. He works on domain decomposition methods, multiscale methods, and high performance parallel scientific computing.

Contact: Martin Lanser, mlanser@uni-koeln.de



and Oliver Rheinbach, Technische Universität Bergakademie Freiberg

Oliver Rheinbach is Professor for High Performance Computing in Continuum Mechanics at Technische Universität Bergakademie Freiberg, Germany.

Contact: Oliver Rheinbach, oliver.rheinbach@math.tu-freiberg.de





Projects

In this section you will find information about current internal (research) projects of GCS.

Human Brain Project: Towards a European infra- structure for brain research

In March of this year, the Human Brain Project (HBP) [1] successfully released initial versions of its six Information and Communication Technology (ICT) Platforms to users outside the project [2]. The HBP Platforms are designed to help brain researchers advance faster and more efficiently, by sharing data and results, and exploiting advanced ICT capabilities. The release marked the end of the HBP's 2.5-year ramp-up phase and the start of the next phase, during which the HBP continues to build an open, community-driven infrastructure for brain research.



Human Brain Project



Fig. 1: A thin slice of human brain tissue, mounted for microscope imaging under polarized light, for the HBP Human Brain Atlas.

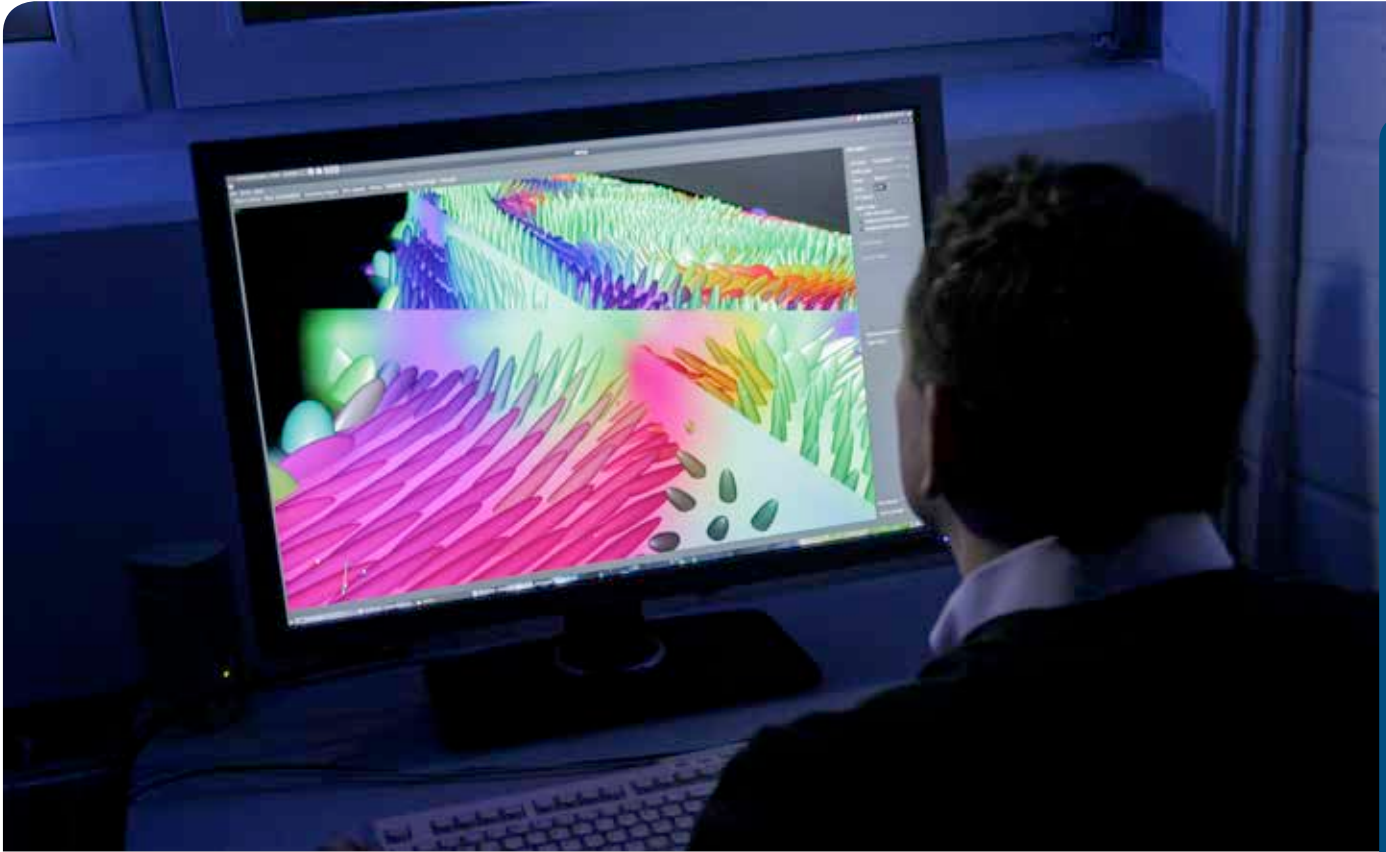


Fig. 2: HPAC Platform resources enable neuroscientists to reconstruct the orientations of nerve fiber tracts.

The HBP is a large-scale European project with over a hundred institutional partners from more than 20 countries in Europe and around the world. It is co-funded by the European Union (EU) within the EU's FET (Future and Emerging Technologies) Flagships Initiative [3]. Launched in October 2013 under the 7th Framework Programme, it is meanwhile governed by a Framework Partnership Agreement (FPA), which was signed in October 2015 [4]. The FPA describes the HBP's overall objectives, work plan and governance [5] for the remainder of its 10-year duration under Horizon2020 and beyond.

Infrastructure co-design

The major goal of the HBP is the creation of a user-centric Research Infrastructure (RI) for neuroscience and brain-inspired research areas such as neuromorphic computing. This goal has become the main focus of the HBP following recommendations from reviewers [6] and a mediation addressing criticism of the project from parts of the neuroscience community [7].

The HBP RI will emerge from the HBP's six ICT Platforms, dedicated respectively to Neuroinformatics, Brain Simulation, High Performance



Fig. 3: The two pilot systems, developed by Cray (left) and IBM-NVIDIA (right), are designed to meet the specific requirements of neuroscience applications.

Analytics and Computing, Medical Informatics, Neuromorphic Computing, and Neurorobotics. The Platform versions released in March consist of a preliminary hardware infrastructure, software tools, databases and programming interfaces, all of which are now being further developed and expanded in a collaborative manner with users, and integrated within the framework of a European RI. All Platforms can be accessed via the HBP Collaboratory [8], a

web portal where users can also find guidelines, tutorials and information on training seminars.

To ensure that the HBP RI meets the requirements of the user community, the HBP is promoting a co-design approach to technology development. There are currently six major HBP Co-Design Projects (CDPs) for this purpose, which are each co-led by a domain scientist and an infrastructure



expert. The HBP CDPs address challenging scientific problems that cannot be addressed with traditional methods in neuroscience, but which can possibly be solved with advanced technologies developed as part of the HBP RI [9].

Federated data infrastructure

A fundamental role in the HBP RI is played by the High Performance Analytics and Computing (HPAC) Platform, which is coordinated by the JSC at Forschungszentrum Jülich and CSCS, the Swiss National Supercomputing Centre in Lugano. The mission of the HPAC Platform is to provide the basic data and computing infrastructure that will enable scientists to deal with the huge amounts of data on the human brain. Specifically, enabling them to store the data, integrate it into models, use it in simulations, as well as analyze and visualize it. To this end, the participating data centers JSC, CSCS, Cineca and Barcelona Supercomputing Center are working closely together to develop a federated data infrastructure, codenamed FENIX. While strongly driven by HBP use cases, the scope of FENIX goes beyond neuroscience, as it should also benefit other research areas with similar requirements, such as materials science.

Pilot systems for interactive supercomputing

Regarding computing resources, the HPAC Platform currently federates existing HPC systems at the participating centers, including Europe's fastest supercomputer Piz Daint at CSCS and

JUQUEEN at JSC. Two new pilot systems, which were installed at JSC over the summer, have just been integrated into the Platform. The two systems are cutting-edge demonstrators that have been developed by Cray and a consortium of IBM and NVIDIA, respectively, within a Pre-Commercial Procurement (PCP), carried out by Forschungszentrum Jülich on behalf of the HBP. The goal of the HBP PCP is to have suppliers of HPC technology competitively research, develop and integrate novel technologies in the areas of dense memory integration, scalable visualization and dynamic resource management in order to enable "interactive supercomputing", i.e., the interactive use of supercomputers for complex workflows comprising concurrent simulation, analysis and visualization workloads. The systems are currently used for testing and benchmarking, but are also already in productive use for neuroscience applications.

Outlook

The refocusing of the HBP on its infrastructure-building mission during the first phase of the project was accompanied by the introduction of a new governance structure, which is by now in place. The HBP remains open for new partners to join the Core Project through open calls for the next project phases, while Partnering Projects may use the HBP Platforms for their research and contribute to infrastructure development [10].

The HPAC Platform will continuously be improved and expanded to enable neuroscientists to address key challenges. These include the creation of high-resolution brain atlases and the processing of brain images using advanced data analytics methods. Another example is the study of synaptic plasticity as a basis for learning, by combining large-scale simulations on massively parallel HPC systems with ultra-fast simulations enabled by the Neuromorphic Computing Platform.

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Written by Thomas Lippert¹, Anna Lührs¹, Colin McMurtrie², Boris Orth¹, Dirk Pleiter¹ and Thomas Schulthess²

¹ Jülich Supercomputing Centre (JSC), Germany
² CSCS, ETH Zürich, Switzerland

Contact: Boris Orth, b.orth@fz-juelich.de



Fortissimo 2



Factories of the Future Resources, Technology, Infrastructure and Services for Simulation and Modeling 2.

FORTISSIMO

Fortissimo 2 is a project funded by the European Commission under the H2020 Framework Programme for Research and Innovation through Grant Agreement no. 680481 and part of the ICT Innovation for Manufacturing SMEs (I4MS) action (www.i4ms.eu). FORTISSIMO2 is a follow-on action to the Fortissimo project established in 2013.

Project Outline

The success of bringing a new product to the market for a small or medium sized enterprise (SME) depends on its ability to balance innovation, costs, time and quality during product development. With the advent of computer aided engineering, SMEs have started to use simulations to help their engineers to create the most cost-effective products or even products that were not possible before. However, complex simulations need High Performance Computing resources to get results in a reasonable time. But traditionally HPC resources haven't been affordable by SMEs.

Within its predecessor, the Fortissimo project, the principal objective has been not only to enable European SMEs to be more competitive through the use of simulation services running on a High Performance Computing (HPC) Cloud infrastructure, but also to provide them a "one-stop-shop"—the Fortissimo Marketplace—that allows convenient access to such HPC Cloud infrastructure and in addition to expert support, third-party applications, tools and helpdesk in one place.

In the Fortissimo 2 project, the Fortissimo Marketplace is continued and enhanced with advanced HPC-Cloud services based on High Performance Data Analytics (HPDA) and Coupled HPC Simulations. Any kind of sensor network, like weather or traffic flow control ones, produces a lot of data continuously. Many internet services store a lot of tracking data used later to optimize the service itself. Also complex simulations, like Coupled HPC Simulations, create big data sets in a short time. Coupled HPC Simulations are used nowadays to study complex models in science, for example, a heart and a blood flow simulation running together for a better understanding of the human circulatory system. Somewhere in this big amount of data there is valuable information, however, the analysis to find this information is quite compute intense and can't be handled by traditional data analysis tools. HPDA becomes here necessary to handle and analyse this vast amount of data in a reasonable time.



Detail of the Fortissimo portal. SMEs can sign up into the Fortissimo Marketplace for access to HPC-Cloud services.

As its predecessor, the Fortissimo 2 project is driven by the requirements of Fortissimo 2 experiments (about 35 experiments in total), which will be brought into the project in three tranches, two of them open calls for proposals to solve real-world customer problems. An initial set of 14 experiments has started on February 1st, 2016 and two further sets will be started also in 2016. Details on the call procedure and documentation is available in the Fortissimo website here (www.fortissimo-project.eu).

Fortissimo 2 Experiments

The following table summarizes the 14 initial experiments in Fortissimo 2. These experiments cover a wide range of topics in engineering and

manufacturing, from gas and flame detector layouts simulations to railways infrastructure for high speed train simulations. Partners involved on each experiment are shown in the last column with the leader partner in bold. The High Performance Computing Center Stuttgart of Stuttgart University (HLRS - USTUTT) is the leading partner in experiments E703 and E704 related to the foundry industry and aeroacoustics CFD simulations respectively.

Role of HLRS

In the Fortissimo 2 project, the High Performance Computing Center of Stuttgart University (HLRS), is in charge of the Fortissimo Marketplace development and operations. Therefore,

No.	Title	Partners
E701	Cloud based simulation application for vehicle product engineering	UEDIN , ICONCFD, KOENIGSEGG
E702	Build and HPC-Cloud service for optimizing gas and flame detector layouts in hazardous manufacturing and production plants	UEDIN , GEXCON, MICROPACK
E703	FUSION – HPC Cloud services for the foundry industry	USTUTT , PROSERV, FRAUNHOFER, NOESIS
E704	Aeroacoustics CFD-simulations using open source software and their analysis using big data approaches	USTUTT , FRAUNHOFER, CFDSCHUCK
E705	CLOUDGEAR – HPC Cloud based engineering design and optimization of high performance gears	ARCTUR , STAM, NOESIS
E706	High-resolution magnet modeling and automated production yield prediction	ARCTUR , XLAB, MAGNETI
E707	Cyber-physical laser metal deposition (CyPLAM)	CESGA , AIMEN, EMO
E708	Advance dimensional data analytics for knowledge generation in camshaft manufacturing	CESGA , TRIMEIK, EPC
E709	Computing simulation of box framed timber beams	COMPUTE , USC, MADERAS
E710	Near real-time analysis of airframe certification test data	COMPUTE , COLOSSO, KEWORKS
E711	Big data inside a crankshaft machining center	BULL , ATOS, ETX, VICOM
E712	Improved data handling in global analysis of risers, moorings and flow lines	BULL , PRINCIPIA
E713	HPC Cloud based simulation in railways infrastructure for high speed train	CINECA , ALSTOM, HYPERTEC
E714	Predictive diagnosis services for automotive industry (PRESERVE)	CINECA , TEXA, T2I



HLRS will not only operate and maintain the Fortissimo Marketplace, but also will extend it based on the requirements of the new experiments in Fortissimo 2. The main topics covered by these new requirements, obtained from the first initial experiments and later on, the open calls, focus on the use of high performance data analytics, data stream processing and an enhanced remote visualization of partial and final results if possible in real time.

Partners

The project is coordinated by the University of Edinburgh and involves initially 38 partners. There are 13 core partners: University of Edinburgh, Scapos, University of Stuttgart, Sicos BW, Intel, Actur, XLAB, CESGA, Gompute, Bull, Atos, SURFsara and CINECA. There are also 25 experiment partners working since February 1st, 2016 on their experiments (see table in the Fortissimo 2 Experiments section).

Key Facts

Fortissimo 2 has a total cost of 11.1 M€ and an EU contribution of 10 M€ over a duration of three years, commensurate with achieving its ambitious goals. The project has started in November 1st, 2015 and will finish therefore in October 31st, 2018.

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Additional contact at HLRS:

Michael Gienger: gienger@hlrs.de

Nico Struckmann: struckmann@hlrs.de



Written by Jochen Buchholz, HLRS

Jochen Buchholz is involved for ten years in many national and european research projects on HPC and Cloud computing infrastructures. The covered areas reach from infrastructure provisioning to energy saving aspects, to end user support. His major interest is on network related aspects. Within Fortissimo 2 Jochen Buchholz is in charge of the Marketplace Development and Operations work package.

Contact: Jochen Buchholz, buchholz@hlrs.de



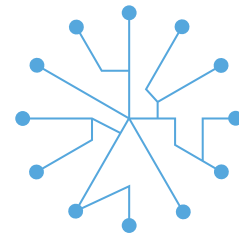
and Carlos Díaz, HLRS

Carlos Diaz has a Master in Innovation and Research in Informatics with specialization in High Performance Computing, by the Polytechnic University of Catalonia, Spain. Previously to join the Stuttgart Supercomputing Center (HLRS), he has been working in the Barcelona Supercomputing Center (BSC) in projects for cloud computing like EU Brazil Cloud Connect among others. Carlos Diaz currently participates in the Marketplace Development and Operations work package in the Fortissimo 2 project.

Contact: Carlos Díaz, diaz@hlrs.de

EuroLab-4-HPC

**Foundations of a European Research Center
of Excellence in High Performance Computing Systems**



EUROLAB-4-HPC

Project outline

The EuroLab-4-HPC project's overall goal is to build connected and sustainable leadership in high-performance computing systems by bringing together the different and leading performance orientated communities in Europe working across all layers of the system stack and, at the same time, fuelling new industries in HPC. Thus, to tackle the long-term challenges of HPC the project brings together European research groups to compete internationally.

The EuroLab-4-HPC project targets the vital importance to the progress of science and technology for HPC systems in Europe. In this scope, a collaboration to the ETP4HPC [2] project driving a European HPC vision towards exascale systems will be established. EuroLab-4-HPC purpose is to develop a long-term research agenda promoting innovation and education for HPC systems. The EuroLab-4-HPC project will achieve its objectives through:

- defining an HPC curriculum in HPC technologies and best-practice education/training methods to foster future European technology leaders.
- joining HPC system research groups around a long-term HPC research agenda by forming an HPC research roadmap and joining forces behind it.
- accelerating commercial uptake of new HPC technologies.
- building an HPC ecosystem with researchers and other stakeholders, e.g. HPC system providers and venture capital.

- forming a business model and organization for the EuroLab-4-HPC excellence center in HPC systems.

The EuroLab-4-HPC project considers latest training activities and research by using the expertise of the involved partners and encouraging the scientific exchange between EuroLab-4-HPC and projects such as PRACE [1] and ETP4HPC. Further, the consortium brings in specific HPC and Training expertise.

EuroLab-4-HPC addresses major gaps in implementing an effective European HPC strategy concerning industrial and academic leadership in the supply of HPC systems. EuroLab-4-HPC builds a HPC research community by consideration of ongoing activities. In this scope, ETP4HPC is taking a lead in building an HPC ecosystem. From a user perspective, PRACE offers a Europe-wide e-Science infrastructure and, as such, connects the scientific users. What is lacking is a consolidated research community in HPC systems motivated to drive innovations. What is needed for a European HPC strategy to be effective, is establishing links between a wide range of HPC stakeholders. Thus, the project triggers cross stack research and innovation. Additionally, in terms of roadmap and technology challenges it is important to form an agile process for long-term roadmapping of what are the major technological challenges facing HPC as well as having agile processes for bringing promising research ideas on a fruitful path to commercialization. The EuroLab-4-HPC objectives lead to the need



of enhancing existing approaches and deploy new ones for training purposes for future HPC technology leaders.



As presented in figure 1 the EuroLab-4-HPC consortium combines aspects of research, education and innovation for achieving its goal to join forces among excellent research institutions in HPC systems across the system stack towards a long-term research agenda that drives innovation and education. For reaching this goal EuroLab-4-HPC takes into account sustainability and community building.

The EuroLab-4-HPC Roadmap

The EuroLab-4-HPC roadmap targets a long-term roadmap from 2022 to 2030 for the HPC domain. Due to the long-term view of the roadmap the EuroLab-4-HPC project started with an assessment of future computing technologies that could be relevant for HPC hardware and software.

Beyond the future computing technologies there is an ever growing need of current and new applications for the HPC domain. However, it is not restricted to only HPC. Typically, HPC targets simulations using numerical programs. EuroLab-4-HPC expects a continuous scaling of such applications to continue beyond exascale computers. Generally the roadmap targets two major trends being relevant for HPC and supercomputers. First, the emergence of data analytics completing simulation in scientific discovery is handled and second, the trend of cloud computing and warehouse scale computers will be targeted.

The EuroLab-4-HPC Curriculum

A major goal of the EuroLab-4-HPC project is to establish a HPC curriculum for HPC. Thus, the curriculum is a combination of courses that can be delivered in a traditional form and online. The online courses can be supported by a few limited physical presence sessions as needed, collocated with regularly occurring global events of the EuroLab-4-HPC project.



When thinking of relevant topics for the EuroLab-4-HPC curriculum, courses should cover following contents:

- Parallel Computer Architectures
- Scalable Parallel Algorithms
- Programming with MPI
- Parallel Computing with Hadoop
- Programming Shared Memory Parallel Systems
- Programming Multi-core and Many-core Systems
- Performance Engineering
- Programming Heterogeneous Systems with OpenCL/CUDA
- Large Scale Scientific Computation

In addition, the suggested courses of the curriculum are mapped with programmes for student training. In this scope it is distinguished between three programme proposals:

1. A two-year MSc level program for CS/ECE and Science (Physics/Math) majors consisting of 9 courses and a semester thesis.
2. A two-year MSc level program for CS/ECE and Science (Physics/Math) majors consisting of 9 courses and a semester thesis. However, this program varies from the first program through offering partially a different set of courses than the first program proposal.
3. A single-year MSc level program for CS/ECE majors. It is Bologna-aligned and includes 7 core courses, 2 elective ones and a two-course equivalent thesis (60 ECTS).

Of course the above examples can be tailored in many ways. The Bologna agreement ECTS are a useful metric in gauging the level of the course at least in terms of student effort.

Besides the MSc level programs the curriculum covers courses for experts by figuring out and proposing needed courses being relevant for the HPC domain. In this scope, existing course offers and curricula are considered such as the ACM Computer Science Curricula 2013 [3], course offers of HLRS [4], PRACE or EIT [5]. The curricula will be constantly adapted to address latest educational and training challenges and technological developments. In addition to the curriculum, best practices will be developed in EuroLab-4-HPC, giving guidelines for offering courses and for taking care about customized demands for online courses and training activities.

Role of HLRS in the Project

The role of the High Performance Computing Center is about the educational aspect such as training activities. In this scope HLRS offers its long-term experience and a broad set of courses being physical ones and online training activities. Besides coordination activities, HLRS is deeply involved in offering its expertise regarding HPC training achieved through training activities offered for academia and industry as well as through projects such as PRACE or bwHPC-C5 [6].



Key Facts

The EuroLab-4-HPC project is funded by the European Commission within the Horizon 2020 FET Proactive Programme being a research and innovation action. It has started at the 01.09.2015 and will run until the 31.08.2017.

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<http://www.eitdigital.eu/>, last visited: 25.08.2016.
- [6] **The bwHPC-C5 project web site:**
<https://www.bwhpc-c5.de/>, last visited: 25.08.2016.

EuroLab-4-HPC Project Website

eurolab4hpc.eu

EuroLab-4-HPC Partners

- Chalmers University of Technology
- Barcelona Supercomputing Center
- Foundation for Research and Technology Hellas
- University of Stuttgart
- INRIA - Institut National de Recherche Eninformatique et Automatique
- University of Manchester
- ETHz - Eidgenoessische Technische Hochschule Zuerich
- EPFL - Ecole Polytechnique Federale de Lausanne
- Technion – Israel Institute of Technology
- Rheinisch-Westfalische Technische Hochschule Aachen
- Ghent University

Additional contact at HLRS:

Bastian Koller: koller@hlrs.de

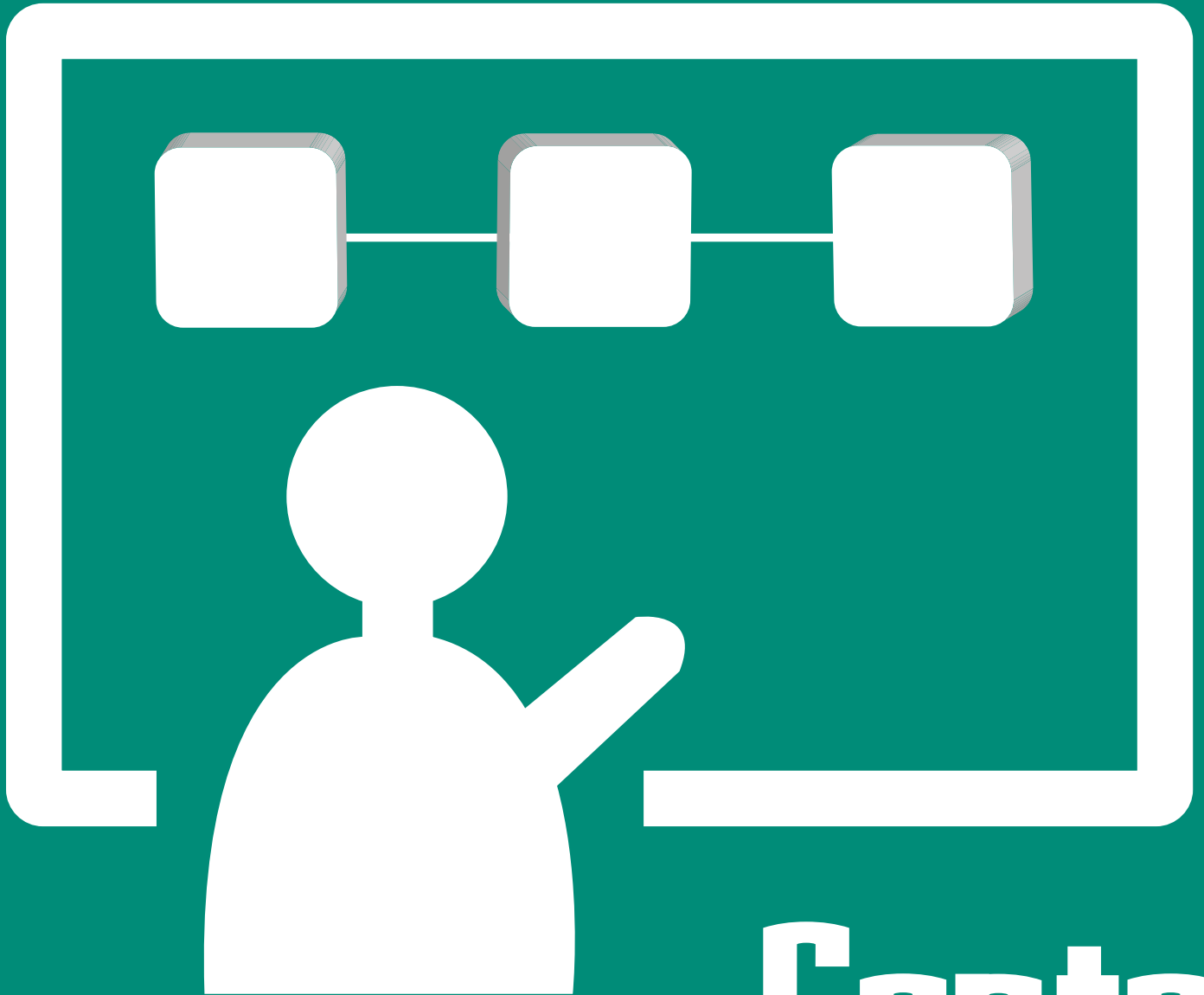


Written by Axel Tenschert, HLRS

M. A. Axel Tenschert has studied at the University of Bielefeld German philology, computer sciences and text technology. He started work as a computer scientist at the High Performance Computing Center Stuttgart (HLRS) in 2007 and is deputy of the SANE research group. Beside this, he has been involved in various national and European research projects in the area of semantic information management and distributed computing (such as grid and cloud computing).

Additionally, he is performing training activities and has submitted his PhD thesis focusing on semantic technologies in terms of distributing ontology matching strategies in an HPC environment.

Contact: Axel Tenschert, tenschert@hlrs.de



Center

rs & Trainings

In this section you will find an overview about the upcoming training program and information about the members of GCS.



Leibniz Supercomputing Centre

Prof. Dr. Arndt Bode

Boltzmannstr. 1

85748 Garching near Munich

Germany

Phone +49-89-358-31-80 00

bode@lrz.de

www.lrz.de

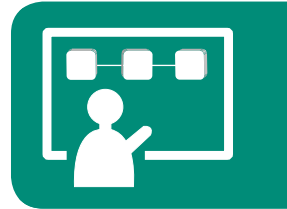
The Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities (Leibniz-Rechenzentrum, LRZ) provides comprehensive services to scientific and academic communities by:

- giving general IT services to more than 100,000 university customers in Munich and for the Bavarian Academy of Sciences
- running and managing the powerful communication infrastructure of the Munich Scientific Network (MWN)
- acting as a competence centre for data communication networks
- being a centre for large-scale archiving and backup, and by
- providing High Performance Computing resources, training and support on the local, regional, national and international level.

Research in HPC is carried out in collaboration with the distributed, statewide Competence Network for Technical and Scientific High Performance Computing in Bavaria (KONWIHR).



Picture of the Petascale system SuperMUC at the Leibniz Supercomputing Centre.



Compute servers currently operated by LRZ

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
IBM/Lenovo System x Cluster "SuperMUC Phase 1"	■ 18 thin node islands ■ IBM iDataPlex ■ 512 nodes, 147,456 cores ■ Sandy Bridge EP ■ 288 TByte, FDR 10 IB	3,185	Capability Computing	German universities and research institutes, PRACE (Tier-0 System)
	■ 1 fat node island with ■ 205 nodes, 8,200 cores ■ IBM Bladecenter HX5 ■ Westmere EX ■ 52 TByte, QDR IB	78	Capability Computing	
	■ 32 accelerated nodes ■ Intel Ivy Bridge EP, ■ Intel Xeon Phi ■ 76 GByte, ■ Dual-Rail FDR 14 IB	100	Prototype System	
Lenovo/IBM Nextscale Cluster "SuperMUC Phase 2"	■ 6 medium node islands ■ Lenovo/IBM Nextscale ■ 512 nodes, 86,016 cores ■ Haswell EP ■ 197 TByte, FDR 14 IB	3,580	Capability computing	German universities and research institutes, PRACE (Tier-0 System)
Lenovo/IBM Nextscale Cluster "CoolMUC2"	■ 252 nodes, 7,056 cores ■ Haswell EP ■ 16.1 TByte ■ FDR 14 IB	270	Capability computing	Bavarian Universities
Megware IB-Cluster "CoolMUC"	■ 178 nodes, 2,848 Cores ■ AMD Magny Cours ■ 2.8 TByte ■ QDR IB	22.7	Capability Computing, PRACE Prototype	Bavarian Universities
SGI Altix Ultraviolet	■ 2 partitions, 2,080 cores ■ Intel Westmere EX ■ 6.0 TByte main memory	20.0	Capability Computing	Bavarian Universities
Linux-Cluster	■ 510 nodes, 2,030 cores ■ Intel Xeon EM64T/ ■ AMD Opteron ■ 2-, 4-, 8-, 16-, 32-way ■ 4.7 TByte main memory	13.2	Capability Computing	Bavarian and Munich Universities, LCG Grid

A detailed description can be found on LRZ's web pages: www.lrz.de/services/compute

HLRS

Hochleistungsrechenzentrum Stuttgart
(HLRS), Universität Stuttgart

Prof. Dr.-Ing. Dr. h.c. Dr. h.c. Prof. E.h.
Michael M. Resch

Nobelstr. 19 | 70569 Stuttgart, Germany
Phone +49 - 711 - 685 - 8 72 69
resch@hlrs.de
www.hlrs.de

First German National Center

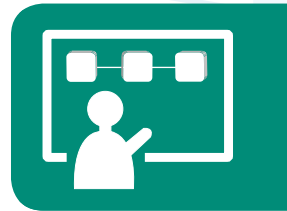
Based on a long tradition in supercomputing at University of Stuttgart, HLRS (Hochleistungsrechenzentrum Stuttgart) was founded in 1995 as the first German federal Centre for High Performance Computing. HLRS serves researchers at universities and research laboratories in Europe and Germany and their external and industrial partners with high-end computing power for engineering and scientific applications.

Service for Industry

Service provisioning for industry is done together with T-Systems, T-Systems sfr, and Porsche in the public-private joint venture hww (Hochleistungsrechner für Wissenschaft und Wirtschaft). Through this co-operation industry always has access to the most recent HPC technology.



View of the HLRS Cray XC40 "Hazel Hen"



Bundling Competencies

In order to bundle service resources in the state of Baden-Württemberg HLRS has teamed up with the Steinbuch Center for Computing of the Karlsruhe Institute of Technology. This collaboration has been implemented in the non-profit organization SICOS BW GmbH.

World Class Research

As one of the largest research centers for HPC HLRS takes a leading role in research. Participation in the German national initiative of excellence makes HLRS an outstanding place in the field.

Compute servers currently operated by HLRS

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
Cray XC40 "Hazel Hen"	■ 7,712 nodes ■ 185,088 cores 1 PB memory	7,420	Capability Computing	German and European (PRACE) Research Organizations and Industry
NEC Cluster (Laki, Laki2) heterogenous computing platform of 2 independent clusters	■ 911 nodes 9,988 cores ■ 23 TB memory	170	Capacity Computing	German Universities, Research Institutes and Industry
NEC SX-ACE	■ 64 nodes 256 cores ■ 4 TB memory	16	Vector Computing	German Universities, Research Institutes and Industry

A detailed description can be found on HLRS' web pages: www.hlr.de/systems



Jülich Supercomputing Centre (JSC)
Forschungszentrum Jülich

Prof. Dr. Dr. Thomas Lippert

Wilhelm-Johnen-Straße

52425 Jülich, Germany

Phone +49 - 24 61-61-64 02

th.lippert@fz-juelich.de

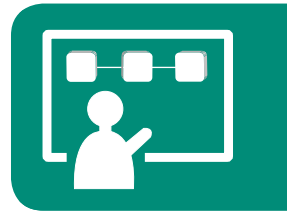
www.fz-juelich.de/jsc

The Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich is committed to enabling scientists and engineers explore some of the most complex grand challenges facing science and society. Our research is performed through collaborative infrastructures exploiting extreme-scale supercomputing and federated data services.

Provision of supercomputer resources of the highest performance class for projects in science, research and industry in the fields of modeling and computer simulation including their methods. The selection of the projects is performed by international peer-review procedures implemented by the John von Neumann Institute for Computing (NIC), GCS, and PRACE.



JSC's supercomputer "JUQUEEN", an IBM Blue Gene/Q system.



Supercomputer-oriented research and development in selected fields of physics and other natural sciences by research groups and in technology, e.g. by doing co-design together with leading HPC companies.

Higher education for master and doctoral students in close cooperation with neighbouring universities.

Implementation of strategic support infrastructures including community-oriented simulation laboratories and cross-sectional teams, e.g. on mathematical methods and algorithms and parallel performance tools, enabling the effective usage of the supercomputer resources.

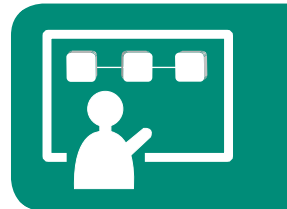
Compute servers currently operated by JSC

System	Size	Peak Performance (TFlop/s)	Purpose	User Community
IBM Blue Gene/Q "JUQUEEN"	■ 28 racks ■ 28,672 nodes ■ 458,752 processors ■ IBM PowerPC® A2 ■ 448 Tbyte main memory	5,872	Capability Computing	European Universities and Research Institutes, PRACE
Intel Linux Cluster "JURECA"	■ 1,884 SMT nodes with 2 Intel Haswell 12-core 2.5 GHz processors each ■ 150 graphics processors (NVIDIA K80) ■ 281 TByte memory	2,245	Capacity and Capability Computing	European Universities, Research Institutes and Industry
IBM Cell System "QPACE"	■ 1,024 PowerXCell 8i processors ■ 4 TByte memory	100	Capability Computing	QCD Applications SFB TR55, PRACE

Timetable

High Performance Computing courses and tutorials

Course Title	Location	Date
Advanced C++ with Focus on Software Engineering	Garching	Nov 22–24, 2016
Introduction to the Programming and Usage of the Supercomputer Resources at Jülich	Jülich	Nov 24–25, 2016
Elmer FEM Course	Garching	Nov 28–29, 2016
Advanced Parallel Programming with MPI and OpenMP	Jülich	Nov 28–30, 2016
Advanced C++, Focus on Software Engineering	Stuttgart	Nov 28–Dec 1, 2016
Node-Level Performance Engineering (PATC course)	Garching	Dec 1–2, 2016
Fortran for Scientific Computing (PATC course)	Stuttgart	Dec 12–16, 2016
Introduction to hybrid programming in HPC (PATC course)	Garching	Jan 12, 2017
Introduction to parallel programming with MPI and OpenMP	Jülich	Jan 31–Feb 3, 2017
Intel MIC Programming Workshop (PATC course)	Ostrava	Feb 2017
Introduction to Computational Fluid Dynamics	Siegen	Feb 13–17, 2017
Parallel Programming (MPI, OpenMP) and Tools	Dresden	Feb 20–24, 2017
Programming with Fortran	Garching	Mar 1–3, 2017
Parallel Programming of High Performance Systems	Garching	Mar 6–10, 2017
OpenMP and OpenACC GPU Directives for Parallel Accelerated Supercomputers (PATC course)	Stuttgart	Mar 7–8, 2017
Parallel I/O and Portable Data Formats (PATC course)	Jülich	Mar 13–15, 2017
Parallelization with MPI and OpenMP	Frankfurt a. M.	Mar 13–15, 2017
Advanced C++, Focus on Software Engineering	Stuttgart	Mar 14–17, 2017
Vectorisation and Portable Programming Using OpenCL	Jülich	Mar 16–17, 2017
Fortran for Scientific Computing (PATC course)	Stuttgart	Mar 20–24, 2017
Iterative Linear Solvers and Parallelization	Stuttgart	Mar 27–31, 2017
Advanced Topics in High Performance Computing (PATC course)	Garching	Apr 3–6, 2017
CFD with OpenFOAM®	Stuttgart	Apr 3–7, 2017
GPU Programming with CUDA (PATC course)	Jülich	Apr 24–26, 2017
Node-Level Performance Engineering (PATC course)	Stuttgart	Apr 27–28, 2017
Cray XC40 Workshop on Optimization at Scale	Stuttgart	May 2–5, 2017
Introduction to the Programming and Usage of the Supercomputer Resources at Jülich	Jülich	May 22–23, 2017
Cluster Workshop	Stuttgart	May 29–30, 2017
Scientific Visualization	Stuttgart	May 31–Jun 1, 2017
Intel MIC Programming Workshop (PATC course)	Garching	Jun 2017
Introduction to hybrid programming in HPC	Stuttgart	Jun 12, 2017
High-performance Computing with Python (PATC course)	Jülich	Jun 12–13, 2017
Introduction to UPC and Co-Array Fortran (PATC course)	Stuttgart	Jun 29–30, 2017
Efficient Parallel Programming with GASPI (PATC course)	Stuttgart	Jul 3–4, 2017
Introduction to Cluster Filesystems	Stuttgart	Jul 6, 2017
NEC SX-ACE – Vectorization and Optimization	Stuttgart	Jul 11–12, 2017
Guest Student Programme at JSC	Jülich	Aug 6–Oct 13, 2017



Advanced C++ with Focus on Software Engineering

Nov 22–24, 2016 | LRZ, Garching near Munich
see also Nov 28–Dec 1, 2016 in Stuttgart (4 days) and Mar 14–17, 2017 in Stuttgart (4 days)

This advanced C++ training is a course on object-oriented (OO) software design with the C++ programming language. The focus of the training are the essential OO and C++ software development principles, concepts, idioms, and best practices, which enable programmers to create professional, high-quality code. The course will not address special areas and applications of C++, such as for instance Template Meta Programming (TMP), or the quirks and curiosities of the C++ language. It rather teaches guidelines to develop mature, robust, and maintainable C++ code. The following topics will be covered:

- Essential object-oriented design principles
- Concepts and the STL
- Class design
- Robust code
- Proper use of dynamic Inheritance
- Dependency-breaking techniques
- Non-Intrusive design
- C++11/14 update

Prerequisites

Solid base on C++ and at least one year of experience with the language is needed. Participants have to bring their own laptop for the hands on sessions.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Introduction to the Programming and Usage of the Supercomputer Resources at Jülich

Nov 24–25, 2016 | JSC, Forschungszentrum Jülich
see also May 22–25, 2017 in Jülich

Forschungszentrum Jülich provides two major high-performance computing resources to scientific user groups from throughout Germany and Europe. The aim of this course is to give new users of the supercomputing resources an introductory overview of the systems and their usage, and to help them in making efficient use of their allocated resources.

Prerequisites:

Basic knowledge of Unix, knowledge of either C, C++ or Fortran

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/sc-nov>

Elmer FEM Course

Nov 28–29, 2016 | LRZ, Garching near Munich

The Elmer FEM course is intended for persons with none or some prior knowledge of Elmer but some background on the solution of partial differential equations. The course will cover the use of Elmer through its graphical user interface, ElmerGUI. Also command-line operation of Elmer will be explained. The course will also include the basics of parallel computing and writing user subroutines with Elmer. After the course the participants should be able to solve basic modelling problems themselves, modify them manually, and have basic knowledge on the general features of Elmer software.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Advanced Parallel Programming with MPI and OpenMP

Nov 28–30, 2016 | JSC, Forschungszentrum Jülich

The focus is on advanced programming with MPI and OpenMP. The course addresses participants who have already some experience with C/C++ or Fortran and MPI and OpenMP, the most popular programming models in High Performance Computing (HPC). It will teach newest methods in MPI-3.0/3.1 and OpenMP-4.5, which were developed for the efficient use of current HPC hardware. Topics with MPI are the group and communicator concept, process topologies, derived data types, the new MPI-3.0 Fortran language binding, one-sided communication and the new MPI-3.0 shared memory programming model within MPI. Topics with OpenMP are the OpenMP-4.0 extensions, as the vectorization directives, thread affinity and OpenMP places. The course also contains performance and best practice considerations, e.g., with hybrid MPI+OpenMP parallelization. The course ends with a section presenting tools for parallel programming. The course is given in German. This course is organized by JSC in collaboration with HLRS. Presented by Dr. Rolf Rabenseifner, HLRS.

Prerequisites:

Knowledge in Unix, in either C, C++ or Fortran; familiar with the principles of MPI, i.e., point-to-point message passing, datatypes, nonblocking communication, collective communication; familiar with OpenMP 3.0

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/mpi>

Advanced C++, Focus on Software Engineering

Nov 28–Dec 01, 2016 | HLRS, Stuttgart
see also Nov 22–24, 2016 in Garching (3 days) and Mar 14–17, 2017 in Stuttgart (4 days)

This advanced C++ training is a course on object-oriented (OO) software design with the C++ programming language. The focus of the training are the essential OO and C++ software development principles, concepts, idioms, and best practices, which enable programmers to create professional, high-quality code. Additionally, the course gives insight into kernel development with C++. The course will not address special areas and applications of C++, such as for instance Template Meta Programming (TMP), or the quirks and curiosities of the C++ language. It rather teaches guidelines to develop mature, robust, maintainable, and efficient C++ code.

After this course, participants will:

- have a detailed understanding of the essential OO design principles
- have gained knowledge about fundamental C++ programming concepts and idioms
- be able to properly design classes and class interfaces
- know about the importance of exception safe programming
- have gained insight into kernel development with C++
- avoid the usual pitfalls in the context of inheritance
- comprehend the advantages of non-intrusive design
- understand the virtue of clean code

Prerequisites

Basic UNIX/Linux knowledge (login with secure shell, shell commands, simple scripts, editor vi or emacs), solid base on C++ and at least one year of experience with the language

Webpage for further information:

<http://www.hlrs.de/training/2016-11-28-cpp2/>

Node-Level Performance Engineering (PATC course)

Dec 1–2, 2016 | LRZ, Garching near Munich
see also Apr 27–28, 2017 in Stuttgart

This course teaches performance engineering approaches on the compute node level. "Performance engineering" as we define it is more than employing tools to identify hotspots and bottlenecks. It is about developing a thorough understanding of the interactions between software and hardware. This process must start at the core, socket, and node level, where the code gets executed that does the actual computational work. Once the architectural requirements of a code are understood and correlated with performance measurements, the potential benefit of optimizations can often be predicted. We introduce a "holistic" node-level performance engineering strategy, apply it to different algorithms from computational science, and also show how an awareness of the performance features of an application may lead to notable reductions in power consumption.

Prerequisites

Participants must have basic knowledge in programming with Fortran or C.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Fortran for Scientific Programming (PATC course)

Dec 12–16, 2016 | HLRS, Stuttgart
see also Mar 20–24, 2017 in Stuttgart

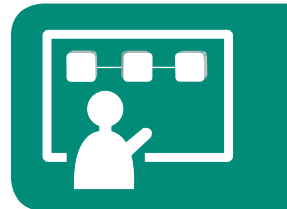
This course is dedicated for scientists and students to learn (sequential) programming with Fortran of scientific applications. The course teaches newest Fortran standards. Hands-on sessions will allow users to immediately test and understand the language constructs. This workshop provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves. (This course has the same content as the course in spring.)

Prerequisites

Familiarity with Linux and Linux editors is recommended. Basics/principles of programming (in any language). Basic mathematics (integration and differentiation).

Webpage for further information:

<https://www.hlrs.de/training/2016-12-12-ftn2/>



Introduction to hybrid programming in HPC (PATC course)

Jan 12, 2017 | LRZ, Garching near Munich
see also Jun 12, 2017 in Stuttgart

Most HPC systems are clusters of shared memory nodes. Such SMP nodes can be small multi-core CPUs up to large many-core CPUs. This course analyses the strengths and weaknesses of several parallel programming models on clusters of SMP nodes. Multi-socket-multi-core systems in highly parallel environments are given special consideration. MPI-3.0 has introduced a new shared memory programming interface, which can be combined with inter-node MPI communication. It can be used for direct neighbour accesses similar to OpenMP or for direct halo copies, and enables new hybrid programming models. These models are compared with various hybrid MPI+OpenMP approaches and pure MPI. Numerous case studies and micro-benchmarks demonstrate the performance-related aspects of hybrid programming.

Prerequisites

Participants must have basic knowledge in programming with MPI and OpenMP.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Introduction to parallel programming with MPI and OpenMP

Jan 31–Feb 3, 2017 | JSC, Forschungszentrum Jülich

An introduction to the parallel programming of supercomputers is given. The focus is on the usage of the Message Passing Interface (MPI), the most often used programming model for systems with distributed memory. Furthermore, OpenMP will be presented, which is often used on shared-memory architectures.

Prerequisites

Knowledge of Fortran, C or C++

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/mpi-intro>

Intel MIC Programming Workshop (PATC-Course)

Feb 2017, 2 days | IT4Innovations, Ostrava
see also Jun 2017, in Garching (3 days)

These workshops discuss Intel's Many Integrated Core (MIC) architecture. They cover various programming and optimisation techniques for Intel Xeon Phi based systems. While the course taking place at IT4Innovations in February will concentrate on the Knights Corner based system Salomon - currently the largest Intel Xeon Phi based system in Europe - the course at LRZ in June will focus on Intel's new Knights Landing architecture.

The workshops are developed within PRACE and the joint German-Czech Republic project CzeBaCCA.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Introduction to Computational Fluid Dynamics

Feb 13–17, 2017 | University of Siegen

The course deals with current numerical methods for Computational Fluid Dynamics in the context of high performance computing. An emphasis is placed on explicit methods for compressible flows, but classical numerical methods for incompressible Navier-Stokes equations are also covered. A brief introduction to turbulence modelling is also provided by the course. Additional topics are high order numerical methods for the solution of systems of partial differential equations. The last day is dedicated to parallelization.

Hands-on sessions will manifest the contents of the lectures. In most of these sessions, the application Framework APES will be used. They cover grid generation using Seeder, visualization with ParaView and the usage of the parallel CFD solver Ateles on the local HPC system.

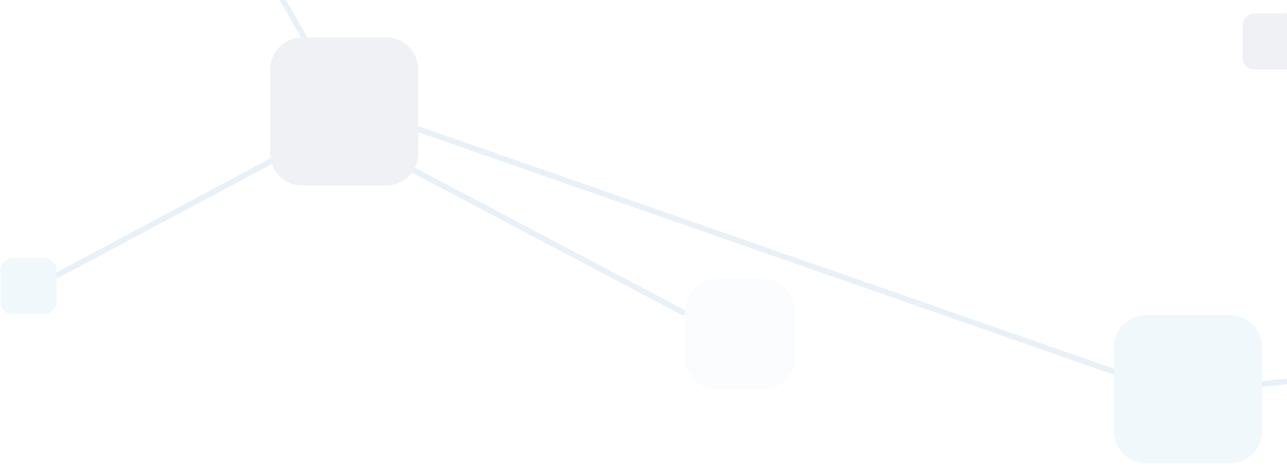
The course is organized by HLRS, IAG (University of Stuttgart) and STS, ZIMT (University of Siegen).

Prerequisites

Basics of partial differential equations and physics, programming experience in Fortran or C

Webpage for further information:

<http://www.hlr.de/training/2017-02-13-cfd-siegen/>



Parallel Programming (MPI, OpenMP) and Tools

Feb 20–24, 2017 | ZIH, TU Dresden

The focus is on programming models MPI and OpenMP. Hands-on sessions (in C and Fortran) will allow users to immediately test and understand the basic constructs of the Message Passing Interface (MPI) and the shared memory directives of OpenMP. The last part is dedicated to tools. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves. It is organized by ZIH in collaboration with HLRS. (Content Level: 70% for beginners, 30% advanced)

Prerequisites

Unix / C or Fortran

Webpage for further information:

<https://www.hlr.de/training/2017-02-20-zih/>

Parallel Programming of High Performance Systems

Mar 6–10, 2017 | LRZ, Garching near Munich

This course, a collaboration of Erlangen Regional Computing Centre (RRZE) and LRZ, is targeted at students and scientists with interest in programming modern HPC hardware, specifically the large scale parallel computing systems available in Jülich, Stuttgart and Munich. Each day is comprised of approximately 4 hours of lectures and 3 hours of hands-on sessions.

Prerequisites

Participants must have good knowledge of at least one of the standard HPC languages: Fortran 95, C or C++.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

Programming with Fortran

Mar 1–3, 2017 | LRZ, Garching near Munich

This course is targeted at scientists with little or no knowledge of the Fortran programming language, but need it for participation in projects using a Fortran code base, for development of their own codes, and for getting acquainted with additional tools like debugger and syntax checker as well as handling of compilers and libraries. The language is for the most part treated at the level of the Fortran 95 standard; features from Fortran 2003 are limited to improvements on the elementary level. Advanced Fortran features like object-oriented programming or coarrays will be covered in a follow-on course in autumn.

To consolidate the lecture material, each day's approximately 4 hours of lecture are complemented by 3 hours of hands-on sessions.

Prerequisites

Course participants should have basic UNIX/Linux knowledge.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

OpenMP and OpenACC GPU Directives for Parallel Accelerated Supercomputers (PATC course)

Mar 7–8, 2017 | HLRS, Stuttgart

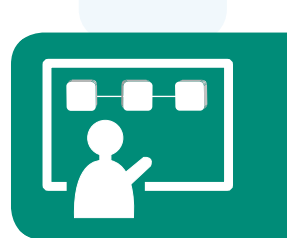
This workshop will cover the directive-based programming model based on OpenMP v4 and OpenACC v2 whose multi-vendor support allows users to portably develop applications for parallel accelerated supercomputers. The workshop will also demonstrate how to use the Cray Programming Environment tools to identify application bottlenecks, facilitate the porting, provide accelerated performance feedback and to tune the ported applications. The Cray scientific libraries for accelerators will be presented, and interoperability of the directives approach with these and with CUDA will be demonstrated. Through application case studies and tutorials, users will gain direct experience of using both OpenMP and OpenACC directives in realistic applications. Users may also bring their own codes to discuss with Cray specialists or begin porting. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Programming experience in C or Fortran, some knowledge about parallel programming.

Webpage for further information:

<https://www.hlr.de/training/2017-03-07-gpu/>



Parallel I/O and Portable Data Formats (PATC course)

Mar 13–14, 2017 | JSC, Forschungszentrum Jülich

This course will start with an introduction to the basics of I/O, including basic I/O-relevant terms, an overview over parallel file systems with a focus on GPFS, and the HPC hardware available at JSC. Different I/O strategies will be presented. The course will introduce the use of the HDF5, the netCDF and the SIONlib library interfaces as well as MPI-I/O. Optimization potential and best practices will be discussed. Participants should have experience in parallel programming in general, and either C/C++ or Fortran in particular.

Prerequisites

Experience in parallel programming with MPI, and either C/C++ or Fortran in particular.

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/parallelio>

Parallelization with MPI and OpenMP

Mar 13–15, 2017 | Goethe University of Frankfurt

The focus is on the programming models MPI and OpenMP. Hands-on sessions (in C and Fortran) will allow users to immediately test and understand the basic constructs of the Message Passing Interface (MPI) and the shared memory directives of OpenMP. This course is organized by HKHLR and CSC, Goethe University Frankfurt in collaboration with HLRS. (Content Level: 70% for beginners, 30% advanced)

Prerequisites

Unix / C or Fortran

Webpage for further information:

<http://www.hlr.de/training/2017-03-13-fra/>

Advanced C++, Focus on Software Engineering

Mar 14–17, 2017 | HLRS, Stuttgart

see also Nov 22–24, 2016 in Garching (4 days) and Nov 28–Dec 01, 2016 in Stuttgart (3 days)

This advanced C++ training is a course on object-oriented (OO) software design with the C++ programming language. The focus of the training are the essential OO and C++ software development principles, concepts, idioms, and best practices, which enable programmers to create professional, high-quality code. Additionally, the course gives insight into kernel development with C++. The course will not address special areas and applications of C++, such as for instance Template Meta Programming (TMP), or the quirks and curiosities of the C++ language. It rather teaches guidelines to develop mature, robust, maintainable, and efficient C++ code.

After this course, participants will:

- have a detailed understanding of the essential OO design principles
- have gained knowledge about fundamental C++ programming concepts and idioms
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- know about the importance of exception safe programming
- have gained insight into kernel development with C++
- avoid the usual pitfalls in the context of inheritance
- comprehend the advantages of non-intrusive design
- understand the virtue of clean code

Prerequisites

Basic UNIX/Linux knowledge (login with secure shell, shell commands, simple scripts, editor vi or emacs), solid base on C++ and at least one year of experience with the language

Webpage for further information:

<http://www.hlr.de/training/2017-03-14-cpp1/>

Vectorisation and Portable Programming Using OpenCL

Mar 16–17, 2017 | JSC, Forschungszentrum Jülich

OpenCL provides an open, portable C-based programming model for highly parallel processors. In contrast to NVIDIA's proprietary programming API CUDA, a primary goal of OpenCL is portability across a diverse set of computing devices including CPUs, GPUs, and other accelerators.

Topics covered will include an introduction to vectorisation, the programming model of OpenCL, data-types and OpenCL vectorisation features, the tuning for architectures like CPUs, accelerators (GPUs), and co-processors (Xeon Phi), and heterogeneous multi-device programming.

Prerequisites

Some knowledge about Linux, e.g. make, command line editor, Linux shell, experience in C

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/opengl>

Iterative Linear Solvers and Parallelization

Mar 27–31, 2017 | HLRS, Stuttgart

The focus is on iterative and parallel solvers, the parallel programming models MPI and OpenMP, and the parallel middleware PETSc. Thereby, different modern Krylov Subspace Methods (CG, GMRES, BiCGSTAB ...) as well as highly efficient preconditioning techniques are presented in the context of real life applications. Hands-on sessions (in C and Fortran) will allow users to immediately test and understand the basic constructs of iterative solvers, the Message Passing Interface (MPI) and the shared memory directives of OpenMP. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves. It is organized by HLRS, IAG, Uni. Kassel, and SFB/TRR30.

Prerequisites

Wednesday+Thursday: Basics of linear algebra
Monday+Tuesday+Friday: Unix / C or Fortran

Webpage for further information:

<https://www.hlrs.de/training/2017-03-27-iter-s/>

Fortran for Scientific Computing (PATC course)

Mar 20–24, 2017 | HLRS, Stuttgart

see also Dec 12–16, 2016, HLRS, Stuttgart

This course is dedicated to scientists and students to learn (sequential) programming with Fortran of scientific applications. The course teaches newest Fortran standards. Hands-on sessions will allow users to immediately test and understand the language constructs. This workshop provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Familiarity with Linux and Linux editors is recommended. Basics/principles of programming (in any language). Basic mathematics (integration and differentiation).

Webpage for further information:

<https://www.hlrs.de/training/2017-03-20-ftnl/>

Advanced Topics in High Performance Computing (PATC course)

April 3–6, 2017 | LRZ, Garching near Munich

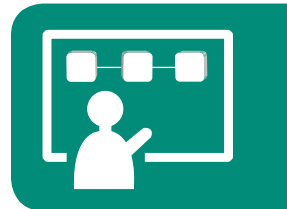
In this add-on course to the parallel programming course special topics are treated in more depth, in particular processor-specific optimisation, I/O, Intel Xeon Phi programming and PGAS concepts. It is provided in collaboration of Erlangen Regional Computing Centre (RRZE) and LRZ within KONWIHR. Each day is comprised of approximately 5 hours of lectures and 2 hours of hands-on sessions.

Prerequisites

Course participants should have good MPI and OpenMP knowledge.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>



CFD with OpenFOAM®

Apr 3–7, 2017 | HLRS, Stuttgart

OpenFOAM® is a widely-used open-source code and a powerful framework for solving a variety of problems mainly in the field of CFD. The five-day workshop gives an introduction to OpenFOAM® applied on CFD phenomena and is intended for beginners as well as for people with CFD background knowledge. The user will learn about case setup, meshing tools like snappyHexMesh and cfMesh. Available OpenFOAM® utilities and additional libraries like swak4Foam, that can be used for pre- and postprocessing tasks, are further aspects of this course. Additionally, basic solvers and major aspects of code structure are highlighted. Lectures and hands-on session with typical CFD examples will guide through this course including first steps in own coding. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Knowledge of using Linux, basics in programming and some insights into CFD theory.

Webpage for further information:

<https://www.hlrs.de/training/2017-04-03-of1/>

Node-Level Performance Engineering (PATC-course)

Apr 27–28, 2017 | HLRS, Stuttgart

see also Dec 1-2, 2016 in Garching

This course teaches performance engineering approaches on the compute node level. "Performance engineering" as we define it is more than employing tools to identify hotspots and bottlenecks. It is about developing a thorough understanding of the interactions between software and hardware. This process must start at the core, socket, and node level, where the code gets executed that does the actual computational work. Once the architectural requirements of a code are understood and correlated with performance measurements, the potential benefit of optimizations can often be predicted. We introduce a "holistic" node-level performance engineering strategy, apply it to different algorithms from computational science, and also show how an awareness of the performance features of an application may lead to notable reductions in power consumption. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Basic knowledge in programming with Fortran or C, and basic OpenMP.

Webpage for further information:

<https://www.hlrs.de/training/2017-04-27-nlp/>

GPU Programming with CUDA (PATC course)

Apr 24–26 2017 | JSC, Forschungszentrum Jülich

see also Dec 12-16, 2016 in Stuttgart

GPU-accelerated computing drives current scientific research. Writing fast numeric algorithms for GPUs offers high application performance by off-loading compute-intensive portions of the code to an NVIDIA GPU. The course will cover basic aspects of GPU architectures and programming. Focus is on the usage of the parallel programming language CUDA-C which allows maximum control of NVIDIA GPU hardware. Examples of increasing complexity will be used to demonstrate optimization and tuning of scientific applications.

Prerequisites

Some knowledge about Linux, e.g. make, command line editor, Linux shell, experience in C

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/cuda>

Cray XC40-Workshop on Optimization at Scale

May 2–5, 2017 | HLRS, Stuttgart

In August 2015, the Cray XC40 supercomputer Hornet at HLRS was upgraded to a new system named "Hazel Hen", featuring 7712 compute nodes, each equipped with two 12 core Intel Haswell processors running at 2.5 GHz. Each node is equipped with 128 GB DDR4 memory and connected to the other nodes through the Cray Aries network. The peak performance amounts to 7.4 PFlops.

In order to help users running efficiently on this new large system, HLRS and Cray offer an optimization workshop for applications running at scale. The intent of this workshop is to tune the performance of such codes by detecting, locating and solving bottlenecks.

Prerequisites

Target audience are users of applications which are already scaling to at least 24000 cores (1000 nodes). In order to attend the workshop, you will have to bring your own code including a dataset which can be used at scale. You will be required to do some work on your application before the workshop. In order to do so, you should already have an account on HAZELHEN and your application should already be able to run on the system.

Webpage for further information:

<https://www.hlrs.de/training/2017-05-02-xc40-1/>

Introduction to the Programming and Usage of the Supercomputer Resources at Jülich

May 22–23, 2017 | JSC, Forschungszentrum Jülich

This course gives an overview of the supercomputers at Jülich. Especially new users will learn how to program and use these systems efficiently. Topics discussed are: system architecture, usage model, compilers, tools, monitoring, MPI, OpenMP, performance optimization, mathematical software, and application software.

Prerequisites: Basic knowledge of Unix, knowledge of either C, C++ or Fortran

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/sc-may>

Cluster Workshop

May 29–30, 2017 | HLRS, Stuttgart

Nowadays, the IT infrastructure of many companies and institutions includes modern compute clusters. The procurement, operation and the efficient usage of such parallel systems introduces new and complex requirements.

To address these emerging requirements, the High Performance Computing Center of the University of Stuttgart (HLRS) offers a vendor-independent workshop. Topics span from the design of compute clusters to details on different hardware components, operating systems, file systems and modes of operation, touching on specific software solutions. Further, typical problems and strategies for their solution will be discussed.

HLRS has been running compute clusters for many years, providing compute resources for scientific and industrial simulations. HLRS is in constant dialogue with users and hardware providers and has accumulated a large knowledge base in cluster computing.

Webpage for further information:

<https://www.hlrs.de/training/2017-05-29-cluster/>

Scientific Visualization

May 31–Jun 1, 2017 | HLRS, Stuttgart

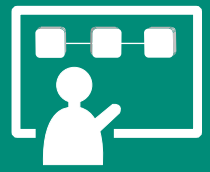
This two day course is targeted at researchers with basic knowledge in numerical simulation, who would like to learn how to visualize their simulation results on the desktop but also in Augmented Reality and Virtual Environments. It will start with a short overview of scientific visualization, following a hands-on introduction to 3D desktop visualization with COVISE. On the second day, we will discuss how to build interactive 3D Models for Virtual Environments and how to set up an Augmented Reality visualization. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Programming experience in Fortran or C

Webpage for further information:

<https://www.hlrs.de/training/2017-05-31-vis1/>



Intel MIC Programming Workshop (PATC-Course)

Jun 2017, 3 days | LRZ, Garching near Munich
see also Feb 2017, 2 days, IT4Innovations, Ostrava

These workshops discuss Intel's Many Integrated Core (MIC) architecture. They cover various programming and optimisation techniques for Intel Xeon Phi based systems. While the course taking place at IT4Innovations in February will concentrate on the Knights Corner based system Salomon - currently the largest Intel Xeon Phi based system in Europe - the course at LRZ in June will focus on Intel's new Knights Landing architecture.

The workshops are developed within PRACE and the joint German-Czech Republic project CzeBaCCA.

Webpage for further information:

<http://www.lrz.de/services/compute/courses/>

High-performance Computing with Python (PATC course)

Jun 12–13, 2017 | JSC, Forschungszentrum Jülich

Python is being increasingly used in high-performance computing projects such as GPAW. It can be used either as a high-level interface to existing HPC applications, as embedded interpreter, or directly. This course combines lectures and hands-on sessions. We will show how Python can be used on parallel architectures and how performance critical parts of the kernel can be optimized using various tools.

Prerequisites

Experience with Python and NumPy

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/events/hpc-python>

Introduction to hybrid Programming in HPC

Jun 12, 2017 | HLRS, Stuttgart
see also Jan 12, 2017 in Garching

Most HPC systems are clusters of shared memory nodes. Such SMP nodes can be small multi-core CPUs up to large many-core CPUs. Parallel programming may combine the distributed memory parallelization on the node interconnect (e.g., with MPI) with the shared memory parallelization inside of each node (e.g., with OpenMP or MPI-3.0 shared memory). This course analyzes the strengths and weaknesses of several parallel programming models on clusters of SMP nodes. Multi-socket-multi-core systems in highly parallel environments are given special consideration. MPI-3.0 has introduced a new shared memory programming interface, which can be combined with inter-node MPI communication. It can be used for direct neighbor accesses similar to OpenMP or for direct halo copies, and enables new hybrid programming models. These models are compared with various hybrid MPI+OpenMP approaches and pure MPI. Numerous case studies and micro-benchmarks demonstrate the performance-related aspects of hybrid programming.

Tools for hybrid programming such as thread/process placement support and performance analysis are presented in a "how-to" section. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Basic MPI and OpenMP knowledge

Webpage for further information:

<https://www.hlrs.de/training/2017-06-12-hy-s/>

Introduction to UPC and Co-Array Fortran (PATC course)

Jun 29–30, 2017 | HLRS, Stuttgart
see also Jan 12, 2017 in Garching

Partitioned Global Address Space (PGAS) is a new model for parallel programming. Unified Parallel C (UPC) and Co-array Fortran (CAF) are PGAS extensions to C and Fortran. UPC and CAF are language extensions to C and Fortran. Parallelism is part of the language. PGAS languages allow any processor to directly address memory/data on any other processors. Parallelism can be expressed more easily compared to library based approaches as MPI. This course gives an introduction to this novel approach of expressing parallelism. Hands-on sessions (in UPC and/or CAF) will allow users to immediately test and understand the basic constructs of PGAS languages. This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Prerequisites

Programming experience in Fortran or C, some knowledge about parallel programming

Webpage for further information:

<https://www.hlrs.de/training/2017-06-29-upcl/>

Efficient Parallel Programming with GASPI (PATC course)

Jul 3–4, 2017 | HLRS, Stuttgart

In this tutorial we present an asynchronous data flow programming model for Partitioned Global Address Spaces (PGAS) as an alternative to the programming model of MPI.

GASPI, which stands for Global Address Space Programming Interface, is a partitioned global address space (PGAS) API. The GASPI API is designed as a C/C++/Fortran library and focused on three key objectives: scalability, flexibility and fault tolerance. In order to achieve its much improved scaling behaviour GASPI aims at asynchronous dataflow with remote completion, rather than bulk-synchronous message exchanges. GASPI follows a single/multiple program multiple data (SPMD/MPMD) approach and offers a small, yet powerful API (see also <http://www.gaspi.de> and <http://www.gpi-site.com>).

GASPI is successfully used in academic and industrial simulation applications. Hands-on sessions (in C and Fortran) will allow users to immediately test and understand the basic constructs of GASPI.

This course provides scientific training in Computational Science, and in addition, the scientific exchange of the participants among themselves.

Webpage for further information:

<https://www.hlrs.de/training/2017-07-03-gaspi/>

NEC SX-ACE – Vectorization and Optimization

Jul 11–12, 2017 | HLRS, Stuttgart

In spring 2015, HLRS installed a next generation vector computer, a NEC SX-ACE. The participants learn about the configuration of the NEC SX-ACE system at HLRS and how to use this cluster of vectorizing shared memory nodes. One focus is an introduction in vectorization. More experienced users can learn how to optimize programs based on performance measurements. Additional topics are I/O and the optimization of application programs. The first day presents an introduction to the NEC SX architecture and vectorization. The second day morning is focused on usage aspects and the differences between the predecessor system (NEC SX-9) and the new NEC SX-ACE. The afternoon is dedicated to hands-on sessions.

Separate registration of individual days is possible. Participants are encouraged to prepare their own applications for use in the hands-on session. Participants familiar with SX vector computers may wish to register only for Day 2.

Prerequisites

Programming experience in C or Fortran, some knowledge about parallel programming

Webpage for further information:

<https://www.hlrs.de/training/2017-07-11-nec/>

Introduction to Cluster Filesystems

Jul 6, 2017 | HLRS, Stuttgart

The one-day workshop will provide an overview and a first deeper insight into the structure, functionality and the differences of the three main cluster file systems, beegfs, IBM Spectrum Scale and Intel Enterprise Edition for Lustre. Experts from the responsible manufacturer will present the file systems in a one and a half hour session, with enough time to respond to the questions of the participants. This workshop will help administrators and technical decision makers to identify the best Cluster File System for the local environment and the specific requirements.

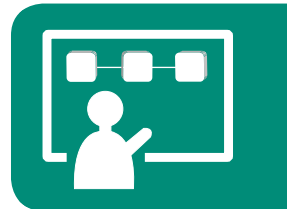
Guest Student Programme at JSC

Aug 6–Oct 13, 2017 | JSC, Forschungszentrum Jülich

Guest Student Programme "Scientific Computing" to support education and training in the field of supercomputing. Students of Computational Sciences, Computer Science and Mathematics can work 10 weeks in close collaboration with a local scientific host on a subject in their field. Application deadline is March 31, 2017.

Webpage for further information:

<http://www.fz-juelich.de/ias/jsc/gsp>



You will also find the detailed course list (as at Oct 2016) online at
<http://inside.hlrs.de/courses.html>
or by scanning the QR-Code with your mobile device.

Complete and updated list of all GCS courses:

http://www.gauss-centre.eu/gauss-centre/EN/Training/Training/_node.html

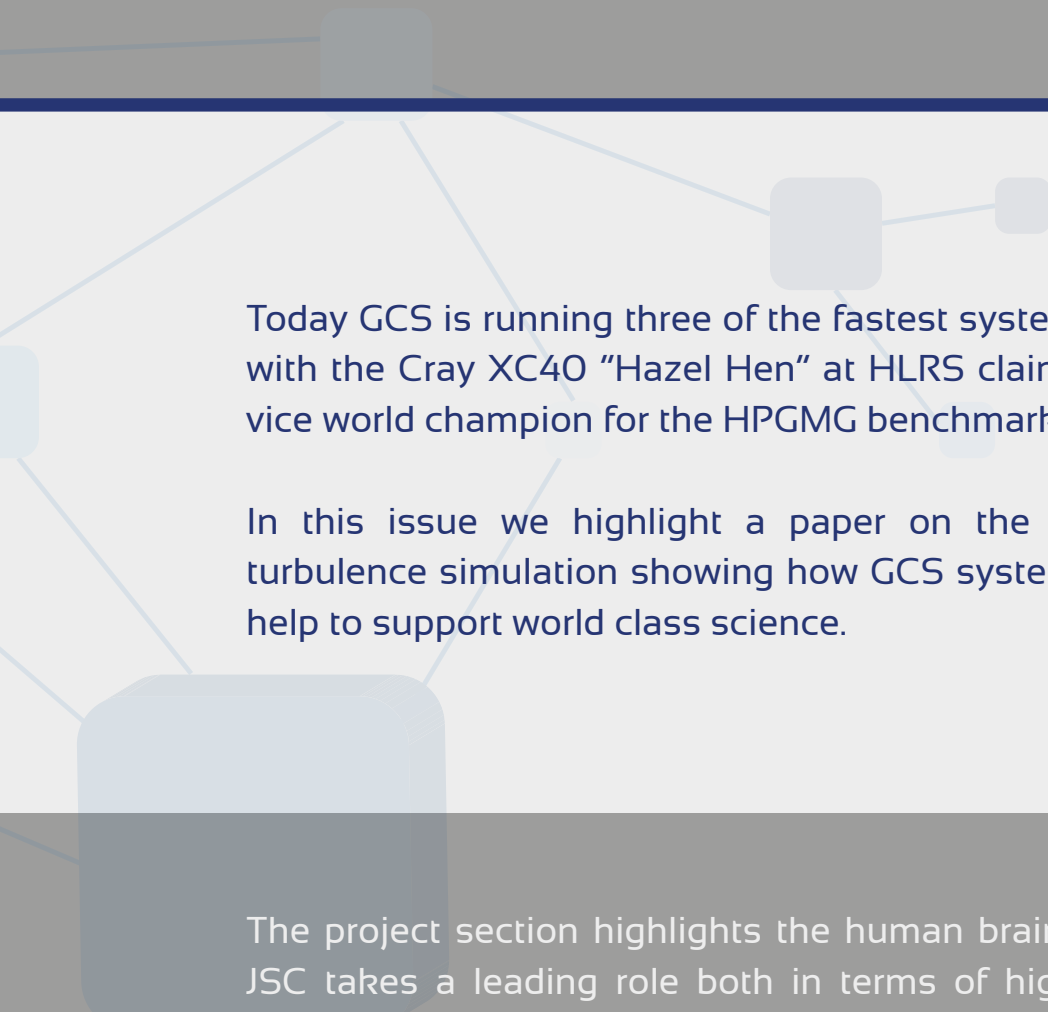
Further training courses at members' sites:

<http://www.fz-juelich.de/ias/jsc/courses>

<http://www.lrz.de/services/compute/courses/>

<http://www.hlrs.de/de/training/>

Get the latest news about innovative High Performance Computing in Germany.



Today GCS is running three of the fastest systems in the world with the Cray XC40 "Hazel Hen" at HLRS claiming the title of vice world champion for the HPGMG benchmark.

In this issue we highlight a paper on the world's largest turbulence simulation showing how GCS systems and centers help to support world class science.

The project section highlights the human brain project where JSC takes a leading role both in terms of high performance computing and in terms of modelling and brain research.

We hope that we have put together again a mix of information on high performance computing systems, applications, projects and HPC activities that our readers enjoy.