


HPC AND LARGE SCALE INSTRUMENTS – FZ JÜLICH'S VIEW

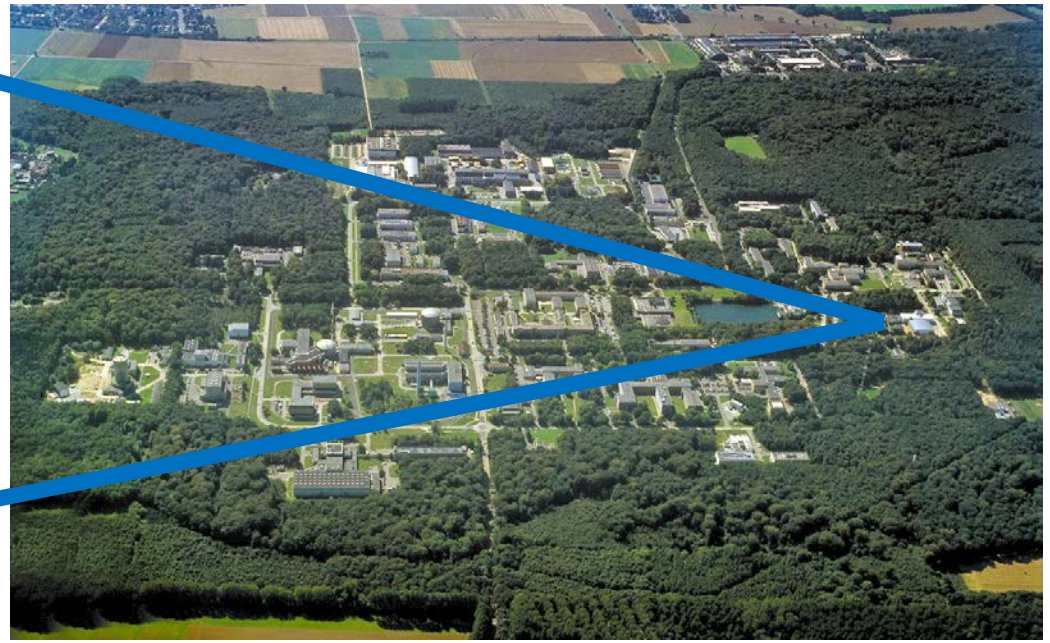
6th Scientific Computing Forum, CERN

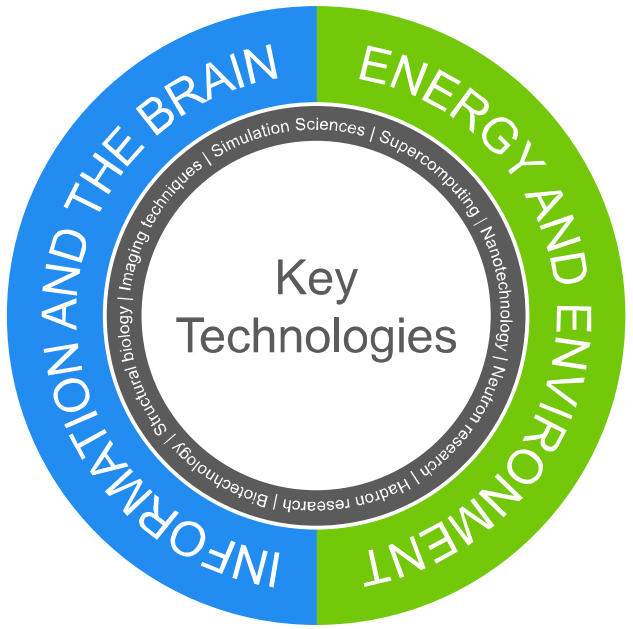
FEBRUARY 25, 2019 I THOMAS EICKERMANN, JSC

JÜLICH Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

FZJ AND JSC AT A GLANCE

FORSCHUNGSZENTRUM JÜLICH BY NUMBERS





- **Budget:** 610 Mio €,
  including 245 Mio € third party funding
  100 Horizon 2020 projects, 420 national projects
- **Employees:** 5.900
  incl. 1.950 scientists including PhD students
  800 guest scientists from 75 countries
- **Publications:** 2.450
  (source: fact sheet 2017)

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

JÜLICH SUPERCOMPUTING CENTRE (JSC)

Facts and Figures

Staff:

220 Total (185 FTE)

160 Scientists

13 PhD Students (+13 external)

Budget:

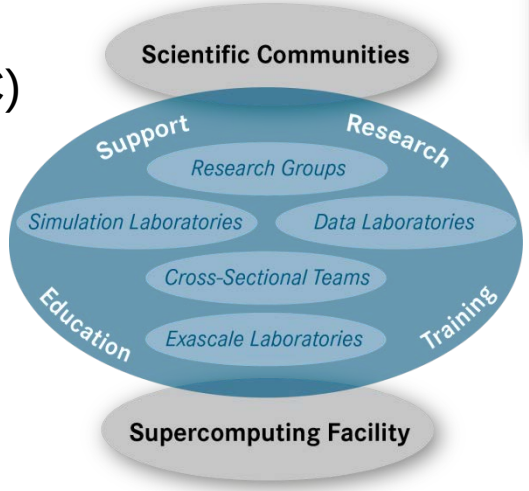
30 Mio. € Institutional Funding (PoF)

15 Mio. € Third Party Funding

JÜLICH SUPERCOMPUTING CENTRE AT A GLANCE

Supercomputer operation for

- Centre – FZJ
- Region – RWTH Aachen University
- Germany – Gauss Centre for Supercomputing (GCS)
  John von Neumann Institute for Computing (NIC)
- Europe – PRACE, EU projects



Application support

- Unique support & research environment at JSC
- Peer review support and coordination

R&D work

- Methods and algorithms, computational science, performance analysis and tools
- Scientific Big Data Analytics with HPC
- Computer architectures, Co-Design, Exascale Labs together with IBM, Intel, NVIDIA

DEEP

Education and training

SUPERCOMPUTER STRATEGY

JÜLICH Forschungszentrum
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JSC‘S ARCHITECTURE STRATEGY - RATIONALE

Dilemma #1

- Grand Challenge applications require extreme performance
- Not achievable with general purpose architectures (x86 Clusters): Cost, Energy
- Highly scalable architectures not suitable for applications requiring high single node performance, large memory per core

Solution: Dual architecture approach

- JUQUEEN - highly scalable system
- JUROPA / JURECA Cluster – general purpose system
- Common Storage

COMPUTER ROADMAP

DUAL ARCHITECTURE

IBM Power 4+
JUMP (2004), 9 TFlop/s

IBM Power 6
JUMP, 9 TFlop/s

JUROPA
200 TFlop/s
HPC-FF
100 TFlop/s

IBM Blue Gene/L
JUBL, 45 TFlop/s

IBM Blue Gene/P
JUGENE, 1 PFlop/s

IBM Blue Gene/Q
JUQUEEN (2012)
5.9 PFlop/s

JURECA Cluster
(2015) 2.2 PFlop/s

JUST Gen 4:
20 PB raw

General Purpose Cluster

Highly scalable

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Dilemma #2

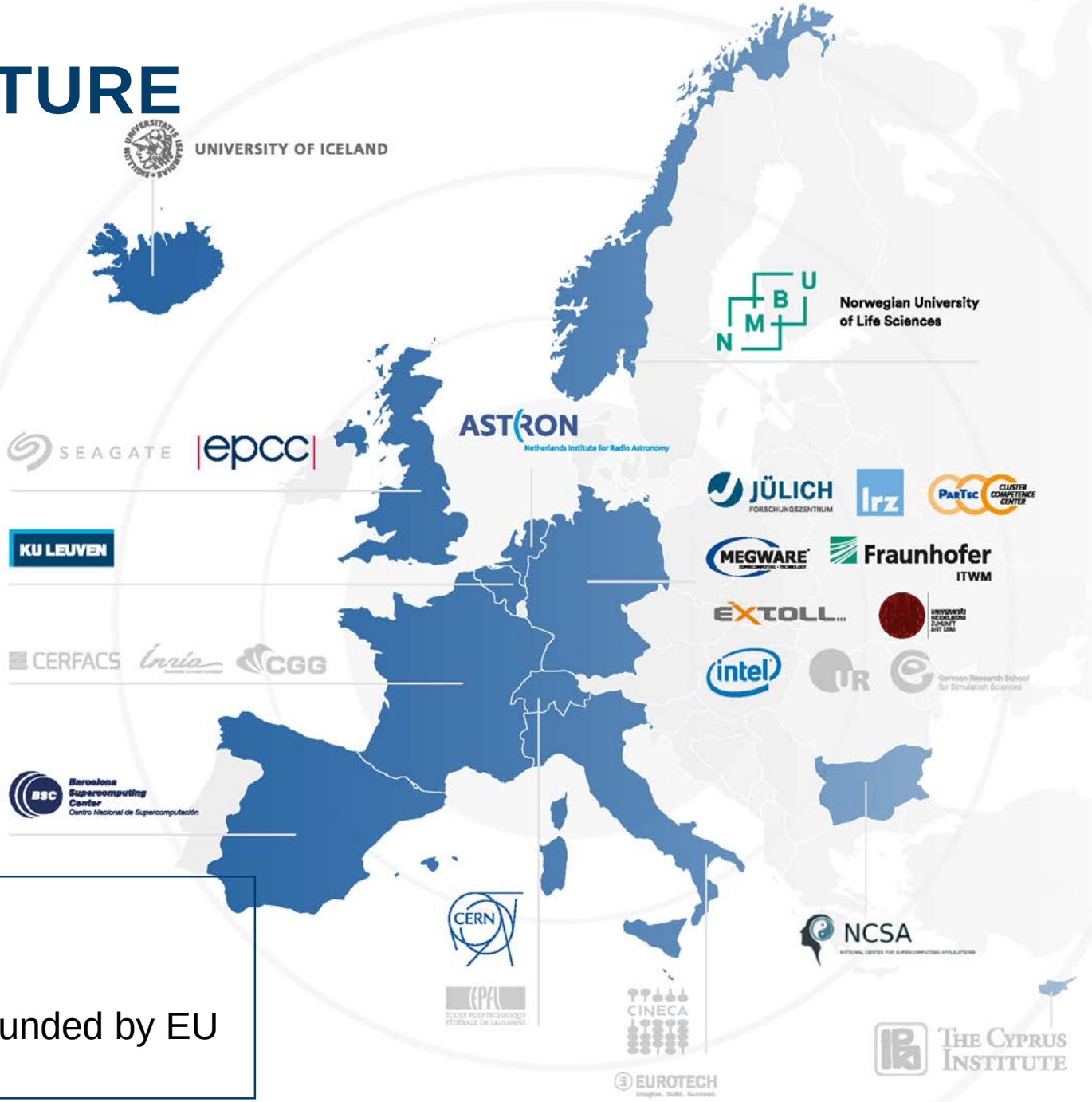
- Parts of complex applications or workflows often have different requirements and scalability properties
- Heterogeneous architectures / clusters with accelerators: static ratio of CPU / Accelerator performance potentially wastes resources and energy

Solution: Modular computing

- Separation of CPU (Cluster) and highly scalable Accelerator (Booster, e.g. GPU-centric system) allows dynamic resource allocation to optimize resource utilization
- Requires substantial application modifications

A EUROPEAN ARCHITECTURE

The DEEP Projects



SEVENTH FRAMEWORK PROGRAMME

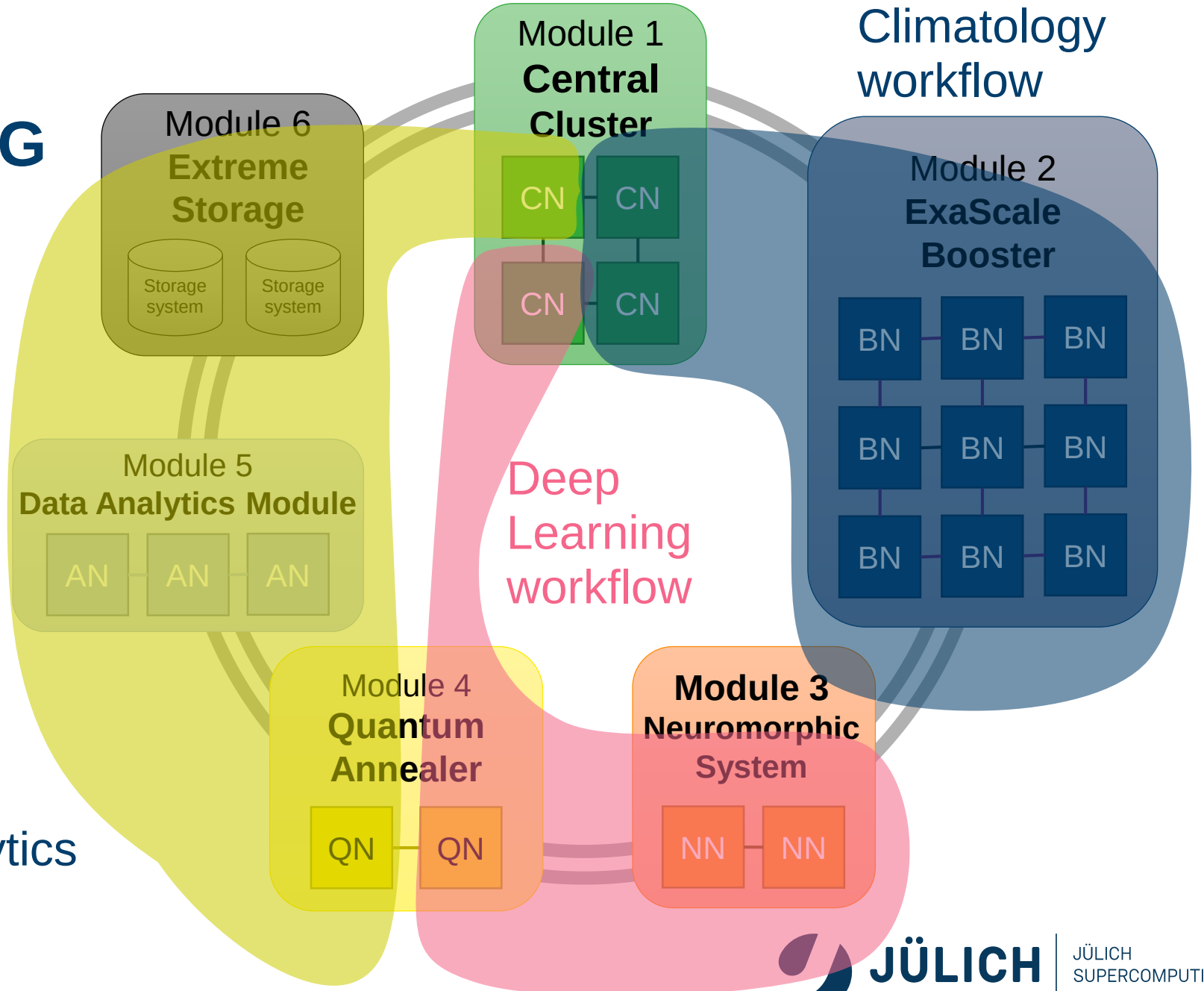
Mitglied der Helmholtz-Gemeinschaft

www.deep-project.eu

- 20 Partners
- 45 Mio € EU
- 30 Mio € EU funded by EU

MODULAR SUPERCOMPUTING

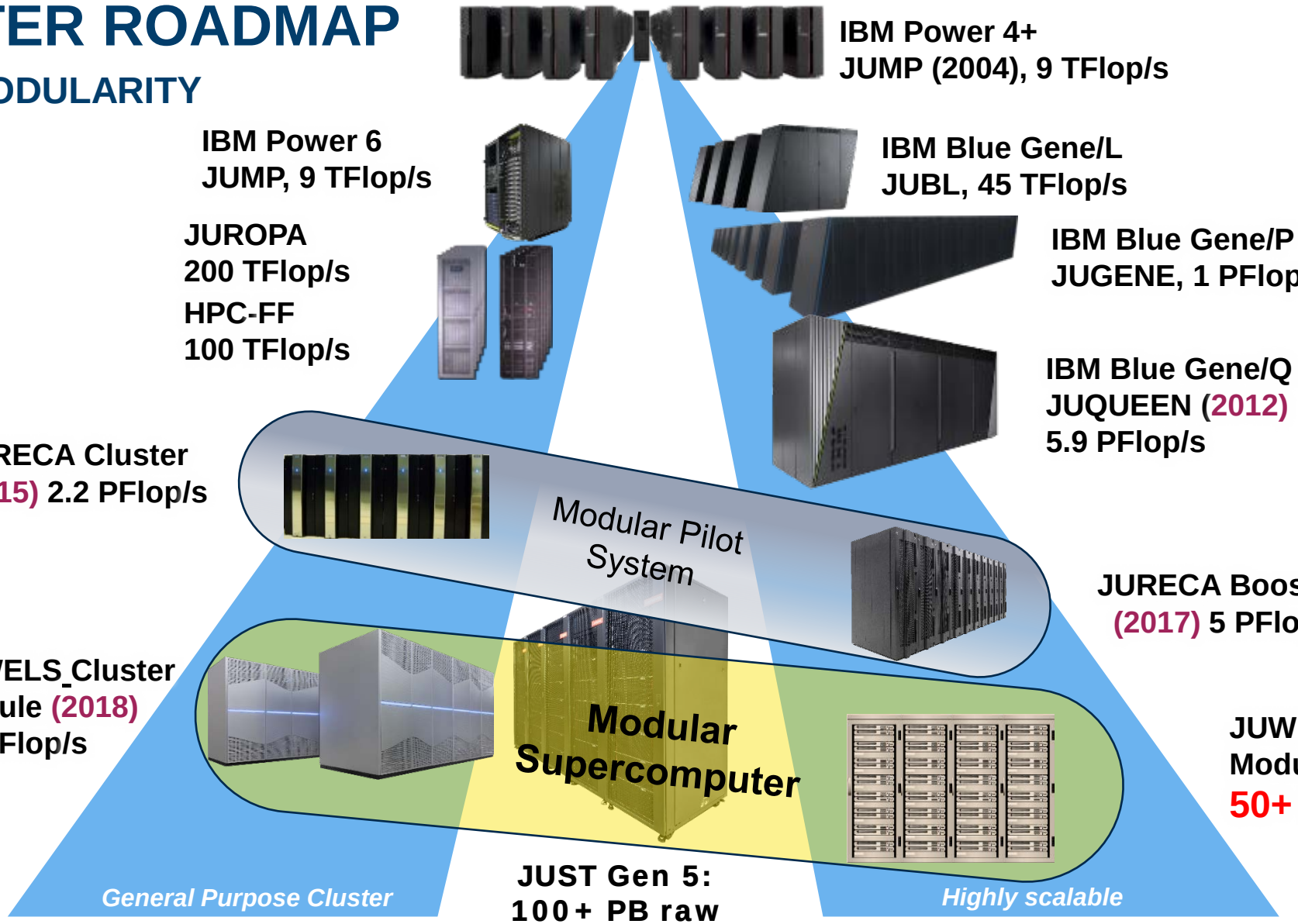
Smart Exascale



HBP
Data Analytics workflow

COMPUTER ROADMAP

TOWARDS MODULARITY



Position 23
in June 2018,
Module I

HPC AND LARGE SCALE INSTRUMENTS

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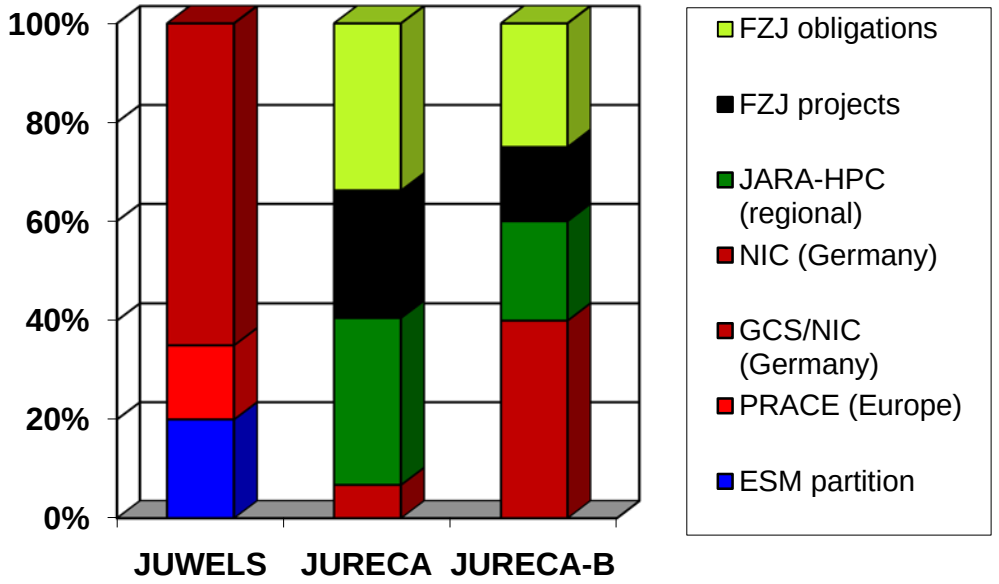
OPPORTUNITIES AND CHALLENGES

Opportunities

- HPC systems provide vast amounts of compute capability and capacity
- HPC centres usually operate high-performance and large capacity storage resources
- Tier-0 / Tier-1 HPC centres typically have excellent NREN / GÉANT connectivity

Challenges

- HPC Systems are optimized for HPC not HTC
  - Applications / workflows may need adaptation
- Existing systems are fully committed and utilized
- Deployment and mode of operation may not be well adapted to requirements of large scale instruments:
  - 1 year project allocations based on Peer Review
    – long-term programme requirements
  - Batch mode with varying turnaround times
    – QoS / near-realtime requirements
  - Compute nodes without Internet Access
    – Access to remote data during runtime



ADDRESSING THE CHALLENGES #1: PILOTS

Demonstrators / Pilot Projects

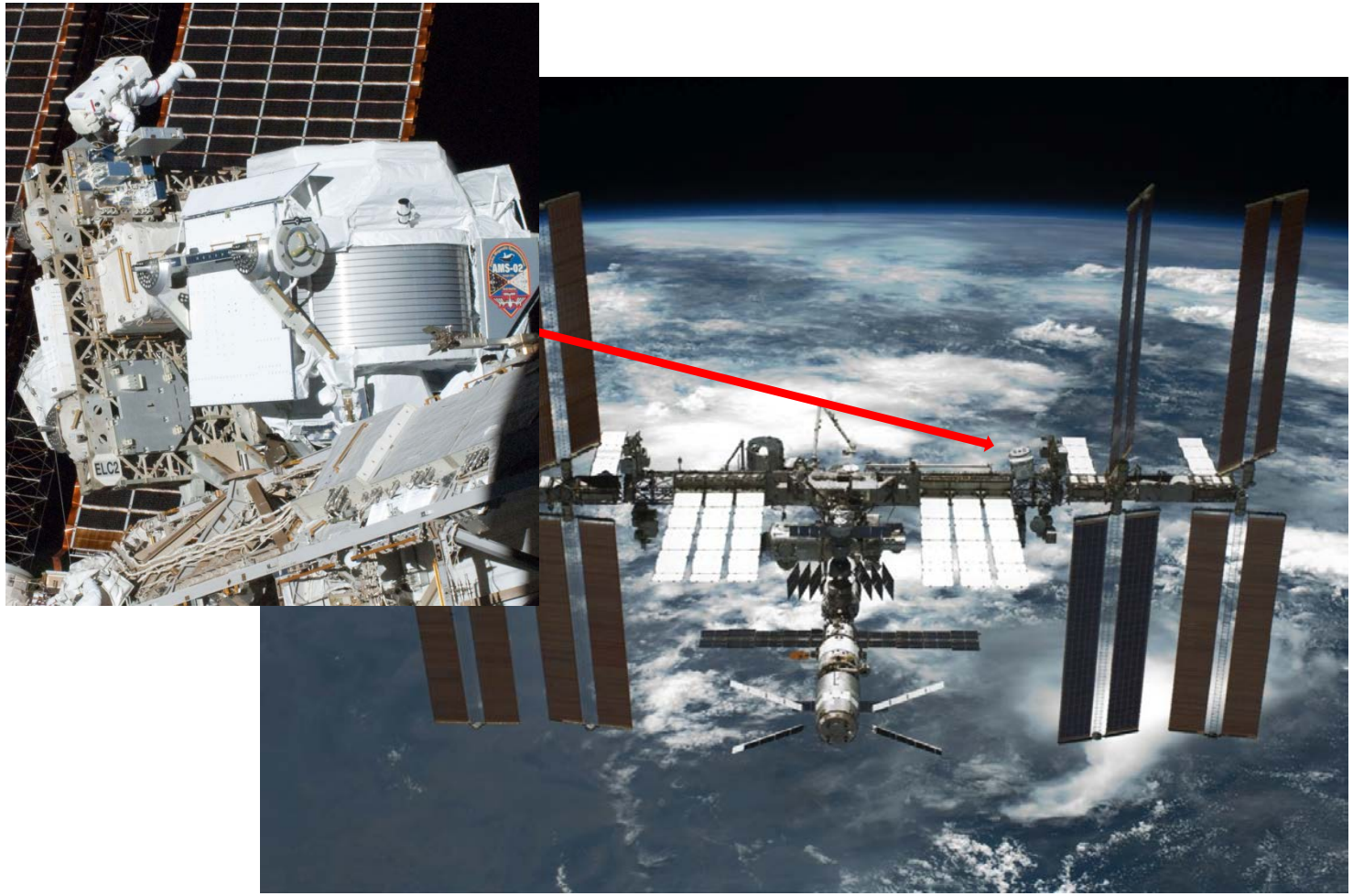
- Address technical challenges and demonstrate feasibility on a small scale
- Postpone policy and financial questions until added value has been proven

PRACE link with Large Scale Scientific Instruments (F.Berberich at CERN on Oct. 22nd, 2018)

- PRACE-5IP Pilot with European Synchrotron Radiation Facility (ESRF)
  - Application Use Cases: Simulation and Data Processing
  - Moderate resource requirement: 256 cores x 2-3 month ~ 500 T core-hours
  - Executed at PSNC (CPU cluster) and MPCDF (GPU cluster)
- First results
  - CPU cluster well suited for use case
  - PRACE's user support beneficial for porting codes and adapting environment to the codes
- **Another Pilot in preparation between CERN and PRACE-6IP**

COSMIC-RAY RESEARCH ON THE ISS – AMS-02

A Production-Level Use-Case at JSC: Alpha Magnetic Spectrometer



- Multi-purpose cosmic-ray detector installed on the ISS
- Indirect search for dark matter and detection of cosmic antimatter as main objectives
- **JSC provides compute and data facilities to support the data analysis of the AMS partner RWTH Aachen (Prof. Dr. S. Schael)**

DATA FLOW AND DATA PROCESSING

Raw Data

DB
CERN

Raw Data

ROOT Files

ROOT Files

ACQT Files

Raw Data
40 TB p.a.
ROOT Files
ca. 160 TB p.a.
ACQT Files
ca. 20 TB p.a.

ADDRESSING THE CHALLENGES #2: PARTIALLY DEDICATED RESOURCES

Use Case Characteristics

- Multi-year project: AMS in operation since 2011; new cooling system planned for 2019
- Plannable IT-resources: data transfer, compute and storage requirements, campaign-oriented mode of operation

JUAMS: dedicated 2000-core CPU Cluster at JSC

- Jointly funded by FZ Jülich and AMS-researchers at RWTH
- Access to JSC's HPC-storage, currently using 2,5 PB
- Leveraging:
  - High-performance Filesystem Access via MPI
  - Plannable (dedicated) CPU capacity, 100% utilized: competitive turnaround times
- JUAMS will be replaced in 2019, new system will be tailored for AMS requirements (same compute, 5 PB)

CLAIX: Tier-2 HPC system at RWTH Aachen

- Relying on project resources granted in competitive Peer Review process via JARA-HPC (11.4 Mio. Core-h recently)
- Leveraging direct access of compute nodes to Internet (Data at CERN)

SUMMARY AND CONCLUSIONS

HPC Trends

- Single core performance gain is slowing down – need to increase level of parallelism
- Accelerators such as GPUs help improving performance / Watt & performance / Euro
- Modular Computing is JSC's approach to address scalability limitations

HPC and Large Scientific Instruments

- HPC can help to address compute demand of large scale instruments
- Challenges
  - Technical: adaptation of applications and workflows
  - When leveraging existing resources at HPC centres: deployment, mode of operation, access policy, …
- There are success stories showing that these challenges can be overcome