

Lattice Practices 2015 @ JSC

The 6th training workshop "Lattice Practices" was held at JSC October 14 to 16, 2015. The scope of the Lattice Practices workshops is to provide training in state-of-the-art numerical techniques and the use of information technologies for research in lattice QCD (LQCD). Geared towards PhD students, young researchers, and other interested LQCD practitioners, the workshops feature lectures on technical topics accompanied by hands on exercises, with strong emphasis on practical training. Furthermore, a few very recent scientific developments are covered, in order to expose the young researchers and students to potential areas of future research.

This year's workshop was organized by the Joint SimLab "Nuclear and Particle Physics" of Cyprus Institute, DESY, and JSC. Speakers from the SimLab partners and other European institutions gave technical lectures and hands-on tutorials on topics commonly dealt with in their field of research. The topics covered ranged from data analysis and numerical techniques over optimization strategies and computer architecture to "hot" LQCD, with accompanying hands on sessions. Here, the participants were given examples on basic techniques such as binning and error and autocorrelation analysis, but also given typical physics tasks they will likely encounter during their own research. A particular emphasis was put on optimal programming, when the course of lectures and exercises went on to introduce the attendees to code optimization techniques

and HPC architectures in general. This was completed by an introduction to numerical linear solver techniques and deepened in the accompanying exercises for both topics. Completing this year's course of lectures were two talks discussing new simulation techniques and LQCD at finite temperature.

This year's participants came from institutions all over Europe, from Italy to Ireland, but also from as far away as India. This interest demonstrates the need for this series of educational workshops, which was initiated in 2006. A next workshop is planned for spring 2017. The slides of the talks and material of the hands on sessions can be found on the web at: <http://www.fz-juelich.de/ias/jsc/lap15>

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Smart Data Innovation Lab



The significantly growing data economy is driven by slogans like "data is the oil of the 21st century" or "the data speaks for itself". But in order to achieve "big insights from data", important research effort still needs to be made, e.g. in terms of parallel, scalable, and even real-time processing of large data quantities ("big data"). Structuring "big data" results in information (called "smart data") which in turn leads to knowledge advantages which can be used to answer important research questions or that contributed to better decision-making processes.

In order to be able to make fast use of this competitive edge for Europe, partners from industry and research have established the Smart Data Innovation Lab (SDIL). The close cooperation between industry and science is intended to improve the conditions for cutting-edge research in the area of data engineering, parallel and scalable machine learning, data mining, and smart data processing. Figure 1 illustrates the conceptual organization of the SDIL initiative.

Besides several important supporting activities with respect to data curation, law, and security, the core benefit of the SDIL initiative is to offer interested communities an SDIL data analytics platform with three cutting-edge industry hardware and software stacks. At the time of writing, the SAP HANA In-Memory database is available on 4 nodes with each 80 CPU-cores, 1 TB RAM, and 20 TB storage. This installation includes software packages like SAP Hana Studio, Client, Smart Data Streaming, Live Tools, and the Predictive Analysis Library. The Software AG Terracotta Big Memory MAX software is available on 8 cores with 64 GB RAM running in a virtual machine. The IBM Watson Foundations is also available with IBM InfoSphere BigInsights on 6 nodes with each 20 cores, 0.5 TB RAM, and over 300 TB space. The Model-based Predictive Analytics system with IBM SPSS Modeler is provided on 1 node with 20 cores and 1 TB of RAM. The SDIL platform thus offers powerful analytics systems without license issues for SDIL users interested in performing research on modern technologies.

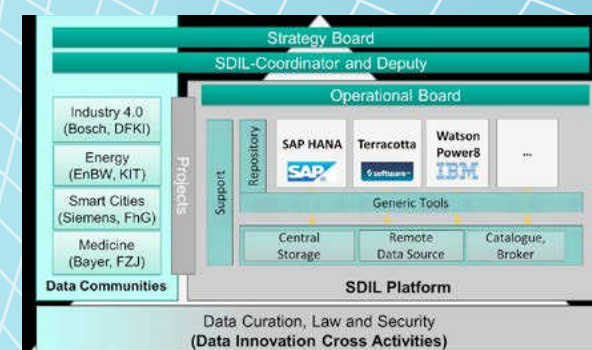


Figure 1: Conceptual organization of the Smart Data Innovation Lab (SDIL).

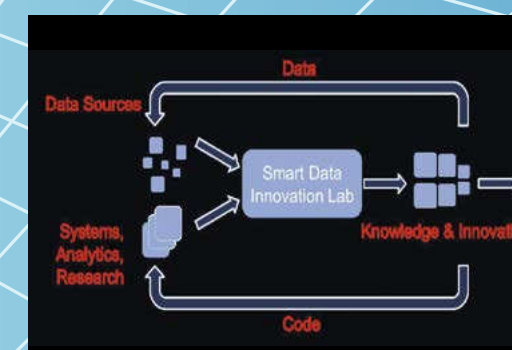


Figure 2: SDIL combines data sources with cutting-edge systems, analytics, and research.

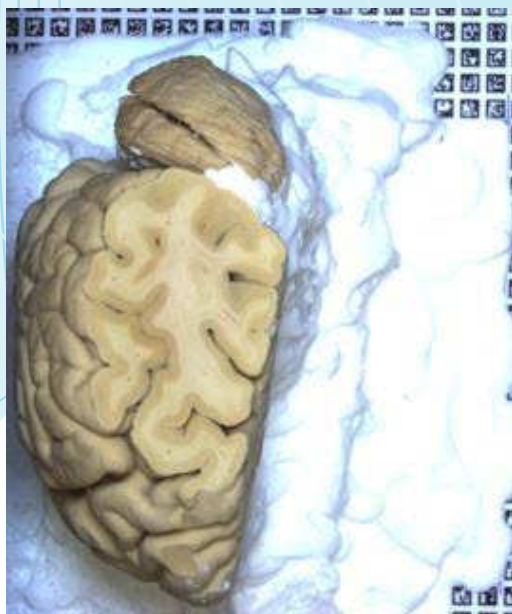


Figure 3: Brain tissue cutted with 80 micrometer into ~700 layers available as block face images.

As shown in Figure 1, currently four data innovation communities (DICs) are using the platform in different topical areas that offer domain-specific data sources for distinct research projects. Interested organizations from industry and academia are welcome to participate in one of the following four topical areas but are particularly encouraged to participate with ready available data, good analytics algorithms, or interesting research questions.

The DIC Energy is headed by KIT and EnBW and explores important data-driven aspects in the area of energy, such as the demand-driven fine-tuning of consumption rate models based on smart metre generated data. The DIC Smart Cities is headed by Fraunhofer IAIS and Siemens explores data-driven aspects of urban life, such as traffic control, but also waste disposal or disaster control. The DIC Industry 4.0 is headed by Bosch and DFKI and explores important data-driven aspects of the fourth industrial revolution (towards Smart Factories), such as proactive

service and maintenance of production resources or finding anomalies in production processes. In one of the projects of this particular DIC, Trumpf is working with SAP and KIT on condition-based monitoring of production systems while Trumpf also is starting to work with IBM, KIT and the Jülich Supercomputing Centre (JSC) on optimizations and classification problems for automatically detecting good or bad welding processes of materials.

The DIC Medicine is headed by Forschungszentrum Jülich and Bayer and works on three different research projects. The JSC and Jülich Institute of Neuroscience and Medicine (INM) closely work together with IBM on a machine learning approach for background segmentation of 3D image volumes of a brain tissue block as shown in Figure 3. The University of Düsseldorf and IBM collaborate on a project about predicting optimal treatment procedures for spinal cord injury patients. In the third project the Ludwig Maximilian University of Munich (LMU) works with JSC and IBM on using machine learning techniques for better supporting the decision-making of doctors when picking patient-specific human eye therapies for patients suffering from eye illnesses such as age-related macular degeneration.

Reference

[1] Smart Data Innovation Lab Website, Online: <http://www.sdil.de/de/>

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JSC to participate in four Horizon2020 Centres of Excellence

On May 8, the results of a keenly contested call for new "Centres of Excellence" within the EU Horizon2020 E-INFRASTRUCTURES Programme were announced [1]. These new funding instruments are intended to harness computational science and big data expertise in HPC in the promotion of scientific discovery and industrial competitiveness. Out of the 20 submitted proposals, 8 projects were approved for initial funding and 4 of these will include active JSC participation – see Table 1 and Ref. [2] for an overview. These four are: POP - Performance Optimisation and Productivity; MaX – Materials Design at the Exascale; E-CAM – an E-infrastructure for Software, Training and Consultancy in Simulation and Modelling; and EoCoE – an Energy-oriented Centre of Excellence. All projects – subject to final approval by all participants – plan to start in the autumn of this year.

EoCoE

EoCoE ("echo"), coordinated by the Maison de la Simulation at CEA, France, received the highest grade of the evaluation, and aims to exploit the prodigious potential offered by the maturing HPC infrastructure to foster and accelerate the European transition to a reliable, low-carbon energy supply. EoCoE will achieve its goal via targeted support of four distinct renewable energy pillars: Meteorology (Wind), Materials (Earth), Hydrology (Water) and Fusion (Fire), each of which boasts activities with a heavy reliance on numerical modelling. From the project outset these four pillars will be anchored within a strong

Coordinator	Partners	Acronym	Proposal Title
CEA	13	EoCoE	Energy oriented Centre of Excellence for computer applications
CNR	12	MaX	Materials design at the eXascale
UCD	18	E-CAM	An e-infrastructure for software, training and consultancy in simulation and modelling
BSC	6	POP	Performance Optimisation and Productivity
DKRZ	16	ESIWACE	Excellence in Simulation of Weather and Climate in Europe
POTSDAM	10	COEGSS	Center of Excellence for Global Systems Science
KTH	11	BioExcel	Centre of Excellence for Biomolecular Research
MPG	11	NoMaD	The Novel Materials Discovery Laboratory

Table 1: Summary of approved EU Centres of Excellence.

transversal multidisciplinary basis providing high-end expertise in applied mathematics and supercomputing science. EoCoE is structured around a central Franco-German hub coordinating a pan-European network, gathering a total of 8 countries and 23 teams, including 5 separate FZJ units from JSC, IEK and IBG. Its partners are strongly engaged in both the HPC and energy fields; a prerequisite for the long-term sustainability of EoCoE and also ensuring that it is deeply integrated in the overall European strategy for HPC.

References

[1] http://ec.europa.eu/research/participants/portal/doc/call/h2020/h2020-einfra-2015-1/1660102-h2020-einfra-2015-1_flash_call_info_en.pdf

[2] <http://www.prace-ri.eu> (needs update)

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