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DEEP-EST Project Started

The aim of DEEP-EST, an EU project launched on 1 July 2017, is to create a modular supercomputer that is able to efficiently run both HPC codes and data analytics applications. Following on from the successfully concluded DEEP and DEEP-ER projects, DEEP-EST will focus on the development of hardware and software components in intensive co-design with applications.

In addition to the Cluster and Booster components of the predecessor projects, which address the needs of low- and high-scalable HPC applications, respectively, the DEEP-EST hardware prototype will include a new computing module tailored to the requirements of high-performance data analytics codes.

DEEP-EST will also create a software environment suitable for enabling the three modules to act jointly as a single system. In particular, the scheduler and resource management software SLURM will be extended to allow applications to allocate nodes in every module. Advanced scheduling techniques will ensure that a diverse portfolio of applications being run simultaneously on the modular supercomputer will be able to fully and efficiently exploit the available resources.

Six co-design applications will influence the hardware and software design, and will also benefit from optimizations over the course of the project. They will reveal to what extent highly complex simulations profit from the modular supercomputer architecture, in which codes can freely select the best-suited mix of nodes.

Coordinated by Forschungszentrum Jülich, the DEEP-EST consortium consists of sixteen partners. Among other activities, JSC participates in the architectural (both hardware and software) designs, the installation of the prototype at Jülich, the extension of SLURM, and the guidance and support of the application developers. Further information can be found at
http://www.deep-projects.eu.
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Helmholtz Analytics Framework

The Helmholtz Analytics Framework is a data science pilot project funded by the Helmholtz Initiative and Networking Fund. Together with five institutes of Forschungszentrum Jülich and five other Helmholtz centres, JSC will pursue the systematic development of domain-specific data analytics techniques in a co-design approach between domain scientists and information experts in order to strengthen the development of data sciences within the Helmholtz Association. In challenging applications such as earth system modelling, structural biology, aerospace, medical imaging, and neurosciences, data analytics methods will be applied to demonstrate their potential in leading to scientific breakthroughs and new knowledge. In addition, the exchange of methods between individual scientific areas should lead to their generalization and standardization.

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The Helmholtz Analytics Framework will be an essential part of the software stack complementing the Helmholtz Data Federation (HDF). The three-year project will start in October 2017.
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New Cross-Sectional Team for Deep Learning

In recent years there has been a radical transformation in the field of machine learning and artificial intelligence, catalyzed by an ensemble of methods now widely known as deep learning. These methods, which are based on adaptive neural network architectures of multiple layers, can be applied to large amounts of raw, unprocessed data to discover hidden complex patterns in the data through learning from labelled or unlabelled training examples. These examples cover a broad range of machine learning tasks such as classification, clustering, prediction, and control. In order to foster research in this area and optimize support for HPC users at JSC, a cross-sectional team (CST) has been formed at JSC dedicated to deep learning.

The team will pursue research and support activities. In addition to basic and applied research, novel architectures will be created for unsupervised and reinforcement learning, and – together with domain scientists – applications will be implemented to analyse and combine large amounts of raw data that contain valuable but hidden information which needs to be revealed. The CST Deep Learning will cooperate closely with data-intensive projects, both within Forschungszentrum Jülich and with international scientific and industrial partners. It will also provide toolsets, support, and optimized infrastructure setups with respect to deep learning methods for end users. While the group is still in the phase of being established, the team has already started to support end users in the field of remote sensing and neurosciences who were chosen through the scientific big data analytics elements in the calls for computing time of the John von Neumann Institute for Computing (NIC). The CST Deep Learning is jointly led by Dr. Jenia Jitsev and Prof. Morris Riedel.

New NIC Research Group "Computational Biophysical Chemistry"

The new NIC research group Computational Biophysical Chemistry began work at Forschungszentrum Jülich at the end of April 2017. The group is headed by Prof. Dr. Holger Gohlke from Heinrich Heine University Düsseldorf. Gohlke obtained his diploma in chemistry from Technische Universität Darmstadt and his PhD from Philipps-Universität Marburg. He subsequently conducted postdoctoral research at The Scripps Research Institute, La Jolla, USA. After appointments as an assistant professor in Frankfurt and a professor in Kiel, he moved to Düsseldorf in 2009. Gohlke was awarded the "Innovationspreis in Medizinischer und Pharmazeutischer Chemie" (innovation award for medicinal and pharmaceutical chemistry) by the German Chemical Society (GDCh) and the German Pharmaceutical Society (DPhG), the Hansch Award of the Cheminformatics and QSAR Society, and the Novartis Chemistry Lectureship. His current research focuses on the understanding, prediction, and modulation of interactions involving biomolecules and supramolecules from a computational perspective. Gohlke's group applies and develops techniques grounded in structural bioinformatics, computational biology, and computational biophysics. In line with these research interests, the group is excited about the possibility of a dual affiliation at JSC and ICS-6. This will pave the way to bridging the supercomputing capabilities of JSC with the structural biochemistry capabilities of ICS-6 in order to address complex questions on the structure, dynamics, and function of biomolecules and supramolecules.
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Godehard Sutmann Appointed Professor at Ruhr University Bochum

In 1998, Godehard Sutmann began his research work at JSC. Since then, he has been working in the field of computational science with a focus on scalable particle-based simulation methods. Since 2003, he has lectured regularly on the Jülich campus of Aachen University of Applied Sciences and has been a member of a number of national and European projects. As of July 2017, Sutmann was appointed professor for High-Performance Computing in Materials Science at Ruhr University Bochum where he is associated with the Faculty of Mechanical Engineering. He is situated at the Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) where scale-bridging techniques are developed and applied to materials. Aside from his work at JSC, Sutmann has been associated with ICAMS since 2012 when he took up work as head of a group for HPC, which was funded by ThyssenKrupp Steel. The focus of the group has been the efficient parallelization of codes developed at ICAMS and the development of new parallelization schemes. In order to exploit HPC architectures most efficiently, dynamic and adaptive load balancing techniques have been developed for different simulation protocols. In his new position, Prof. Sutmann will strengthen the joint work of JSC and ICAMS to advance the field of scalable methods for particle simulations and scale bridging. According to the Jülich model, Prof. Sutmann will lecture and supervise academic research projects at Ruhr University Bochum while also continuing his work at JSC. This will help strengthen JSC's relations with its academic partners.
JSC wishes Godehard all the best in his new position!

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