The German HPC Landscape

The Gauß Alliance as a coordinator in a diverse HPC landscape

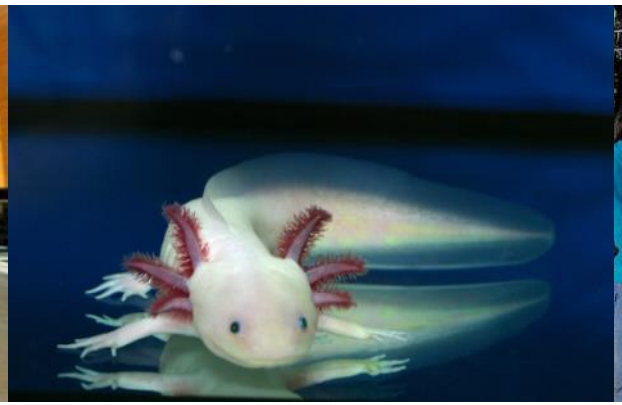
Gauß Alliance
Prof. Dr. Wolfgang E. Nagel
October 2014

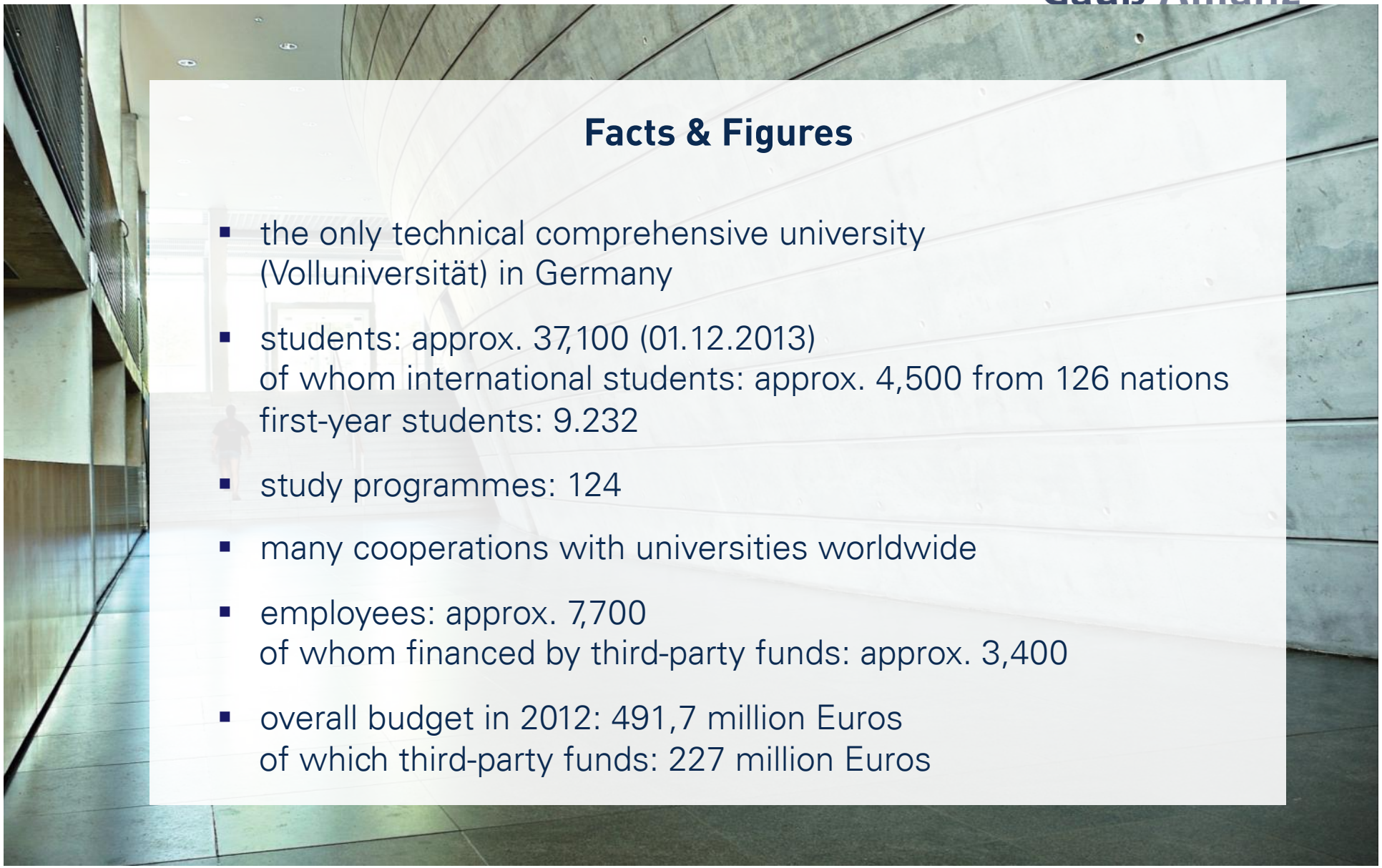
TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept




TU Dresden: University of Excellence

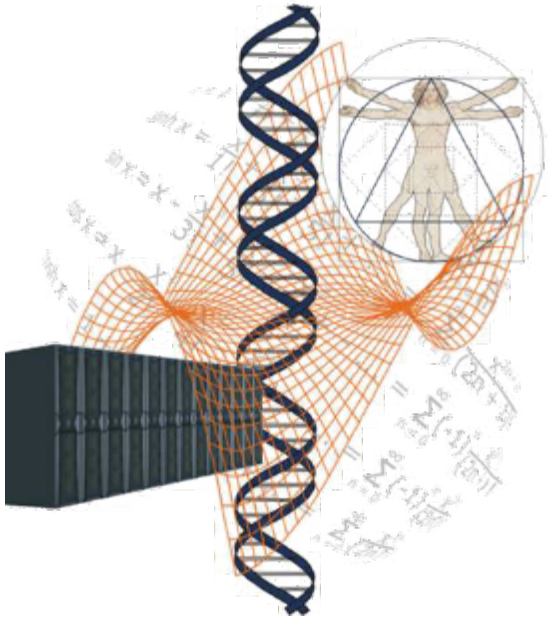


Facts & Figures

- the only technical comprehensive university (Volluniversität) in Germany
- students: approx. 37,100 (01.12.2013)
  of whom international students: approx. 4,500 from 126 nations
  first-year students: 9.232
- study programmes: 124
- many cooperations with universities worldwide
- employees: approx. 7,700
  of whom financed by third-party funds: approx. 3,400
- overall budget in 2012: 491,7 million Euros
  of which third-party funds: 227 million Euros

Center for Information Services and HPC (ZIH)

- Central Scientific Unit at TU Dresden
- Competence Center for „Parallel Computing and Software Tools“
- Strong commitment to support real users
- Development of algorithms and methods: Cooperation with users from all departments
- Providing infrastructure and qualified service for TU Dresden and Saxony



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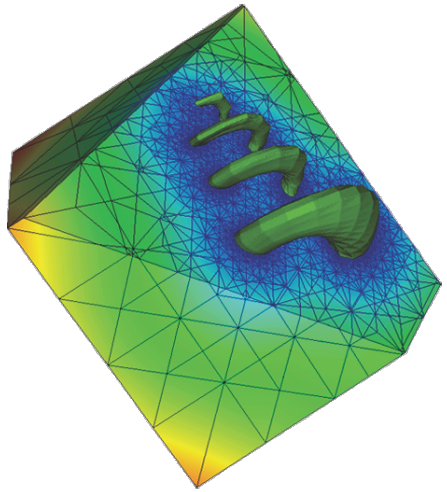
ZIH Areas of Expertise

- Research topics
  - Scalable software tools to support the optimization of applications for HPC systems
  - Data intensive computing and data life cycle
  - Performance and energy efficiency analysis for innovative computer architectures
  - Distributed computing and cloud computing
  - Data analysis, methods and modeling in life sciences
  - Parallel programming, algorithms and methods
- Pick up and preparation of new concepts, methods, and techniques
- Teaching and Education



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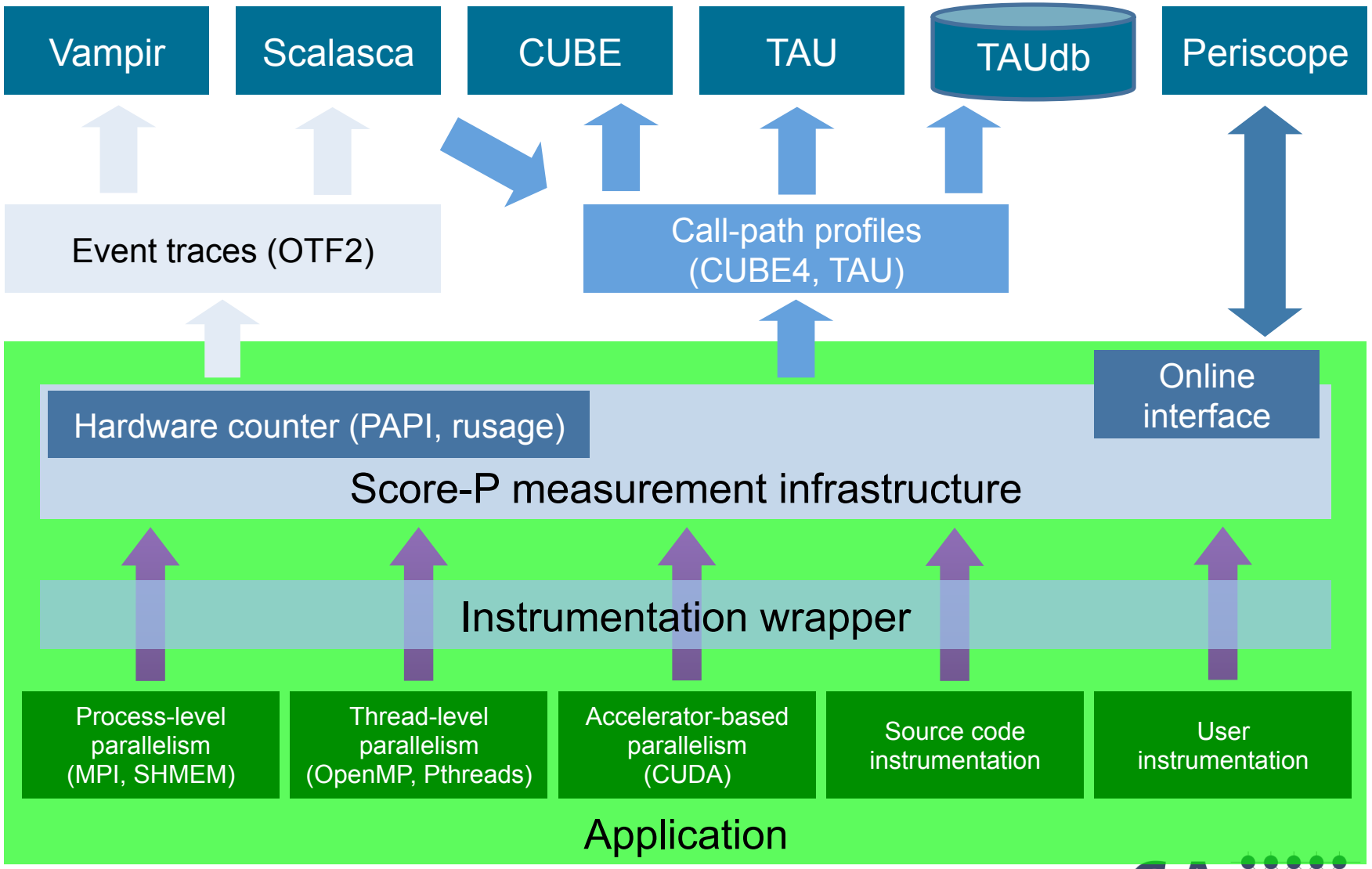
Joint Score-P Architecture for Run-Time Measurement



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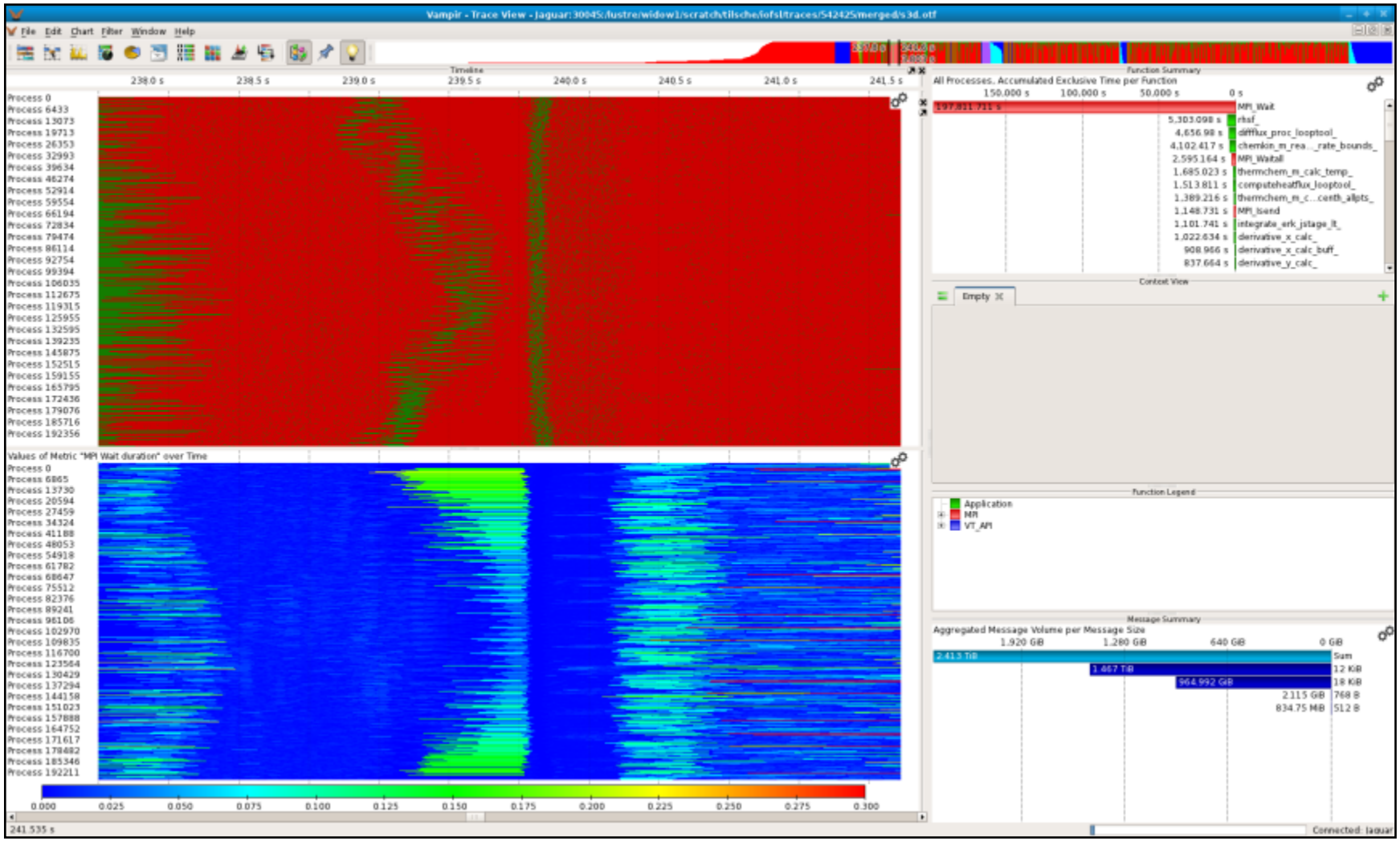
Scalability: 200,000+ Processes in Vampir



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DFG

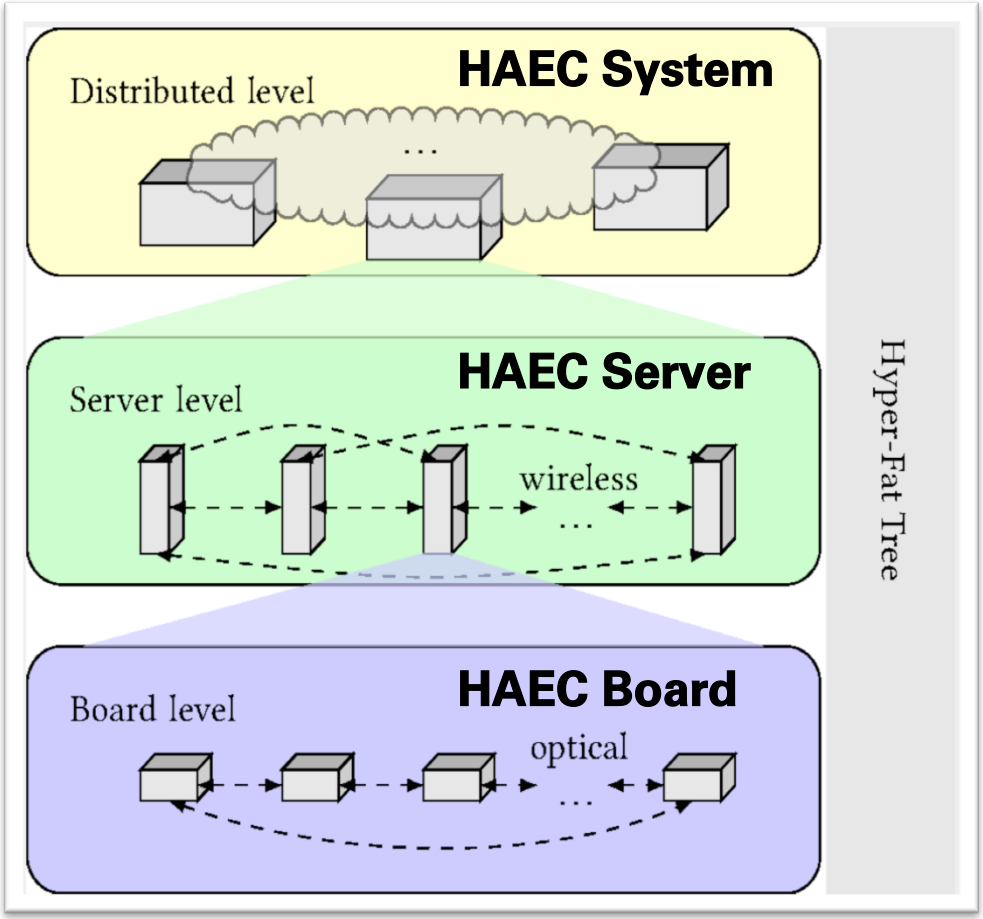
DRESDEN concept

HAEC

Collaborative Research Center 912: HAEC – Highly Adaptive Energy-Efficient Computing

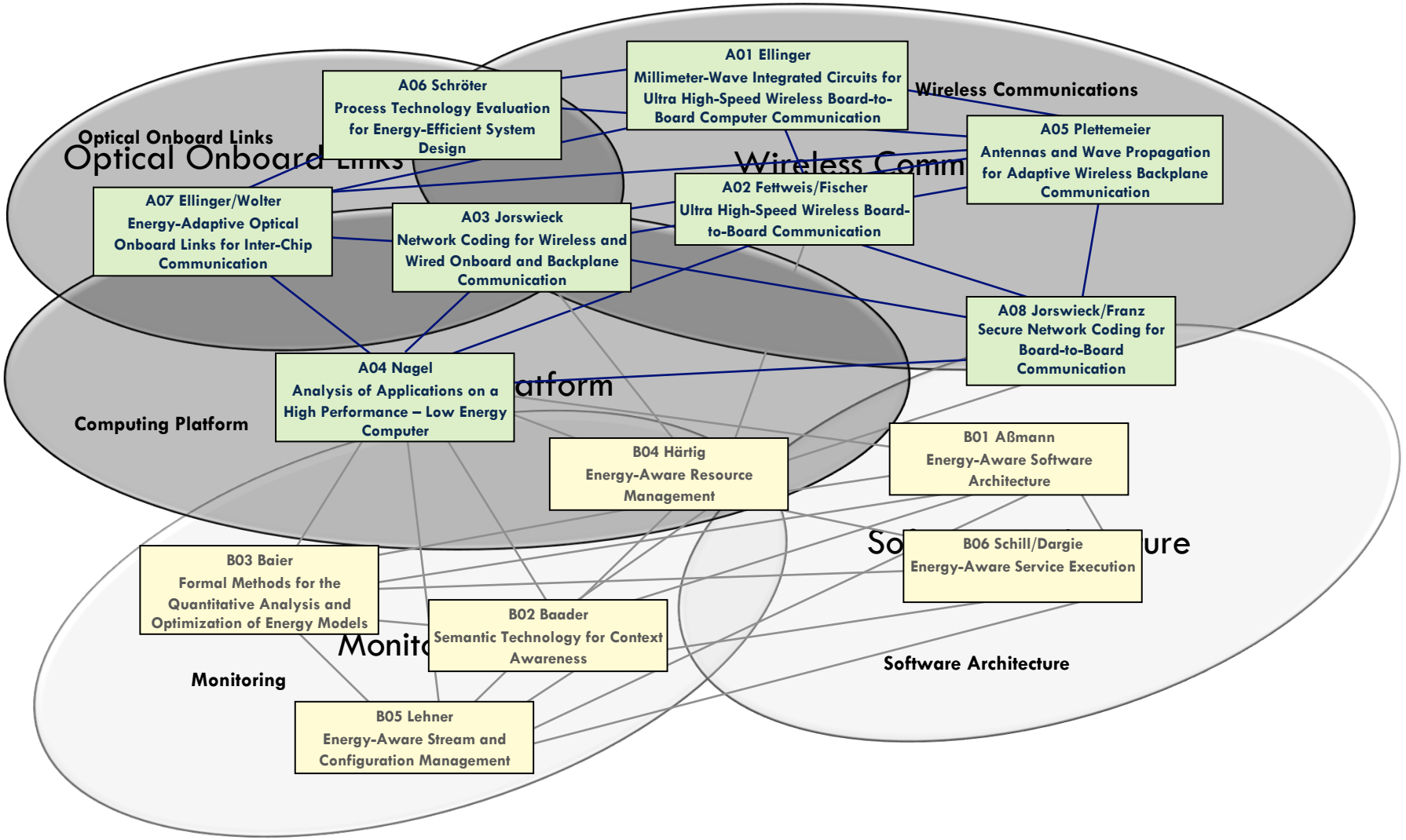
Highly Adaptive Energy-Efficient Computing

- Computing systems tend to become more loosely coupled vs tightly coupled
- Their metabolism is higher than we can/ will be able to afford
- Communication cost tends to dominate cost-to-solution



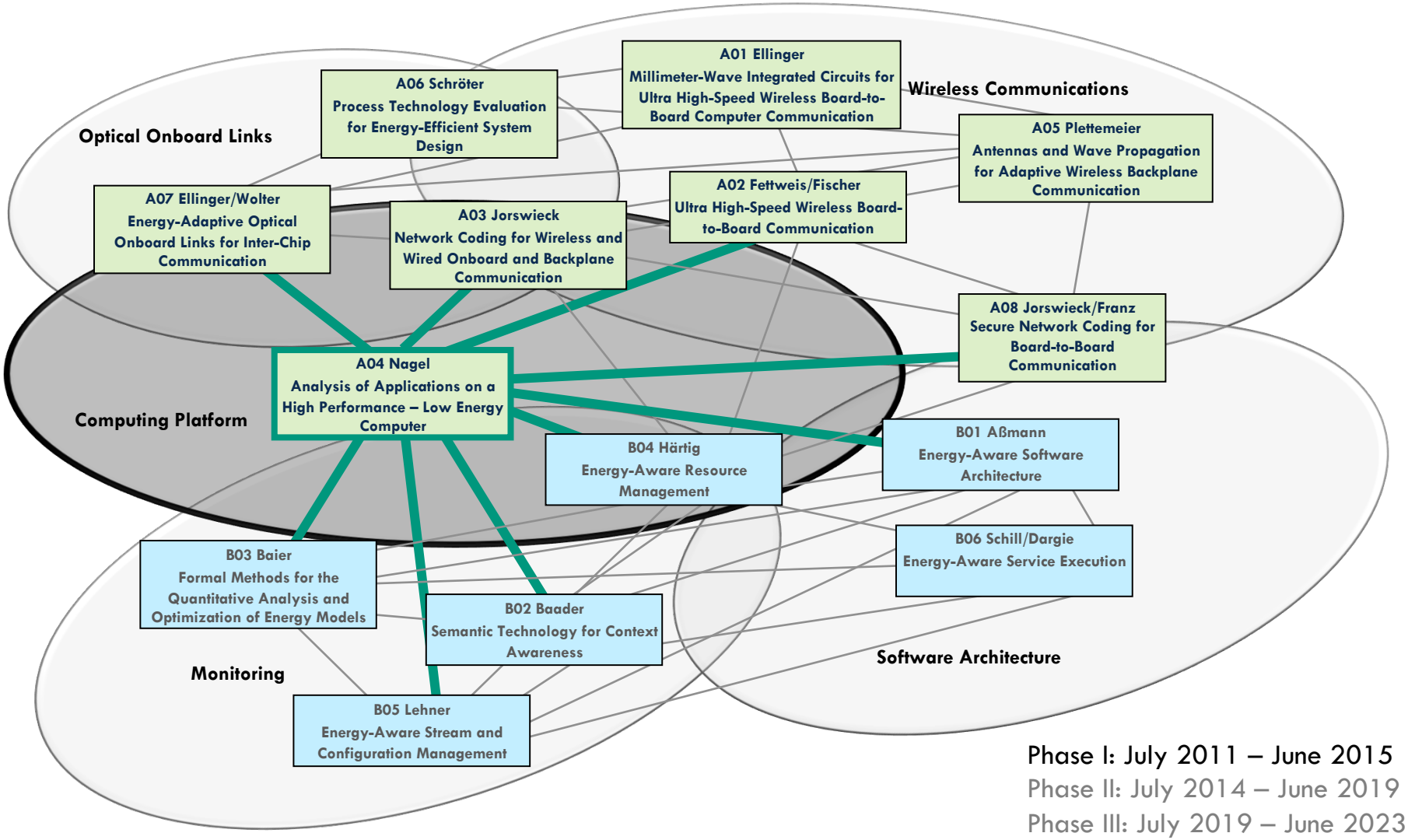
CRC 912 HAEC: http://tu-dresden.de/sfb912

HAEC as Collaborative Research Center



HAEC as Collaborative Research Center

Collaborative Research Center 912: HAEC — Highly Adaptive Energy-Efficient Computing



Phase I: July 2011 – June 2015
Phase II: July 2014 – June 2019
Phase III: July 2019 – June 2023

ScaDS Dresden/Leipzig

Competence Center for Scalable Data Services and Solutions

National Competence Center for Big Data

Prof. Dr. Wolfgang E. Nagel

Center for Information Services and HPC
Technische Universität Dresden

Announcement at CeBIT 2014

March 10th, 2014 – CeBIT Hannover

- Federal Minister Prof. Dr. Johanna Wanka announces the funding of two national competence centers for Big Data in Berlin and Dresden/Leipzig

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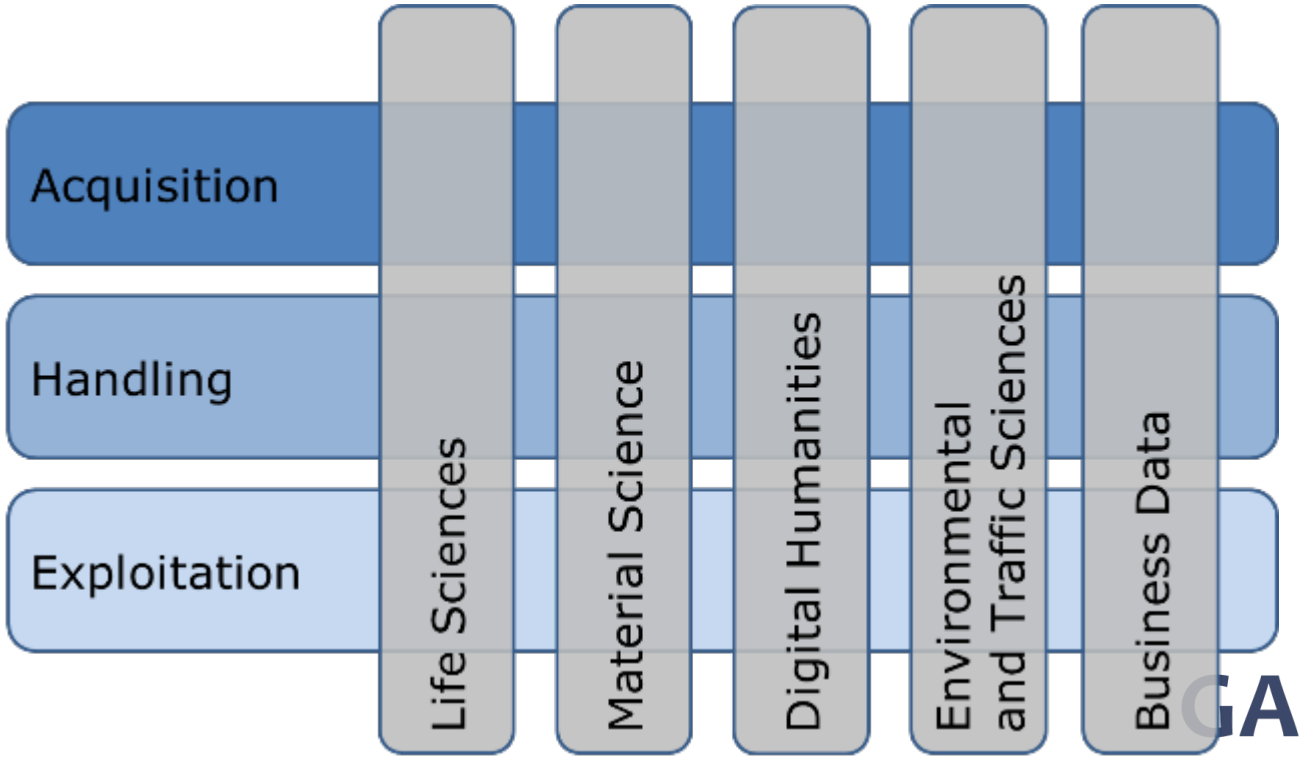
Big Data at ScaDS: Scientific Applications

- Developments of Big Data solutions for a broad field of scientific applications
- Starting with five disciplines in the project, later open to all



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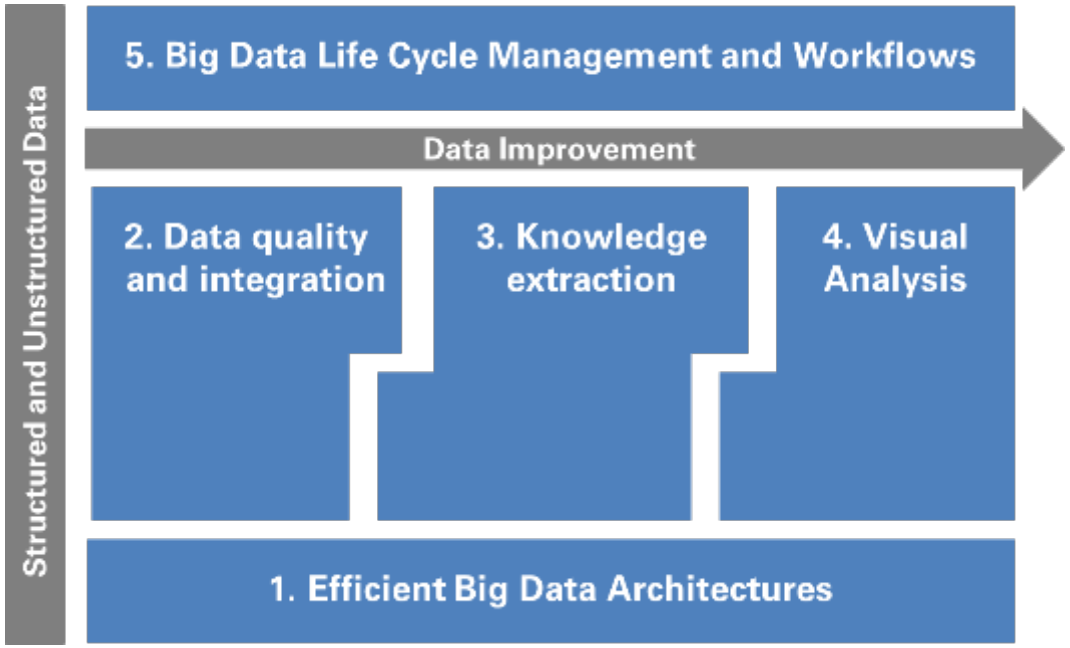
Big Data Research at ScaDS: Innovative Methods

- Cooperation on various topics of computer science
- Methodological focus: data quality and integration, knowledge extraction, visual analysis
- Cross-cutting topics: Big Data architectures and data life cycle management



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ZIH Research Topics (Selection)

- Software Tools for Analysis of Parallel Performance and Energy Efficiency
- Highly Adaptive Energy-Efficient Computing (HAEC) in SFB 912
- National competence center for Big Data “ScaDS Dresden/Leipzig”
- **More topics**
  - Data Lifecycle Management and Archiving
  - Grid middleware and Grid services
  - High Definition Energy Efficiency Monitoring (HDEEM) project with BULL
  - IT Service Management (ITSM) and ITIL
  - University-wide Service Desk
  - Dresden CUDA Center of Excellence, see http://ccoe-dresden.de
  - Intel Parallel Computing Center
  - More …

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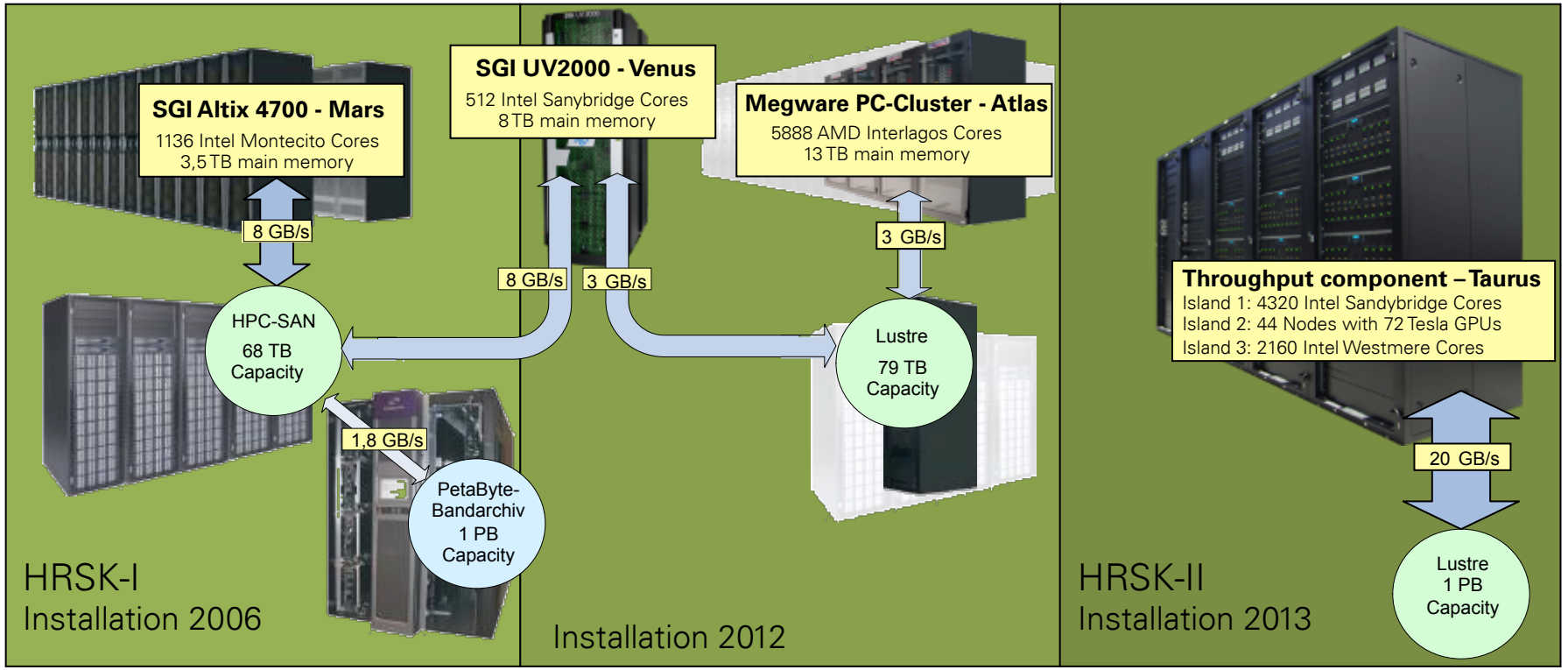
HPC Infrastructure at ZIH/TU Dresden



HRSK-II: Installation in Two Phases

- 1. Phase Q1/2013
  - Current machine room
  - 3.500.000 €
  - <100 m^2
  - <300 kW
- 2. Phase Q4/2014
  - New machine room
  - 11.500.000 €

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New Data Center – German Data Center Award 2014

Winner in the category of energy and resource efficient data centers 2014

- Plenum in the data center: A concept for efficiency and safety

DEUTSCHER
RECHENZENTRUMSPREIS
2014

1. PLATZ KATEGORIE 8:
ENERGIE- UND RESSOURCENEFFIZIENTE
RECHENZENTREN

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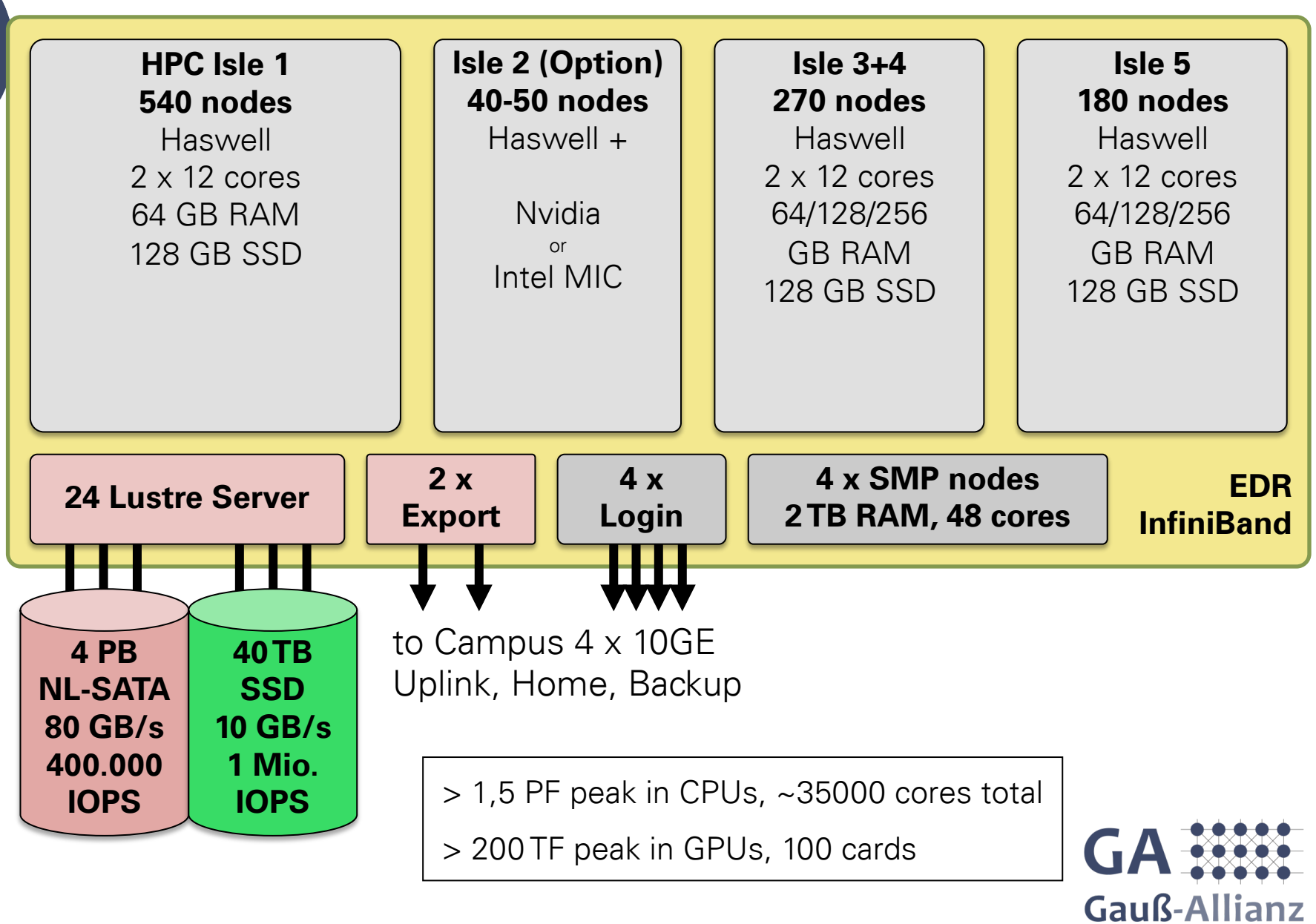
HRSK-II, Phase 2, Q4 2014 (additional to Phase 1)



> 1,5 PF peak in CPUs, ~35000 cores total

> 200 TF peak in GPUs, 100 cards

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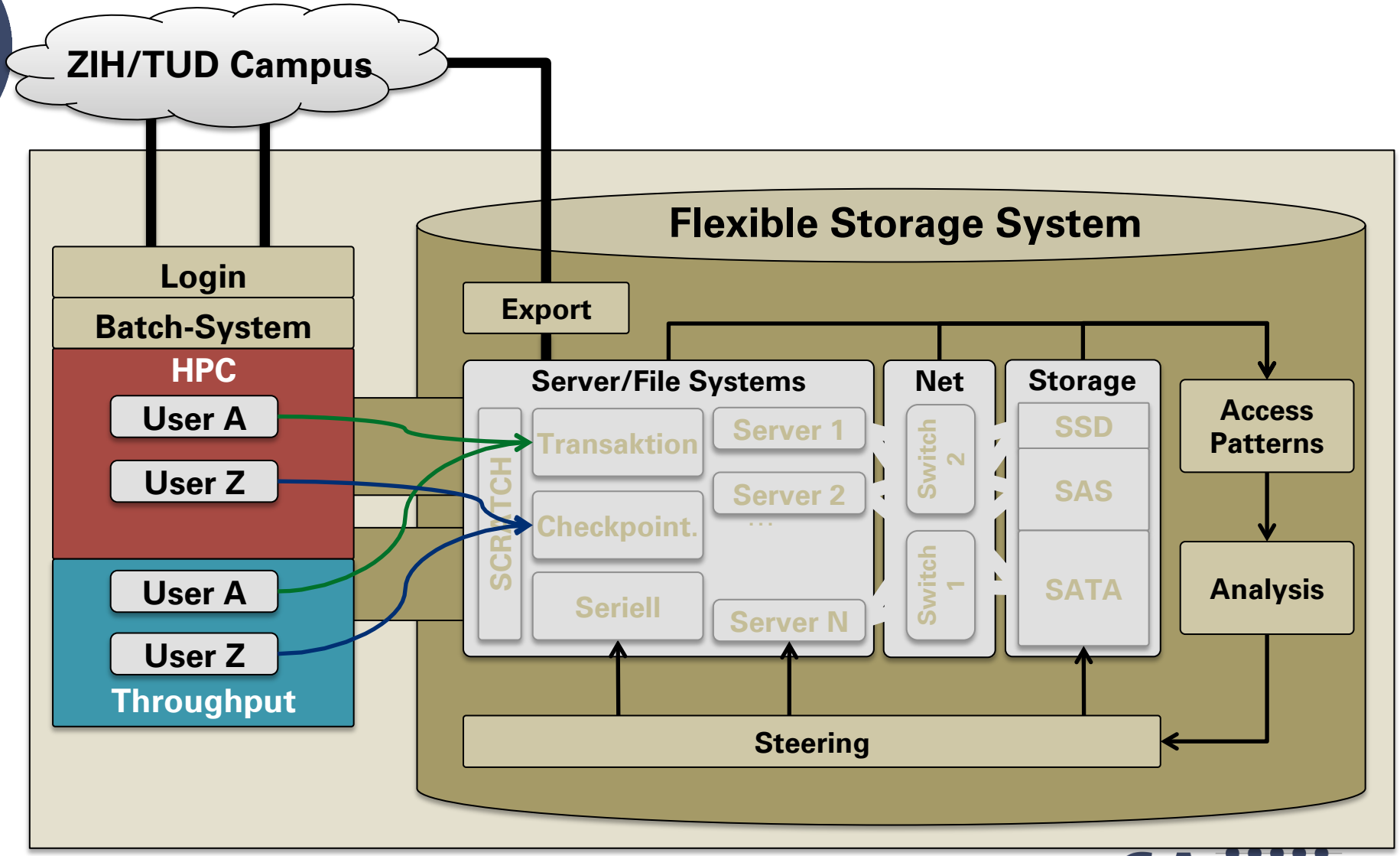
In more detail ...



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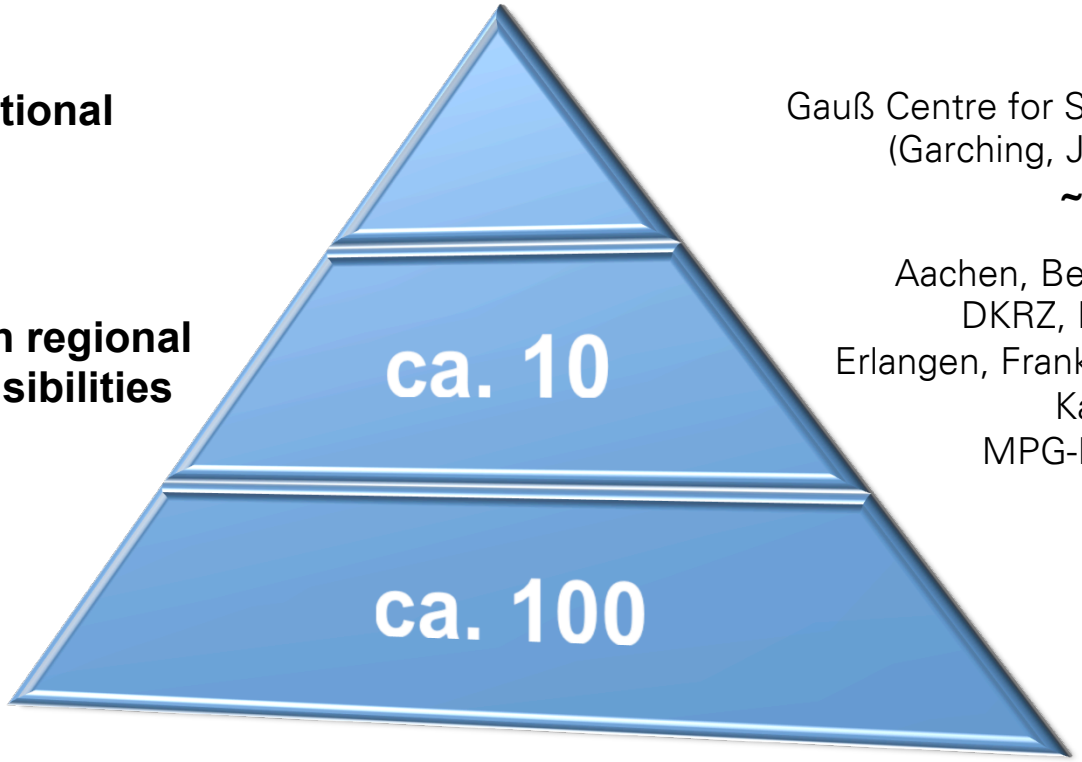
German HPC pyramid structured by capability

European and national HPC Centres

Gauß Centre for Supercomputing (Garching, Jülich, Stuttgart)
~ 12.69 PFLOPS

HPC Centres with regional or topical responsibilities



Aachen, Berlin, Darmstadt, DKRZ, Dresden, DWD, Erlangen, Frankfurt, Hannover, Karlsruhe, Mainz, MPG-RZG, Paderborn
~7.21 PFLOPS

HPC systems at Universities / Institutes

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Infrastructure for the German Scientific Computing

- At every time at least one system in Germany that is compatible with the international top level systems, so far funded by federal and local state.
- within the renewal phase of Tier-1 systems we have to ensure the architecture diversity within the HPC landscape to be able to serve all users equally
- selected Tier-2 systems as data backup systems for the important data of the Tier-1 systems, access to broader user communities with high HPC needs and - especially - potential
- coordinated procurement planning between Tier-1 and Tier 2 necessary

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HPC in Germany: Gauß-Alliance

- Members
  - Gauß Centre for Supercomputing, HLRN (RRZN, ZIB), RWTH, TU Dresden, RZG, TU Darmstadt, DWD, DKRZ, SCC, JGU Mainz
- Associates
  - G-CSC, PC^2, RRZE, DFN, DESY, RRZK, GWDG
- 19 locations – diverse HPC landscape
  - different architectures,
  - different vendors (IBM, Cray, BULL, ...)
  - specialised and supplementing expertise

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Gauss Centre for Supercomputing (www.gauss-centre.eu)

GCS
Gauss Centre for Supercomputing

- **Established: March 2007, 3 centres located in Juelich, Stuttgart, and Garching**
- **International representative of the German HPC** (e.g., within PRACE)
- Chairman: Prof. Resch (HLRS), CEO: Dr. Claus Axel Müller
- Financial budget 2009-2014: 400 Mio. EUR
  200 Mio. Euro from the German Ministry for Education and Science (BMBF)
  200 Mio. Euro, one third from each involved local state NRW, BW, Bavaria

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HPC structure in Germany – Gauß Alliance

- One umbrella organization that brings together all German HPC centres, including
  - Tier-1 High Performance Computing Centres,
  - HPC centres at universities and research institutes
  - topical HPC centres like DWD and the German climate research centre

- Gauß Alliance established in December 2008

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Objective of the Gauß Alliance

- Promotion of the scientific topic "High Performance Computing" (HPC) towards to a key research component
- Set up the requirements for a sustainable and efficient use of the highest level High Performance Computing ressources
  - Coordination and use of synergie effects of the complement expertises and the diverse hardware architectures with their related access policies

- This is done in the time of IT-consolidation and cloud activities

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Coordination between HPC centres

- Germany has three centres to host top level HPC systems
- Each centre (also Tier-2) focusses on distinctive aspects of the scientific High Performance Computing (HPC)
- Coordination not only on technical level, but to also ensure the continuity of user support between the different levels
- Exploitation of new research groups and areas
- Coordination between Tier-1 and Tier-2 centres necessary
- Strategical coordination for a sustainable HPC infrastructure in Germany

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Different coordination levels

- The coordination process has to cover the following topics
  - project engineering
  - ensure the full supply of the customers and users
  - user support
  - task assignment between the different levels of the HPC pyramid
  - education and training for HPC and scientific computing
  - strategic procurement planning
  - guarantee service operation and data life cycle
- Agreement between the sites to support and implement the coordination process and its outcome

- Adequate form of organization for 10-20 different partners and their different aspects

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Mission of the Gauß Alliance

- education and training of HPC specialists
  - use and support of HPC ressources
  - modelling and programming on highly parallel machines; interface between administrators and domain scientists
  - research on HPC relevant topics like scalability and parallel paradigms

- German Competence Network with task and responsibility assignment between the members
- Need for education and research on HPC relevant topics; otherwise the capability of future systems will not be used efficiently

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Financial Situation of the Gauß-Alliance members

Gauss Centre for Supercomputing

- Via a project funding: ca. 400 Mio. EUR
  - For Hardware, operating costs, and third-party costs (office, Cebit etc.)
- additional technical support provided by the involved centres

Gauß Allianz without Gauß Centre for Supercomputing

- three topical centre (DWD, DKRZ, RZ MPG): Finance from BMBF, ...
- Other members: usually universities (budget via Art. 91b GG, Special call for High Performance Computer, 15 Mio EUR every 5 years, only hardware, no staff for service or support, no operational costs)

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Standardized review and approval process

- Quality-driven assignement of computing time on the highest levels of the HPC pyramid (Tier-0,1,2) is essentiell
- Coordinated review and approval process within the Gauss Centre for Supercomputing established
- Gauß Alliance: Investigation of the review processes on the different member sites
- Set up a central review and approval process in close collaboration with the Gauss Centre for Supercomputing for all Gauß Alliance members

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Recommendations for Efficient Usage

For an optimal and efficient use of hardware organized by a pyramid structure the following requirements in addition to the technical requirements have to be addressed:

- Arrangements for cooperative research and development programs that provide/ extend software with focus on scalability and usability for users and also administrators
  Actually there is a strong need for research on this topic, otherwise future systems will be underachieved
- Usage and operation of HPC systems need well trained specialists
- Close collaboration with industry for economical benefit of scientific computing

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Analysis

Imbalance between “racks” and “brains” hampers the efficient use of systems

Software in the applications is huge, complex – and badly prepared

The (non-)availability of highly performing simulation software gets more and more the enabler (or disabler) for leading science

No simple transfer of existing solutions – need for novel approaches

We are at a new era‘s eve – in the applications, in algorithm design, in software complexity, and, in particular, in system architectures (many-core)

Approaches in Germany so far address …

- mono-disciplinary domains (IN, MA, PH, ENG …) – important, but not sufficient
- single steps of the simulation pipeline (modelling, algorithms, implementation, software, data exploration), but do not take into account their interplay
- more applied than fundamental issues (HPC Software program of BMBF – wait for 4th round)

Huge potential for HPC applications in general (capability computing and capacity computing; in science, research, and industry)

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SPPEXA – Software for Exascale Computing

DFG's Priority Program 1648

Hans-Joachim Bungartz, Wolfgang E. Nagel

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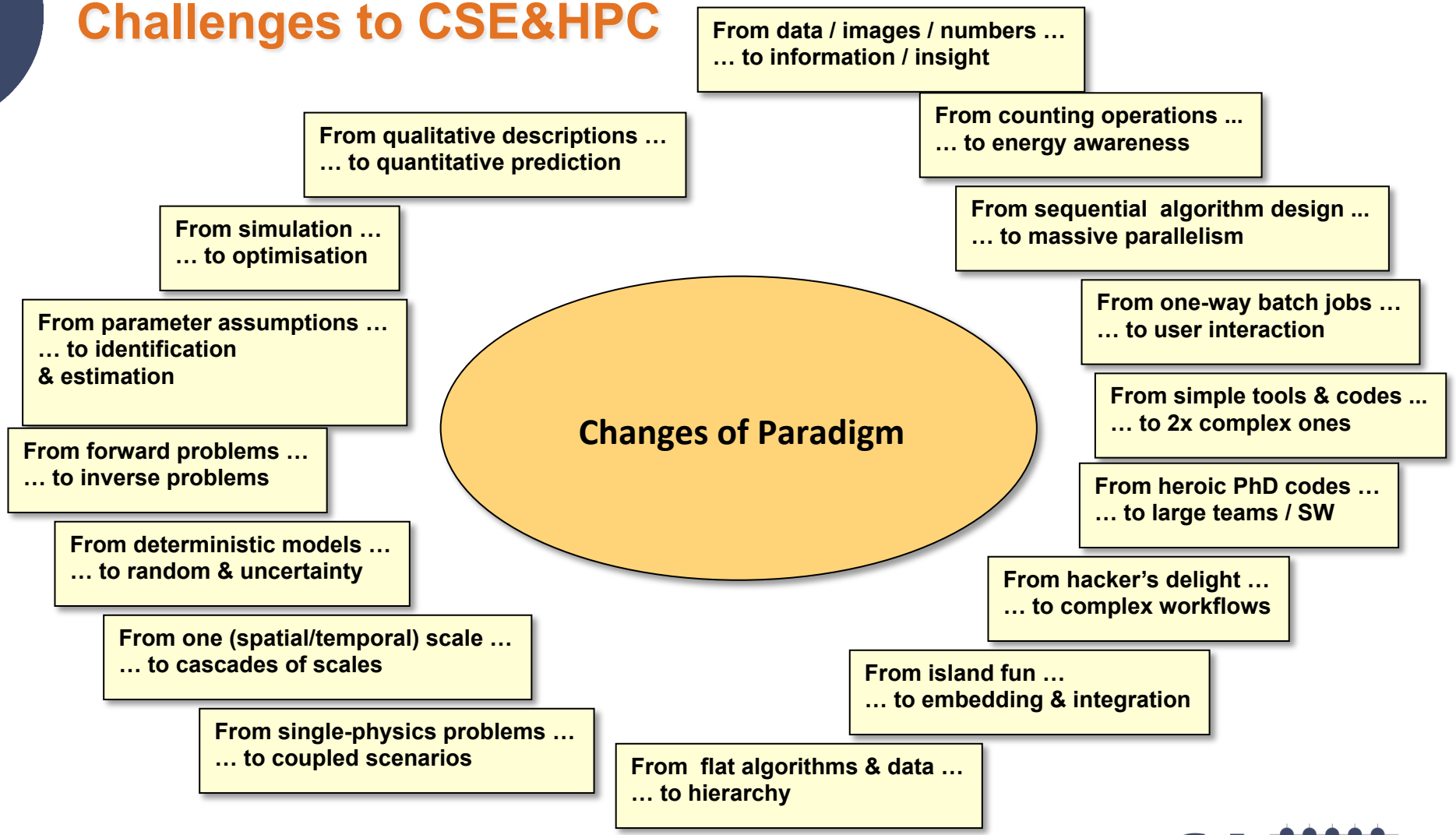
Challenges to CSE&HPC



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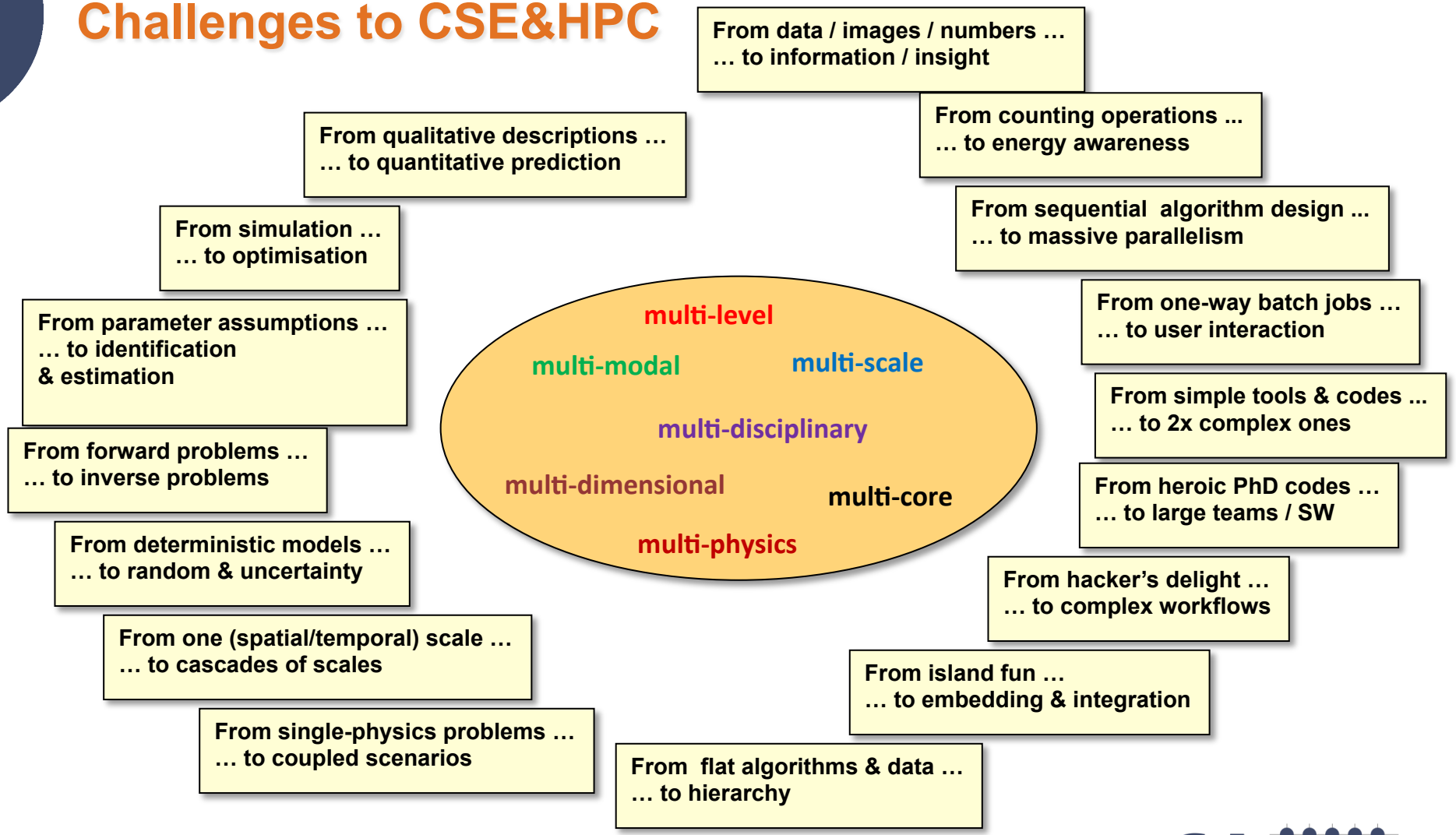
Challenges to CSE&HPC



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The Topics of SPPEXA (13 Funded Projects)

1. Computational Algorithms
2. System software
3. Application software
4. Data management and exploration
5. Programming
6. Software tools

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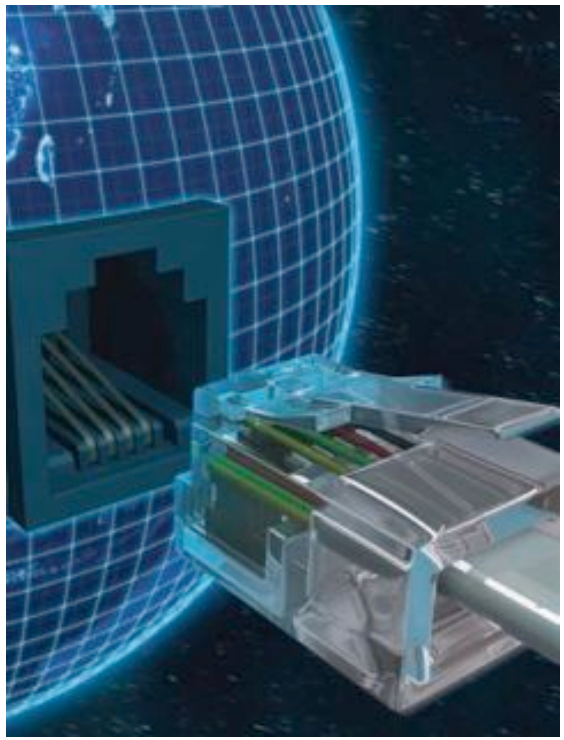
In Design: National HPC ressource portal

Ressource coordination (Tier-2 systems)

- Online portal for the use and support of HPC
- Classification by topical and/or topological aspects
- Documentable and transparent process
- Strategic effort to introduce HPC within small and medium sized companies as well as in “HPC-remote” research areas



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Conclusion

- With the increase of the technological challenges, methodical competences of HPC centers become more and more important:
  - Users need support for hybrid parallel programming (CPU and accelerators) and support for porting their applications to specialized hardware like BlueGene/Q
  - Access to resources (Grid, cloud, clusters)
  - Visualization and data-intensive computing
  - Tools for application optimization on highly parallel systems
- Algorithmic and methodical work are key components for success
- Close coordination between centers is inevitable

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