



SIMDAS & INDUSTRY RELATIONS – EXAMPLES FROM JUELICH

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 HEAD OF CROSS-SECTIONAL TEAM DEEP LEARNING & RDA CO-CHAIR INTEREST GROUP BIG DATA
 3RD MAY SIMDAS & MINISTRY MEETING, NICOSIA, CYPRUS

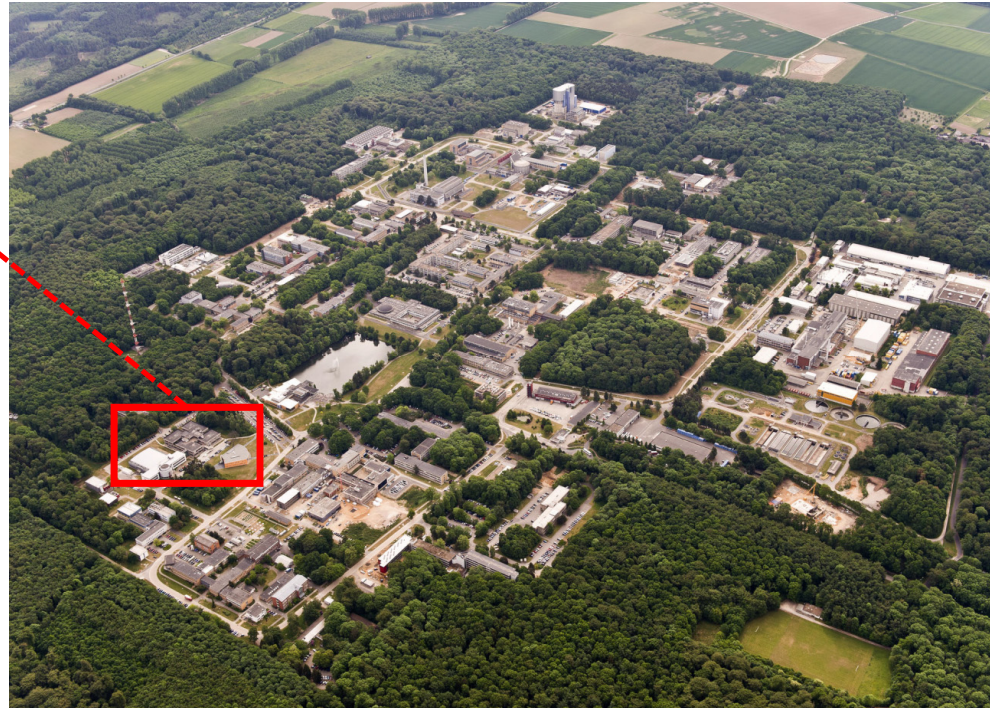


FORSCHUNGSZENTRUM JUELICH (FZJ)

Multi-Disciplinary Research Centre of the Helmholtz Association in Germany

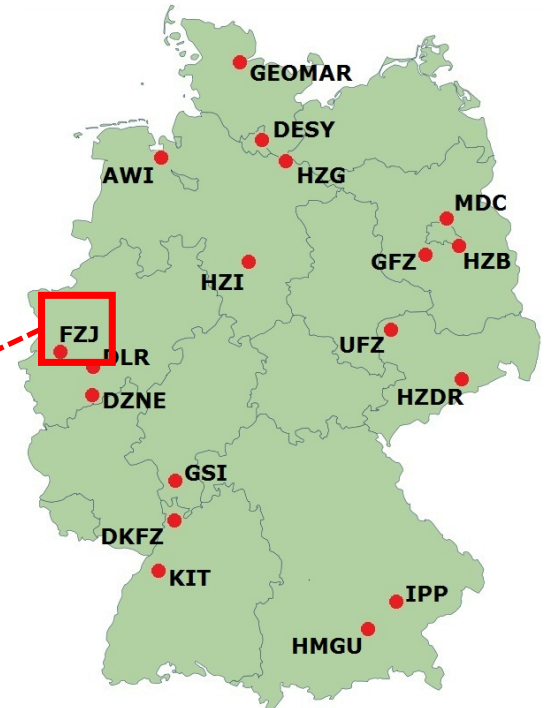


(Juelich Supercomputing Centre known as JSC)



■ Selected Facts

- One of EU largest inter-disciplinary research centres (~5000 employees)
- Special expertise in physics, materials science, nanotechnology, neuroscience and medicine & **information technology (HPC & Data)**



HELMHOLTZ
RESEARCH FOR GRAND CHALLENGES

[1] Helmholtz Association Web Page

HPC & DATA SCIENCE: A FIELD OF CONSTANT EVOLUTION

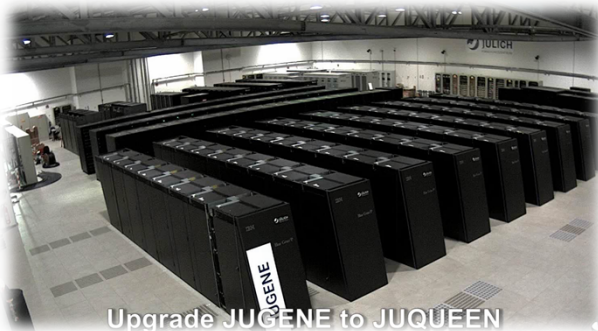
Perspective: Floating Point Operations
per one second (FLOPS or FLOP/s)

1.000.000 FLOP/s
~1984



- 1 GigaFlop/s = 10^9 FLOPS
- 1 TeraFlop/s = 10^{12} FLOPS
- 1 PetaFlop/s = 10^{15} FLOPS
- 1 ExaFlop/s = 10^{18} FLOPS

1.000.000.000.000.000 FLOP/s
~295.000 cores ~2009 (JUGENE)



Upgrade JUGENE to JUQUEEN



>5.900.000.000.000.000
FLOP/s
~ 500.000 cores
~ 2017

EUROPEAN UNION & COMMISSION PLANS

The SIMDAS Project and Objectives are In-line with Strategic Plans

“By supporting strategic projects in frontline areas such as artificial intelligence, supercomputers, cybersecurity or industrial digitisation, and investing in digital skills, the new programme will help to complete the Digital Single Market, a key priority of the Union.”

[11] COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE EUROPEAN COUNCIL, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS, EC, 2018, 2nd May 2018



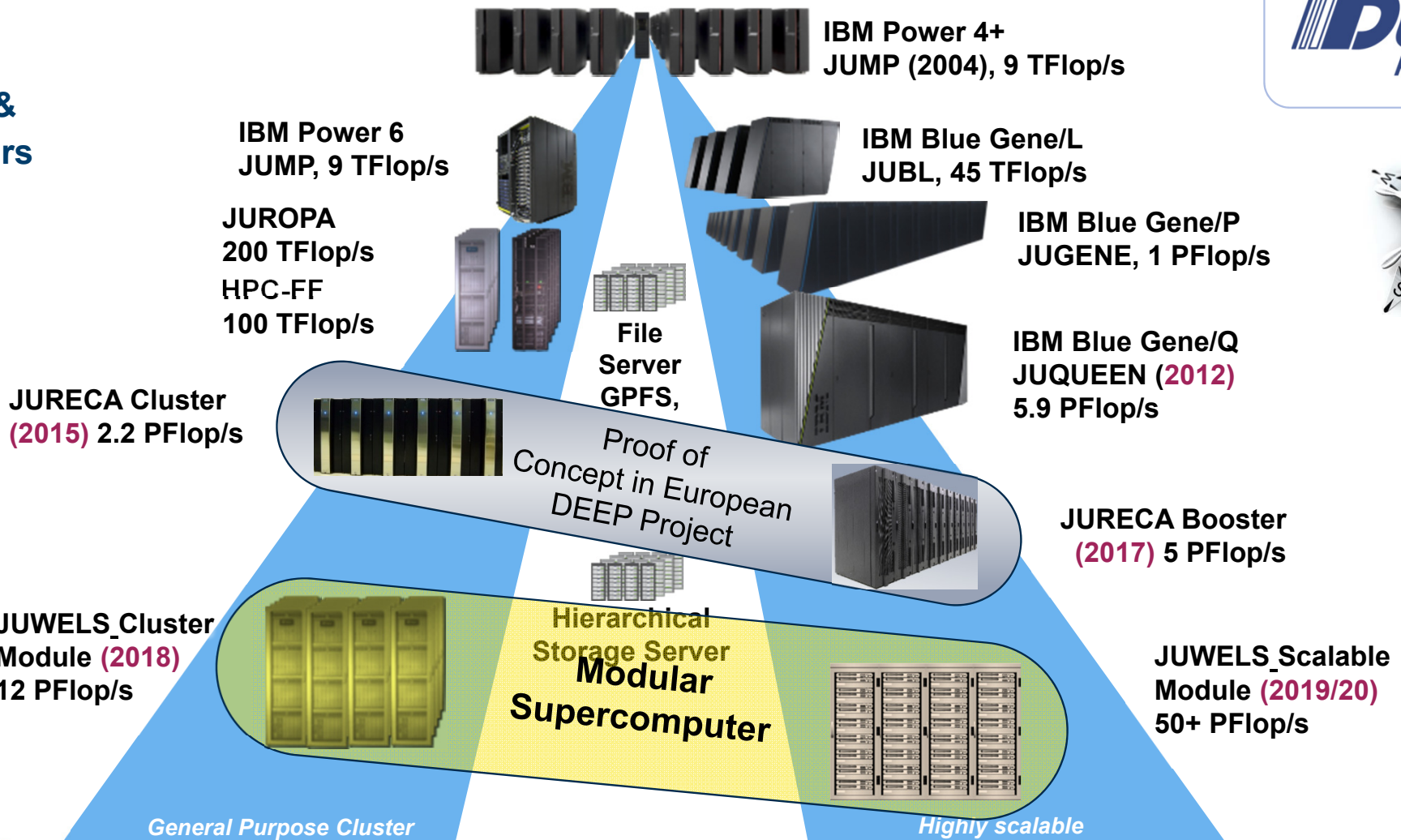
3rd May 2018



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JSC

Roadmap & Key Vendors



EXAMPLE CO-DESIGN APPROACH

Drive Technology Innovation in Different Roles

■ Exascale Labs (or Competence Centres)



- Long-term collaboration with suppliers
- POWER Acceleration and Design Center
- Collaboration between Forschungszentrum Juelich, IBM and NVIDIA
- Mission statement: Provide support to scientists and engineers to target the grand challenges facing society in the fields of energy & environment, information & health care

■ Co-Design Projects

- E.g. DEEP projects



(Selected JSC collaboration partners)

SIMDAS & JSC IMPLEMENT CO-DESIGN APPROACH

Drive Technology Innovation in Different Roles

- Address Future HPC & Data challenges via **Application Co-Design Approach**
 - SIMDAS thematic areas are key to future design
 - Scientific problem requirements influence architecture design & technology
 - Architectural constraints impact formulation & design of innovative algorithms and software



- **Co-Design: work with technology experts on development of HPC technology & companies are partners → use case driven approaches**
- **Techniques to facilitate co-design is to provide mini-applications and performance analysis results → Transfer knowledge to technology experts**
- **Provide performance models and simulators based on new technologies and hardware architectures → Transfer knowledge to application experts**



JÜLICH
SUPERCOMPUTING
CENTRE



Simulation & Data Science
Center of Excellence



EXAMPLE JUELICH SUPERCOMPUTING CENTRE & SIMDAS

Simulation & Data Labs (SDL) using High Performance Computing (HPC)

Smart Data
Innovation Lab

AixCAPE

smith
Smart Medical Information
Technology for Healthcare

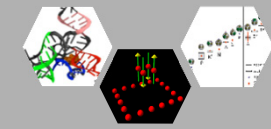
SOCCERWATCH BETA



Communities

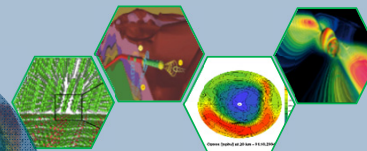
Research
Groups

Research
Group High
Productivity
Data
Processing



Domain-specific
SDLs

Simulation Labs



DEEP-EST
EU
PROJECT

Cross-Sectional Teams

Cross-
Sectional
Team Deep
Learning

Data Life Cycle Labs

Exascale co-Design

DEEP
Projects

Facilities

HPC
Systems
JURECA &
JUQUEEN

Modular
Supercomputer
JUWELS

Industry
Relations
Team



UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES
FACULTY OF INDUSTRIAL ENGINEERING,
MECHANICAL ENGINEERING AND COMPUTER SCIENCE

JÜLICH
Forschungszentrum | JÜLICH
SUPERCOMPUTING
CENTRE

Simulation & Data Science
Center of Excellence

3rd May 2018

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DEEP SERIES OF PROJECTS

EU Projects Driven by Co-Design of HPC Applications



- 3 EU Exascale projects

DEEP
DEEP-ER
DEEP-EST

- 27 partners

Coordinated by JSC

- EU-funding: 30 M€

JSC-part > 5,3 M€

- Nov 2011 – Jun 2020

- Strong collaboration with our industry partners Intel, Extoll & Megware

- Innovative HPC hardware like Intel Nervana Neon and persistent RAMs

- Juelich Supercomputing Centre implements the DEEP projects designs in its HPC production infrastructure



[2] DEEP Projects Web Page

SIMDAS & JSC JOINTLY TOWARDS EXASCALE

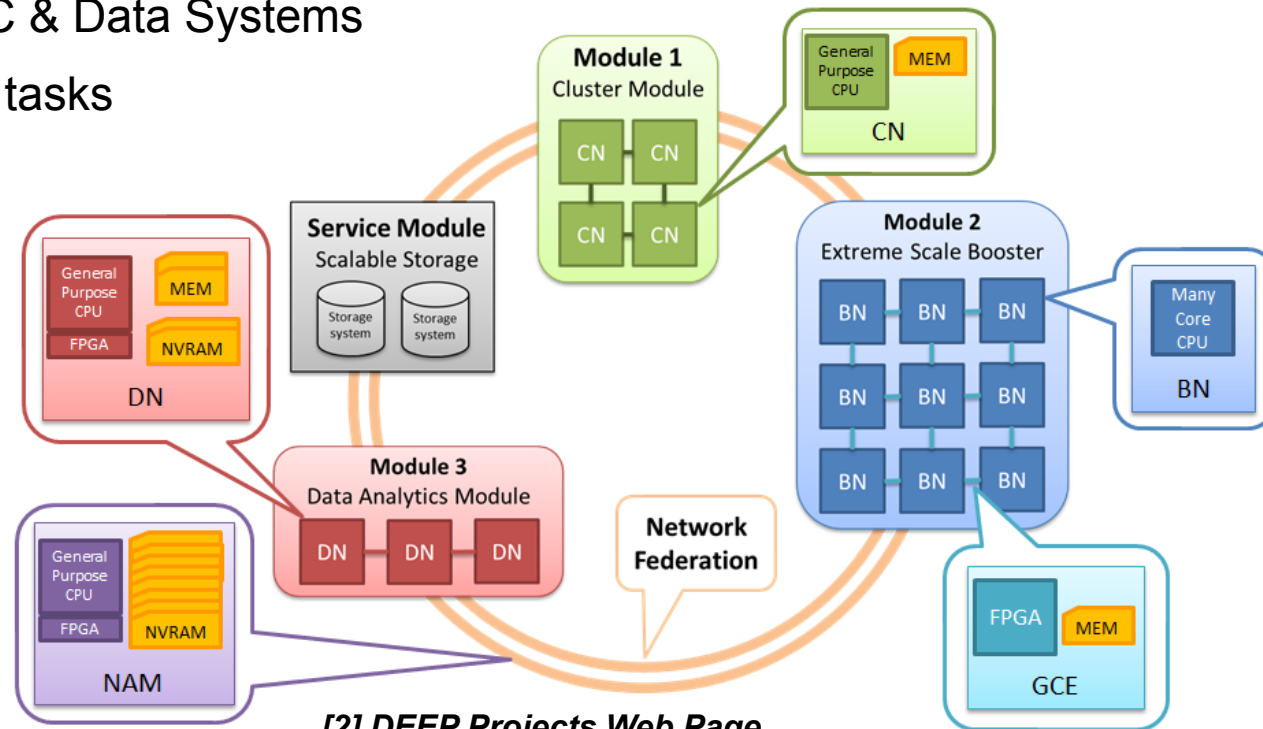
SIMDAS Centre of Excellence will Strengthen the Portfolio of Both Cyprus & Germany



- Flop/s metric will become increasingly less(!) relevant

- Driven by application co-design of HPC & Data Systems
- Support for less regular computational tasks
- Significantly larger memory footprint
- Extreme data processing capabilities
- Improved/optimized data transport capabilities & specialized analytics
- Scalable visualisation capabilities
- Management of complex work-flows

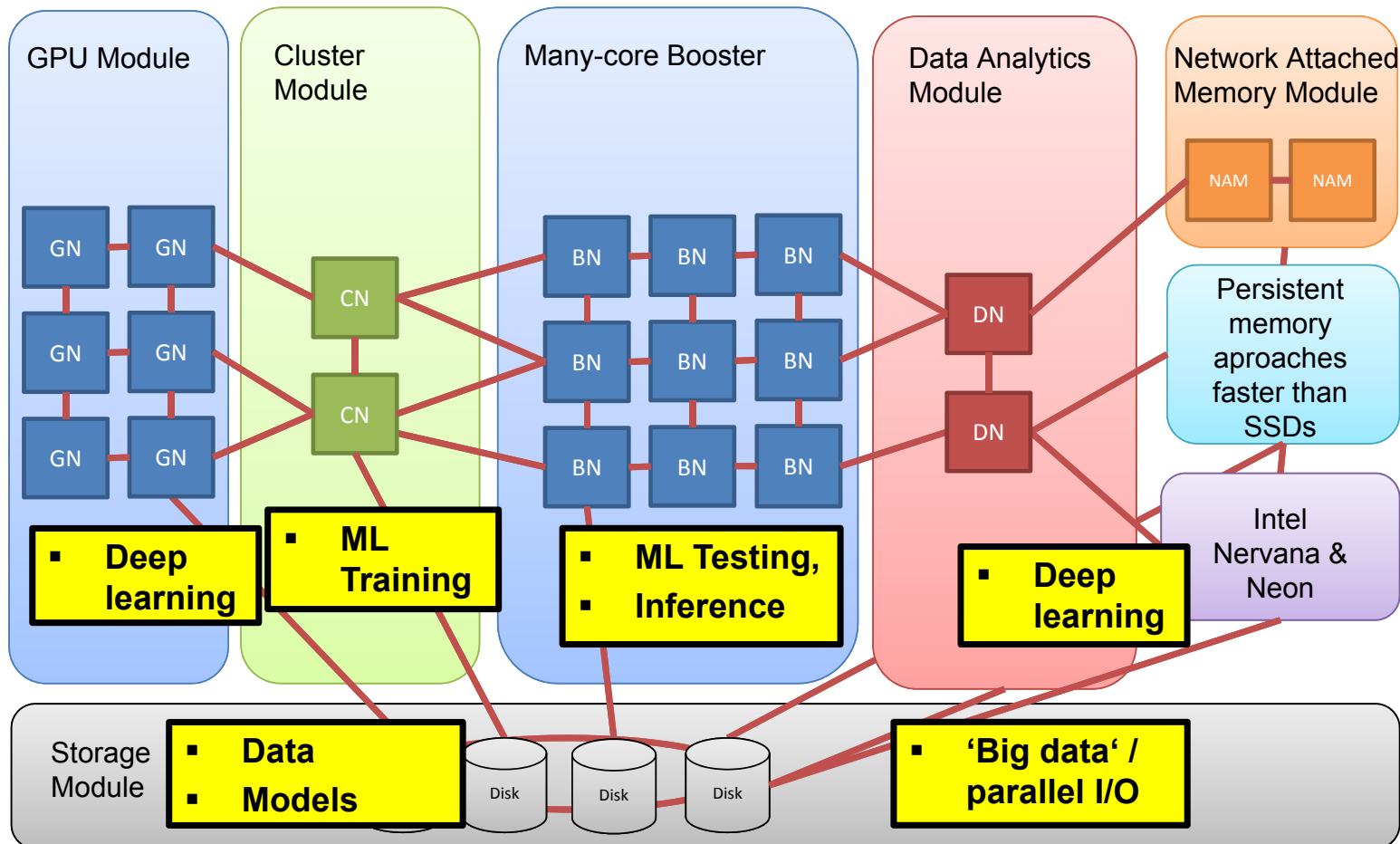
▪ One plausible answer to those facts is the modular supercomputer architecture driven by the JSC & DEEP projects



MODULAR SUPERCOMPUTING ARCHITECTURE



JSC Roadmap

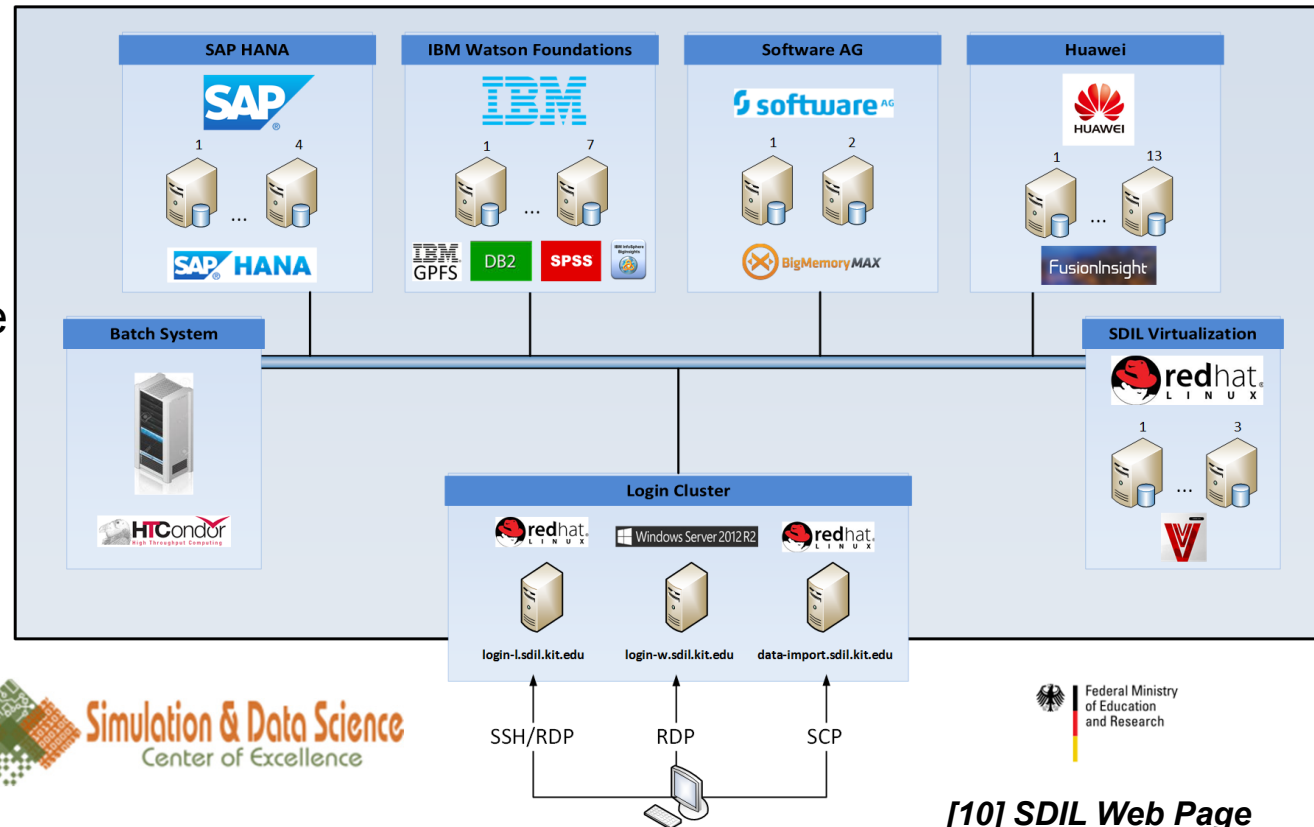


- **Innovative Ideas, e.g. trained models in memory**
- **Innovative memory, e.g. persistent RAM**
- **Innovative chips, e.g. use of deep learning optimized chip designs**

SIMDAS EXAMPLES – TRANSLAB & TOOLS

Joint Use of Smart Data Innovation Lab (SDIL) Platform

- Technology Platform for Data Analytics
- Key technologies from vendors w.r.t. commercial parallel & scalable machine learning tool platforms
- SAP Hana, IBM DB2 & SPSS, Software AG BigMemory MAX, Huawei FusionInsight, etc.
- Data-driven SIMDAS projects can leverage the platform (small proposal needed / case)



[10] SDIL Web Page

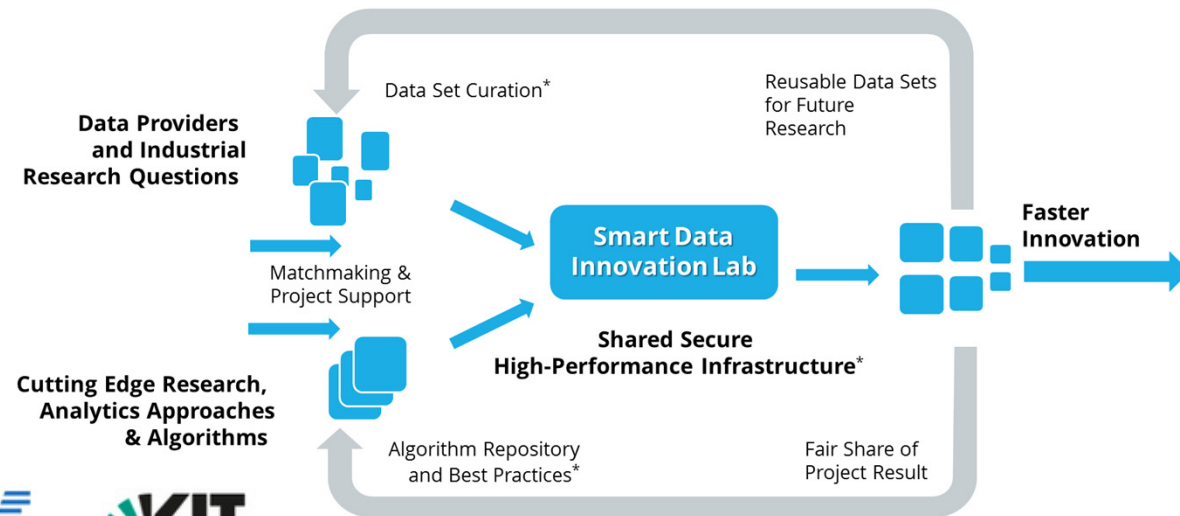
- Letter of intent/support already requested and relevant joint selected work elements have been already discussed

SIMDAS EXAMPLES – TRANSLAB & TOOLS

Joint Use of Smart Data Innovation Lab (SDIL) Platform

■ SDIL Partners

- Key players in German industry
- Head of community Medicine
(Prof. M. Riedel & Prof. A. Schuppert;
both SMITH ASIC Use Case partners)



[10] SDIL Web Page

- Letter of intent/support already requested and relevant joint selected work elements have been already discussed

SIMDAS EXAMPLES – HEALTH AREA

Bayer AG & RWTH Aachen + University Hospital & Forschungszentrum Juelich & Nicosia General Hospital

■ SMITH ASIC Use Case

- ASIC: Algorithmic Surveillance of Intensive Care Unit (ICU) Patients & Focus on Acute Respiratory Distress Syndrome (ARDS)
- University Clinic Aachen (UKA): Machine Learning for patient stratification & virtual ICU patient & risk patterns
- FZJ: Parallel & Scalable Machine Learning & Statistical Modelling via HPC
- Bayer AG: clinical trial optimization in prevention studies & virtual ICU patients & organ models



[3] SMITH Project Web Page

[4] SMITH Methods Journal



■ Letter of intent/support already requested and relevant joint selected work elements have been already discussed

SIMDAS EXAMPLES – HEALTH AREA

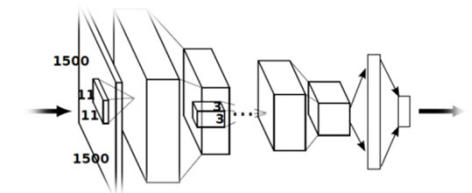
Bayer AG & RWTH Aachen + University Hospital & Forschungszentrum Juelich & Nicosia General Hospital

- MCMC with VP models
 - 1 run for a patient ~ 2 sec (1 core)
 - 10^6 runs required for MCMC
 - 1 patient ~ 1000 core-h

- Markov Chains Monte Carlo (MCMC) with Virtual Patient models
- In clinical practise not feasible with today's computer technology
=> model reduction is necessary
- Virtual Patient (VP) model mapped into a deep learning network

- Good news: 100% parallel → nice scalability and useful for booster
- More data is helpful for more concrete feature selection w.r.t. ARDS

- Compute-intensive part of the Virtual patient model will be mapped onto a deep-learning (DL) network
 - DL-network has is numerically hard to train, but fast to simulate
 - Mapping strategy has been evaluated and applied at partner Bayer
 - Requires HPC (scanning of the full parameter space)



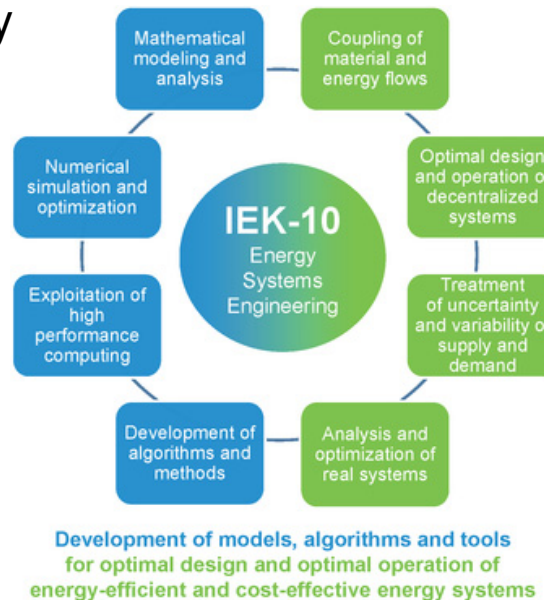
SIMDAS EXAMPLES – ENGINEERING AREA



Exploration of AixCAPE tools & Know-How together with SIMDAS & Various Engineering companies

■ Process Systems Engineering

- Link: Forschungszentrum Juelich (IEK-10) & RWTH Aachen University
- Forschungszentrum Juelich IEK-10 Director & Head of AixCAPE (Prof. A. Mitsos)
- SIMDAS thematic area impact



The Chemical Company



[5] AiXCape Web Page

- Letter of intent/support already requested and relevant joint selected work elements have been already discussed

SIMDAS EXAMPLES – ENGINEERING AREA



Exploration of AixCAPE tools & Know-How together with SIMDAS & Various Engineering companies

- Known player in process engineering
 - Know-How: leverage research transfer projects (aka SIMDAS outcomes)



- Uses phases: Long-term research, prototypes, commercialization for end users



BASF

The Chemical Company



Chemstations™
Europe GmbH



EVONIK
INDUSTRIES

INEOS

THE WORD FOR CHEMICALS

LANXESS

Energizing Chemistry

[5] AiXCape Web Page

- Letter of intent/support already requested and relevant joint selected work elements have been already discussed

INDUSTRY RELATIONS TEAM (IRT) @ JSC

Examples: Selling Computing Time & Offering Code Optimization

■ SIEMENS

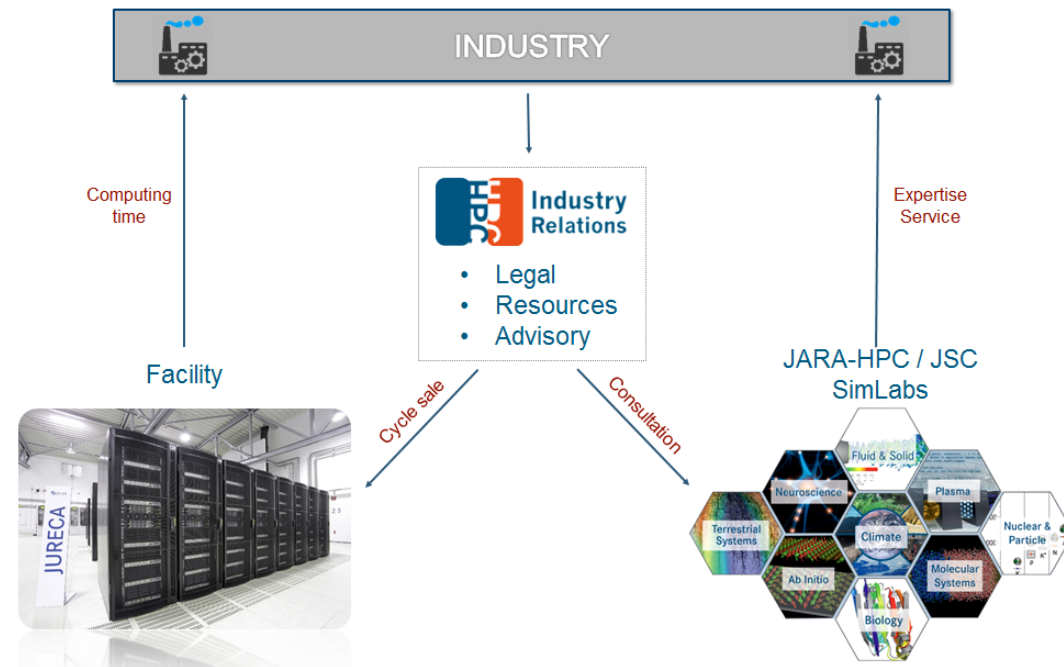
- Long-term cooperation with Siemens Power & Gas Department
- Simulation of combustion processes in turbine systems
- [Computing time on JSC Jureca HPC system](#)
- Take advantage of application support team @ JSC
- Bilateral cooperations and partners in big publicly funded (Germany BMWI) project consortium

■ Outotec

- Global leader in minerals & metals processing technology
- [Computing time on JSC Jureca HPC System](#)
- OpenFOAM computational fluid dynamics (CFD) computations
- Take advantage of application support team @ JSC

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[6] JSC Industry Relations Web Page

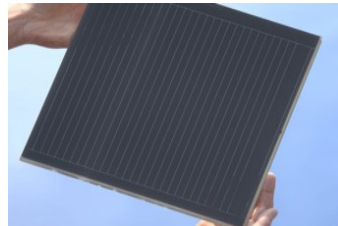
[7] OpenFOAM Web Page

INDUSTRY RELATIONS TEAM (IRT) @ JSC

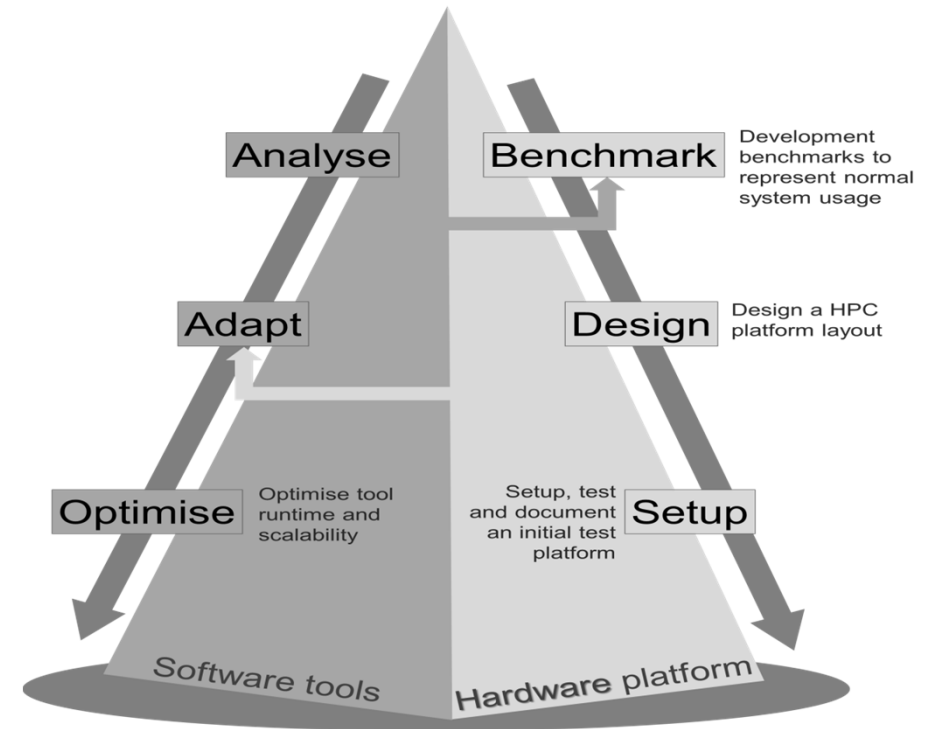
Examples: Selling Computing Time & Offering Code Optimization



- One out of four German Transmission System Operators (TSOs) & designs, builds, and operates high voltage grids
- Selected Consultation & Expertise Services from JSC included software & hardware guidance & support
- Software: code analysis, optimization plan, work-flows
- Hardware: support of a purchase decision & cluster testing



- **Benefit for FZJ/JSC: Work on real industry problem with high societal relevances & follow-up projects discussed like German BMBF projects**

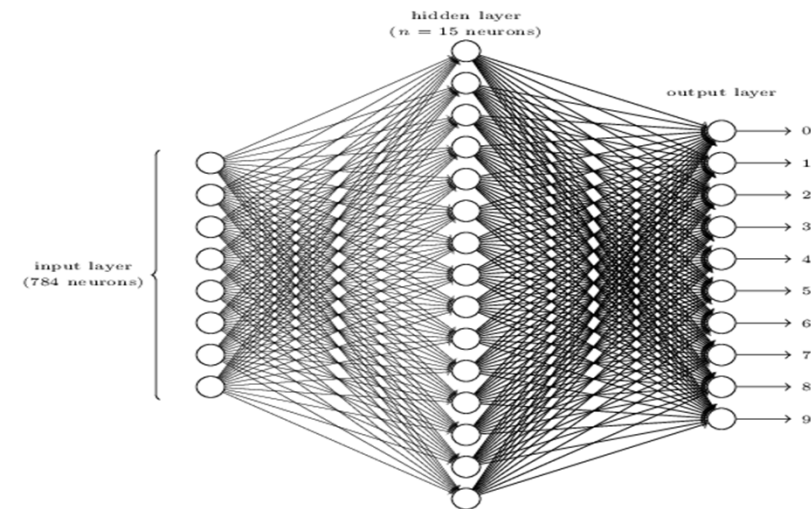


[6] JSC Industry Relations Web Page

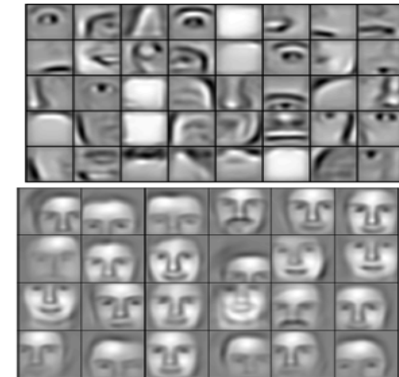
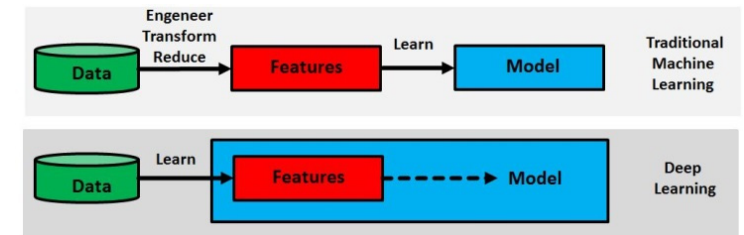
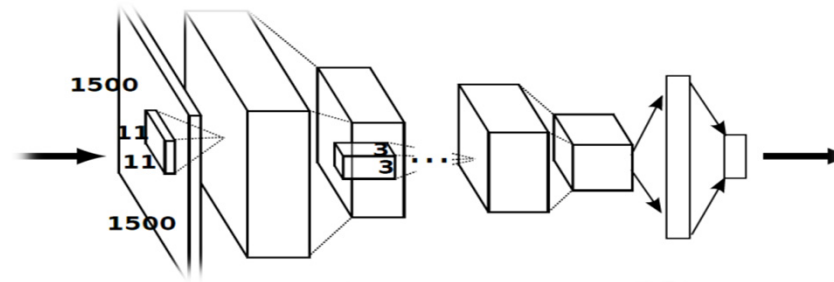
INNOVATIVE DEEP LEARNING TECHNOLOGIES

Short Overview & Role of Team Deep Learning for SIMDAS & Juelich Supercomputing Centre

■ Innovative & disruptive approach



*[8] M. Riedel, Invited
YouTube Tutorial on Deep
Learning, Ghent University*



- Provide deep learning tools that work with HPC machines (e.g. Python/Keras/Tensorflow)
- Advance deep learning applications and research on HPC prototypes (e.g. DEEP-EST, etc.)
- Engage with industry (industrial relations team) & support SMEs (e.g. Soccerwatch)
- Offer tutorials & application enabling support for commercial & scientific users (e.g. YouTube)

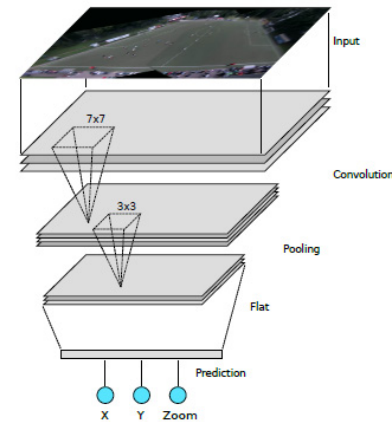
SIMDAS EXAMPLES – INNOVATIVE START-UPS



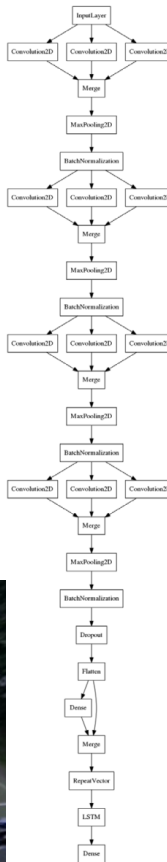
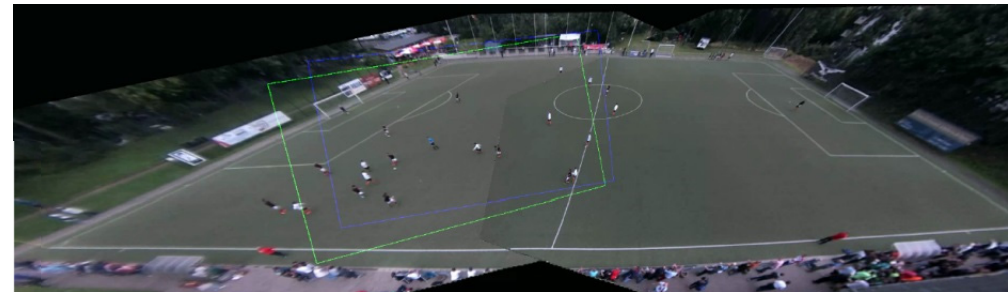
Collaboration in Applying Deep Learning in Commercial Scenarios & Small Start-Up Guidance

■ SoccerWatch.TV

- **Start-up:** created/joined by a 'exit-ing' PHD Student @ JSC
- Besides upper leagues: **80k matches/week**
- Recording too expensive (amateurs) with **camera man needed**
- Approach: Find X,Y center and zoom on panorama camera using **Deep Learning**
- Investor grant (1,5 mio €) **adesso** from Adesso AG



[9] SoccerWatch.TV Web page



- Letter of intent/support already requested and relevant joint selected work elements have been already discussed
- Further German BMBF project has been submitted (NRW-HUB) with relevance to SIMDAS & Retail (with Adesso)

SUMMARY

■ Mindset

- SIMDAS strategic roadmap is long – stay flexible (e.g. new chips or approaches?)
- Engage with commercial partners in Cyprus in co-design applications (e.g. use cases)



■ Skillset

- SIMDAS commercial partners have access to many skills (e.g. how to create a start-up)
- TransLab, thematic share research & industry share approaches (e.g. deep learning)



■ Toolset

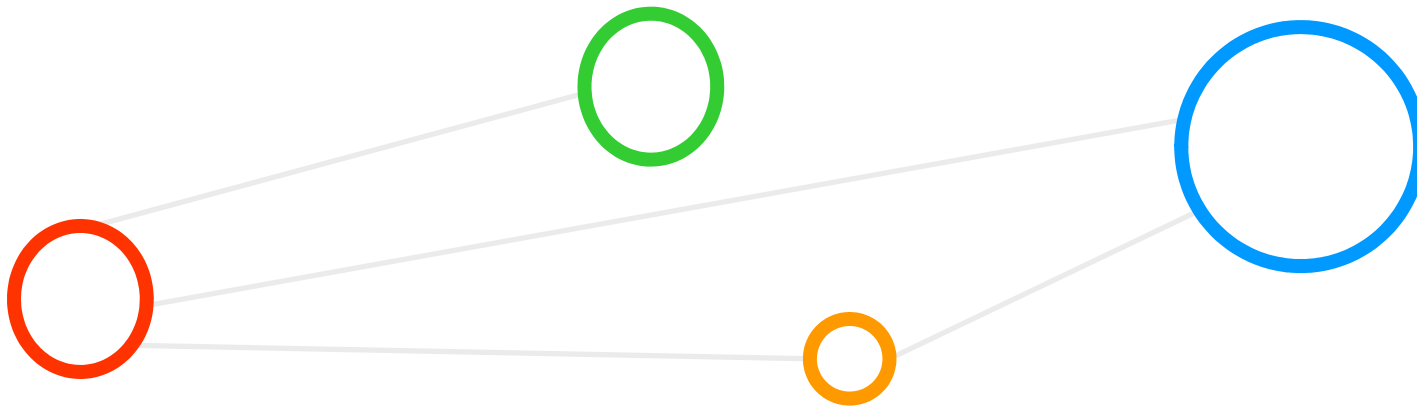
- SIMDAS offers a wide variety of tools/services and underlying infrastructure (e.g. HPC)
- People are key to use tools to engage in application enabling (e.g. consulting users)



THANKS FOR TEAMING WITH US!



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- [2] DEEP Projects Web Page,
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- [3] SMITH Projects Web Page,
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- [4] Alfred Winter et al., 'Smart Medical Information Technology for Healthcare (SMITH) – Data Integration based on Interoperability Standards', submitted to Journal of Methods, 2018, to appear
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Online: https://ec.europa.eu/commission/sites/beta-political/files/communication-modern-budget-may2018_en.pdf?utm_source=POLITICO.EU&utm_campaign=e3a8a86cc6-EMAIL_CAMPAIGN_2018_05_02&utm_medium=email&utm_term=0_10959edeb5-e3a8a86cc6-189710085

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Previous & current members of the High Productivity Data Processing Research Group



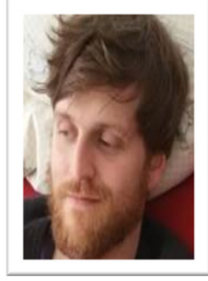
PD Dr.
G. Cavallaro



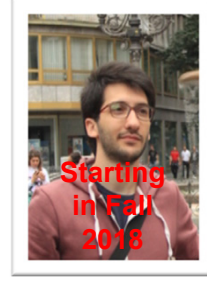
Senior PhD
Student A.S. Memon



Senior PhD
Student M.S. Memon



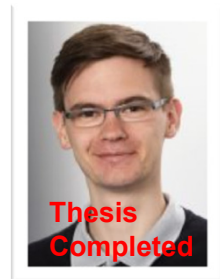
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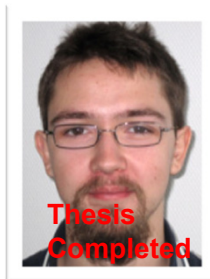
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S. Bakarar



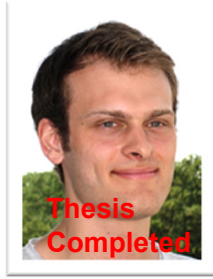
MSc Student
G.S. Guðmundsson
(Landsverkjun)



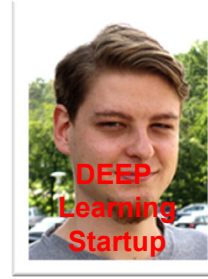
Dr. M. Goetz
(now KIT)



MSc M.
Richerzhagen



MSc
P. Glock
(now INM-1)



MSc
C. Bodenstein
(now Soccerwatch.tv)



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THANKS

Talk shortly available under www.morrisriedel.de

