Kickoff of New SCALEXA Projects

Following last year's "SCALEXA" funding call from the Federal Ministry of Education and Research (BMBF), new collaborative research projects have recently started in the field of software and technology development in high-performance computing (HPC) in the exascale era. The SCALEXA funding guideline supports HPC as a fundamental research method in various scientific disciplines such as astrophysics, biology, Earth system modelling, and nuclear and particle physics. Engineering and industry also have a growing need for computing power. At the same time, research and applications within the field of artificial intelligence (AI) offer new concepts and perspectives for simulation, modelling, and the analysis of large data volumes.

While current supercomputers in Europe achieve performance in the pre-exaflop range, the first computer in the exascale performance class in Europe – JUPITER – is expected to become available in just 1–2 years from now. A variety of technologies is used in modern HPC systems: from new processors, accelerators, and data storage to file systems and operating systems. Programming large, heterogeneous, and modular systems requires new methods and techniques in software development, mainly through an end-to-end co-design approach. At the same time, application requirements are becoming more heterogeneous. For applications to efficiently exploit the capabilities of exascale systems, code and workflow scalability must be improved, especially in use cases combining classical HPC, AI, and data analytics techniques.

The SCALEXA funding guideline complements the infrastructure development and research activities carried out under the EuroHPC Joint Undertaking (JU). The BMBF funding is intended to ensure a good starting position for German participation in these European activities, while at the same time enabling the efficient use of future exascale systems in Germany. JSC is teaming up with project partners all over Germany in six of the new SCALEXA collaborative research projects, which will run over a three-year period from 2022 to 2025. The projects in which JSC is participating mostly focus on HPC software development.

The objective of the **FlexFMM** project led by JSC is the realistic simulation of large interacting biomolecules via GROMACS on upcoming exascale hardware. Emphasis is placed on a scalable and flexible Fast Multipole Method (FMM) as an electrostatic solver. Its low communication complexity, dynamic protonation features, and support for non-periodic and highly inhomogeneous particle systems allow for new biomedical developments. Additionally, the project is focused on fully leveraging SiPearl's upcoming ARM hardware with SVE vector units and HBM memory to future-proof well-established simulation tools and pave the way for exascale.

The goal of the **ADAPTEX** project, led by the Institute for Software Technology at the German Aerospace Center (DLR), is to develop an open-source software framework for exascale-enabled computational fluid dynamics on dynamic adaptive grids and to apply it to the field of Earth System Modelling (ESM). By merging individually specialized HPC software libraries and extending them to heterogeneous exascale computer architectures, the scalability and resource efficiency of current and future ESM applications will be significantly improved.

The goal of the **ExaOcean** project, led by the Institute of Mathematics at TU Hamburg, is to accelerate the ICON-O ocean model by at least a factor of four using a combination of classical discrete algorithms and machine learning methods. The innovative spectral deferred correction (SDC) methods applied in the project are remarkable in that they use accelerators and modular supercomputers more efficiently than simple numerical methods alone could do. Beyond the runtime reduction, this approach will enable better scalability on heterogeneous systems without reducing the accuracy and quality of the simulation.

The **IFCES2** project, led by the Leibniz Institute for Troposphere Research (TROPOS), will develop new methods to optimize the parallel execution of simulation algorithms from the Earth system model ICON on heterogeneous and modular exascale systems. Code parallelism will be improved and methods will be applied to enable better communication between the individual model components as well as dynamic load distribution. The methods will be validated with use cases from cloud

microphysics and ocean biogeochemistry. As a result, the necessary prerequisites will be created for the efficient use of modular exascale systems for complex simulations.

The aim of the **MExMeMO** project is to develop a multi-scale model for the manufacturing processes of soft materials. These applications pose a major challenge for HPC, as complex processes are coupled at very different scales and the associated simulation techniques place very different demands on the hardware. The new, innovative multi-scale model, which uses a special polymer membrane as an example, includes different size and time scales so that flexible computer architectures can be realized. Furthermore, it builds on the concept of modular supercomputer architecture for exascale computing.

The goal of the **StrömungsRaum** project, led by the Department of Mathematics at TU Dortmund, is to methodologically extend the CFD software package FEATFLOW on the basis of parallel near-hardware implementations to enable high-scaling, industrial CFD simulations to be run on future exascale architectures. To ensure the optimal use of heterogeneous hardware components, new geometric multigrid solvers and highly scalable nonlinear domain-decomposition methods for CPU and GPU will be developed. In addition, various time-parallel and time-simultaneous approaches will increase the parallel potential of the algorithms.

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New Projects for Energy-Efficient HPC

JSC is participating in the BMBF funding track "Energy-Efficient HPC (Green HPC)" with two research projects. Data centres operating in Germany currently consume around 3 % of the total electricity produced and are responsible for CO_2 emissions of just over 8 million tonnes per year. As a result, even small energy savings ultimately lead to significant reductions in the total energy consumption of data centres and thus to relevant savings in CO_2. The aim of this funding track is to improve the energy efficiency of high-performance computing, both of high-performance computing centres at universities and research institutions and of commercial computing centres. Both of the projects involving JSC are funded for three years as of 1 October 2022.

The **ENSIMA** project (ENergy-efficient SImulation Methods for Application-oriented computational problems) will use AI methods to improve the determination of design parameters and accelerate the execution time of simulation processes through approximate and heterogeneous computing. For the sample use case – sheet metal forming in the automotive industry – the goal is to reduce computing time by 50 %, leading to a 15 % reduction in steel usage and thus indirectly to a reduction in both manufacturing-related emissions and energy requirements for vehicle production. FZJ will lead work package 2 ("Optimization of Workflow Components"), which will analyse and improve the performance and energy efficiency of the OpenForm user code components used in the project, which is supplied by industry partner GNS. Further project partners are RWTH Aachen University (coordinator) and TU Darmstadt.

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The **STXDemo** project will provide a proof of concept for future energy-efficient high-performance computing. It will develop a hardware prototype made of a motherboard with multiple STX processors, which are processing units optimized to solve stencil algorithms. STXDemo will build on the work done in the EU European Processor Initiative (EPI) project and aims to improve energy efficiency by at least a factor of two compared to competing platforms based on GPUs or x86 processors. The benchmark for the success of the project is the improvement of the energy efficiency of selected computationally intensive simulation applications. FZJ will contribute a co-design application from the field of lattice quantum chromodynamics (LQCD) and will host one hardware prototype at JSC. Further project partners are the Fraunhofer-Gesellschaft (coordinator), TU Kaiserslautern, and Zollner Elektronik AG.

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Research Software Engineering at JSC and FZJ

Since the inception of the term 'Research Software Engineer' (RSE) in the UK in 2012, the RSE community grassroots movement, as well as the importance of research software and those who create it, have gone from strength to strength in gaining recognition around the world. RSEs are increasingly understood as vital in all research disciplines, and JSC has now invested in and committed directly to this cause.

In October, Claire Wyatt joined JSC from the UK as our RSE Community Manager. Claire has very successfully held this role since 2016 at the Software Sustainability Institute in the UK and was a founding member of the Society of Research Software Engineering. She has developed the community in the UK and around the world over these past six years and joins JSC to develop the RSE community here and at FZJ within the OS4FZJ initiative and the HiRSE_PS project. The OS4FZJ initiative is a joint effort from JSC, the Central Library (ZB), and Corporate Development (UE) at FZJ to support open science on the centre level.

To enable you to stay informed about recent activities in the field of RSE, the RSE Rocket.Chat channel is open to all FZJ employees (see https://chat.fz-juelich.de/channel/rse). We post events and news on there regularly, and people can also ask for advice on their current code issues. Next year, JSC will co-organize two RSE conferences in Germany: deRSE 2023 (February 2023 in Paderborn) and the deRSE Unconference 2023 (September 2023 in Jena). For details, see https://de-rse.org/en/events.html.

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JuWinHPC – First German Chapter of Women in HPC Founded

The global organization "Women in High Performance Computing" (WHPC) was founded with the mission to create more equality, diversity, and integration in the male-dominated HPC community. The initiative is active at conferences such as SC and ISC, and offers workshops and mentoring programmes. Anyone who is interested can easily become a WHPC member and benefit from their offerings by registering free of charge on their website. WHPC works with several "chapters" – the official name for WHPC's local networks – on five continents. To become a WHPC chapter, an institution or organization has to prove that they are suitably qualified in an application process.

A team of local WHPC members has now established a local WHPC network on behalf of Forschungszentrum Jülich, called "Jülich Women in HPC" (JuWinHPC). This local network is not only supported by Jülich's Board of Directors in its efforts, but has also already been approved by the global organization as the first German WHPC chapter. JuWinHPC's main goal is to strengthen the local community. For this purpose, the network organizes monthly informational meetings or gatherings. While the chapter members can use the network to meet new colleagues or to strengthen existing contacts, the founders are already working on further tasks in the background: they aim to gain a better understanding of the gender imbalance and make women in the field more visible. Therefore, JuWinHPC will work closely with other chapters on an international level and support the foundation of further chapters on a national level.

JuWinHPC encourages and welcomes anyone interested in the topic of equal opportunities, no matter their gender, to join the initiative.

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New GCS Large-Scale Projects Started in November 2022

Twice a year, the Gauss Centre for Supercomputing (GCS) issues a call for large-scale projects on its petascale supercomputers – Hawk (HLRS), JUWELS (JSC), and SuperMUC-NG (LRZ). Projects are classified as large-scale if they require at least 2 % of the systems' annual production in terms of estimated availability.

Computing time quantities were previously specified in core hours; however, the modularity of JUWELS requires the introduction of a new computing time unit. JSC is currently working with the peak floating point operations per year (FLOP/a) of the computing devices (CPU or GPU) available to approved projects. Computing time on Hawk and SuperMUC-NG continues to be given in core hours. Projects in this case fall into the category of large-scale only if they require at least 100 Mcore-h on Hawk, or 45 x 10^{21} FLOP/a on JUWELS, or 45 Mcore-h on SuperMUC-NG.

The GCS Peer Review Board decided to award the status of "large-scale project" to 21 projects from various scientific fields. In total, five projects were granted 1830 Mcore-h on Hawk, eight projects were granted 480 x 10^{21} FLOP/a on JUWELS, and eight projects were granted 600 Mcore-h on SuperMUC-NG.

For more details about these projects, please visit https://www.gauss-centre.eu/results/large-scale-projects/.

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RISC2 Project Receives 2022 HPCwire Editor's Choice Award

The RISC2 project has been recognized in the annual HPCwire Readers' and Editors' Choice Awards, which were presented at the 2022 International Conference for High Performance Computing, Networking, Storage, and Analysis (SC22) in Dallas, Texas. RISC2 was selected as the Best HPC Collaboration (Academia/Government/ Industry). The RISC2 project aims to promote and improve the relationship between research and industrial communities, focusing on HPC application and infrastructure deployment, between Europe and Latin America. Led by the Barcelona Supercomputing Center (BSC), RISC2 brings together 16 partners from 12 different countries. JSC is RISC2 Event and Training Coordinator.

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2022 End-of-Year Colloquium at JSC

Date: Thursday, 8 December 2022, 14:00–16:45
Venue: online via Zoom
Info: https://go.fzj.de/jsc-eoy-colloq

14:00 Thomas Lippert: *Welcome*
14:20 Kristel Michielsen: *The expansion of a JUNIQ universe*
14:45 Manpreet Jattana: *Noisy quantum computers have arrived. Can we please use them?*
15:10 Alper Yegenoglu: *Optimizing spiking neural networks with L2L on HPC systems*
15:35 Clara Betancourt: *Global air quality mapping with explainable machine learning*
16:00 Mario Rüttgers: *Automated surgical planning for a septoplasty*
16:25 Thomas Lippert: *JUPITER ascending*

All are welcome to participate in the colloquium.