JÜLICH SUPERCOMPUTING CENTRE (JSC) INTRODUCTION

NOV 20, 2023 I BERND MOHR

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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 – EuroHPC JU, EU projects
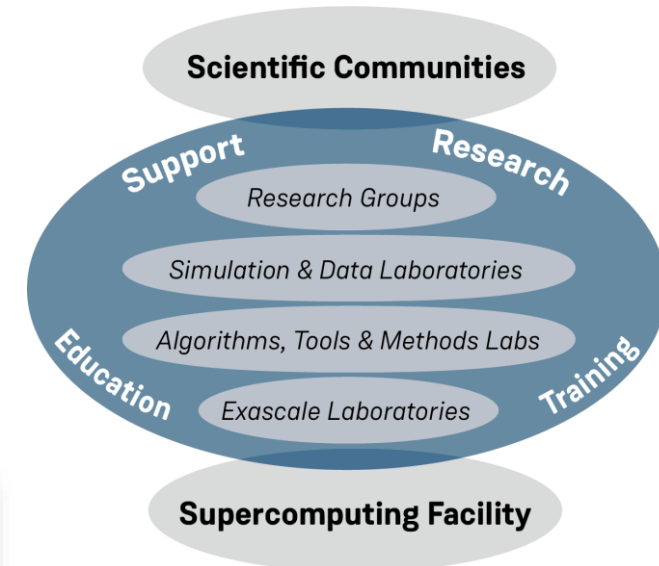- **Application support**
  - Unique support & research environment at JSC
  - Peer review support and coordination
- **R&D work**
  - Methods and algorithms, computational science, performance analysis and tools
  - Scientific Big Data Analytics with HPC
  - Computer architectures, Co-Design, Modularity, Exascale Labs together with IBM, Intel, NVIDIA
- **Education and training**

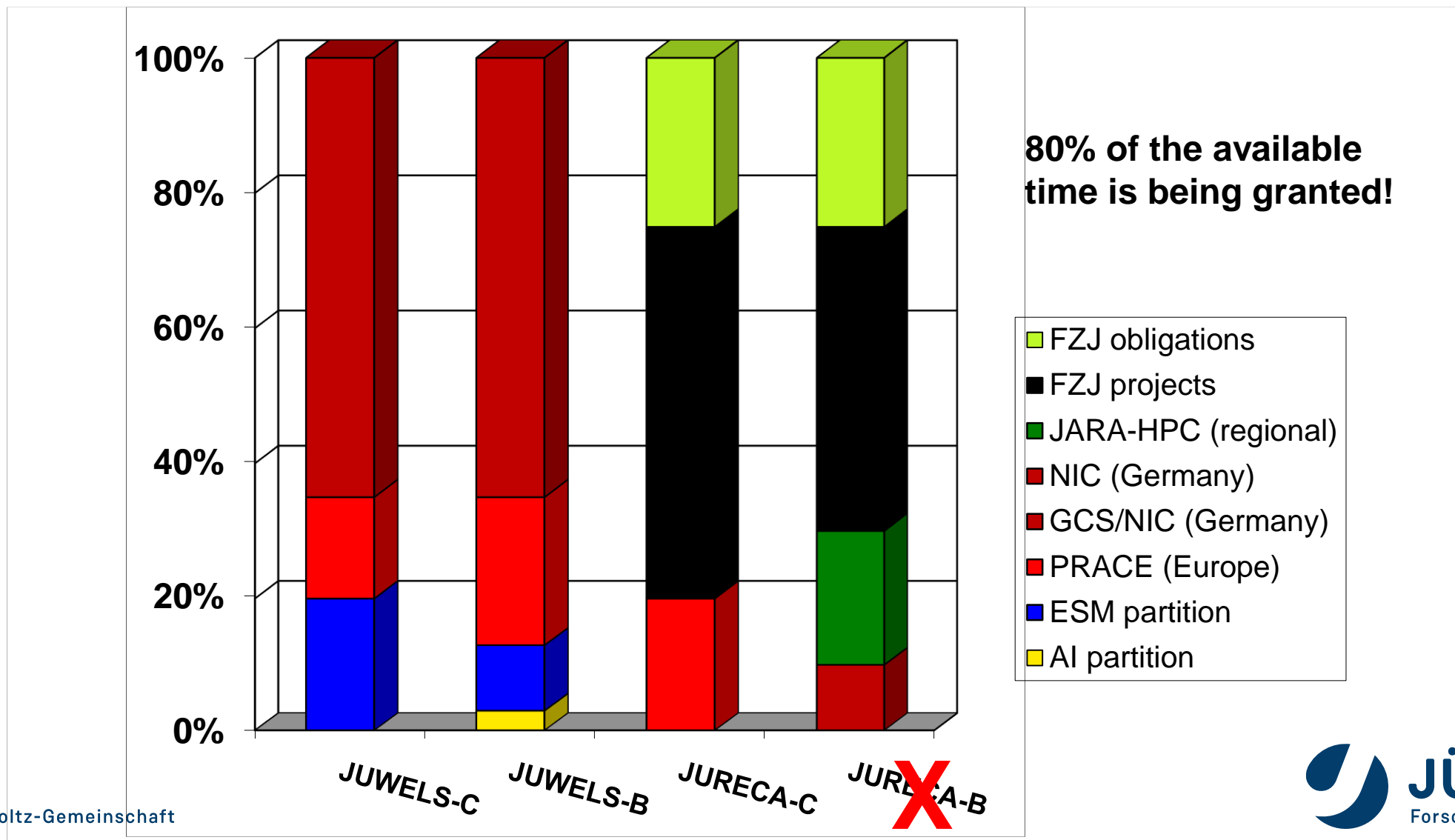# ACCESS TO SUPERCOMPUTING RESOURCES AT JÜLICH

- **Access to JUWELS through biannual Call for Proposals (CfP) via**

  - Gauss Centre for Supercomputing (GCS)
    (JUWELS compute time proposals are evaluated by NIC);
    Large-scale project: >= 2% of expected annual compute power of the total system (cluster + booster)

  - ESM partition for Earth System scientists only (20% of JUWELS Cluster and 10% of JUWELS Booster)
  - AI partition (~2% of JUWELS Booster only)

- **Access to JURECA through biannual CfP via**

  - JARA-HPC Vergabegremium (VGG) for FZJ and RWTH staff members only (JARA-HPC Partition on
    JURECA Booster and D-Wave system JUPSI) and/or Kommission zur Vergabe von SC Ressourcen (VSR)

  - John von Neumann Institute for Computing (NIC)
    - on JURECA Booster (only temporarily)

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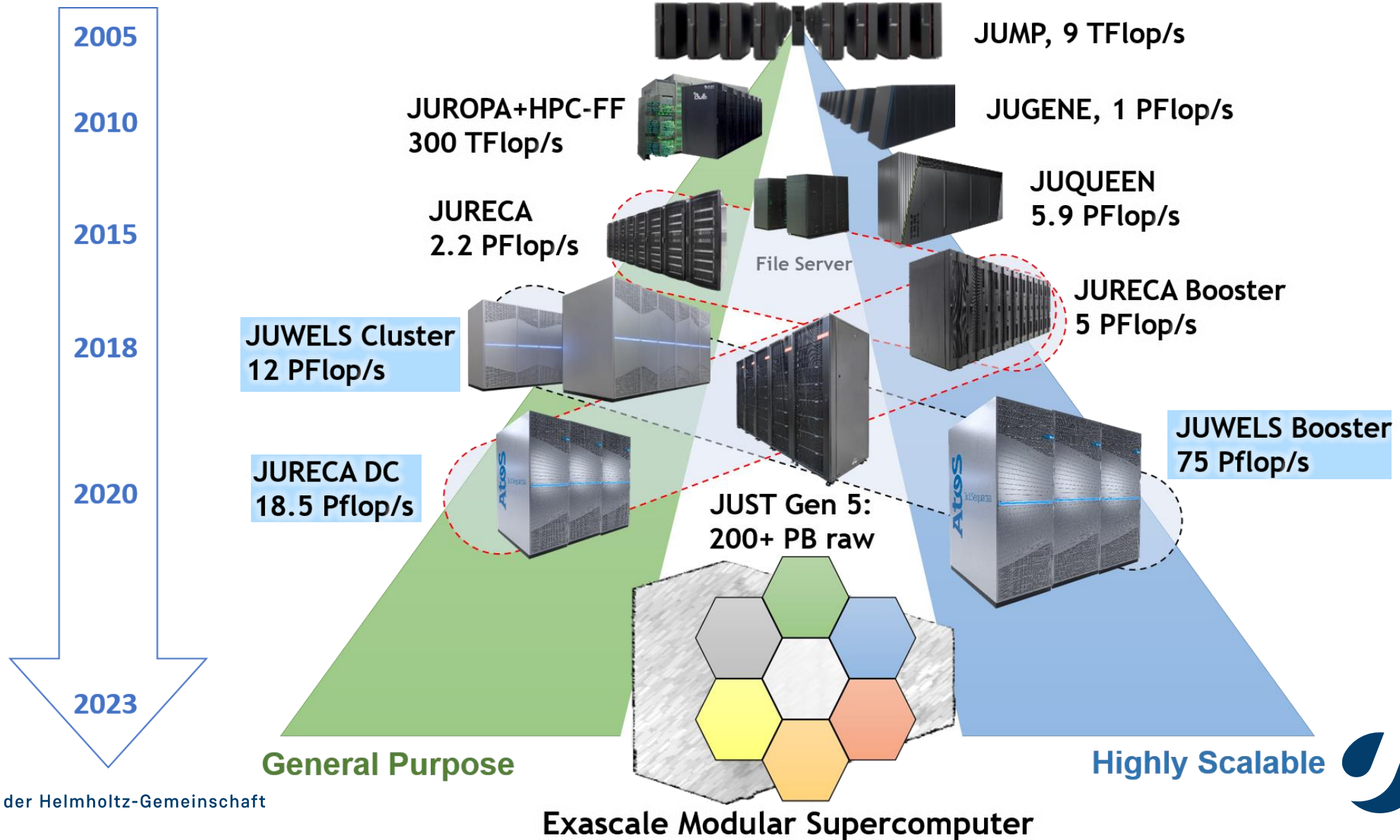
GAUSS CENTRE FOR SUPERCOMPUTING (GCS)

- **GCS is the leading Tier-0 HPC centre in Europe**

  - Alliance of the three German Tier-1 centres
  - High Performance Computing Centre Stuttgart (HLRS)
  - Jülich Supercomputing Centre (JSC)
  - Leibniz Rechenzentrum (LRZ), Garching

- **Key facts**

  - To date in sum more than 140 Petaflops (continuously expanding)
  - 600 people for operation, HPC R&D, services, training
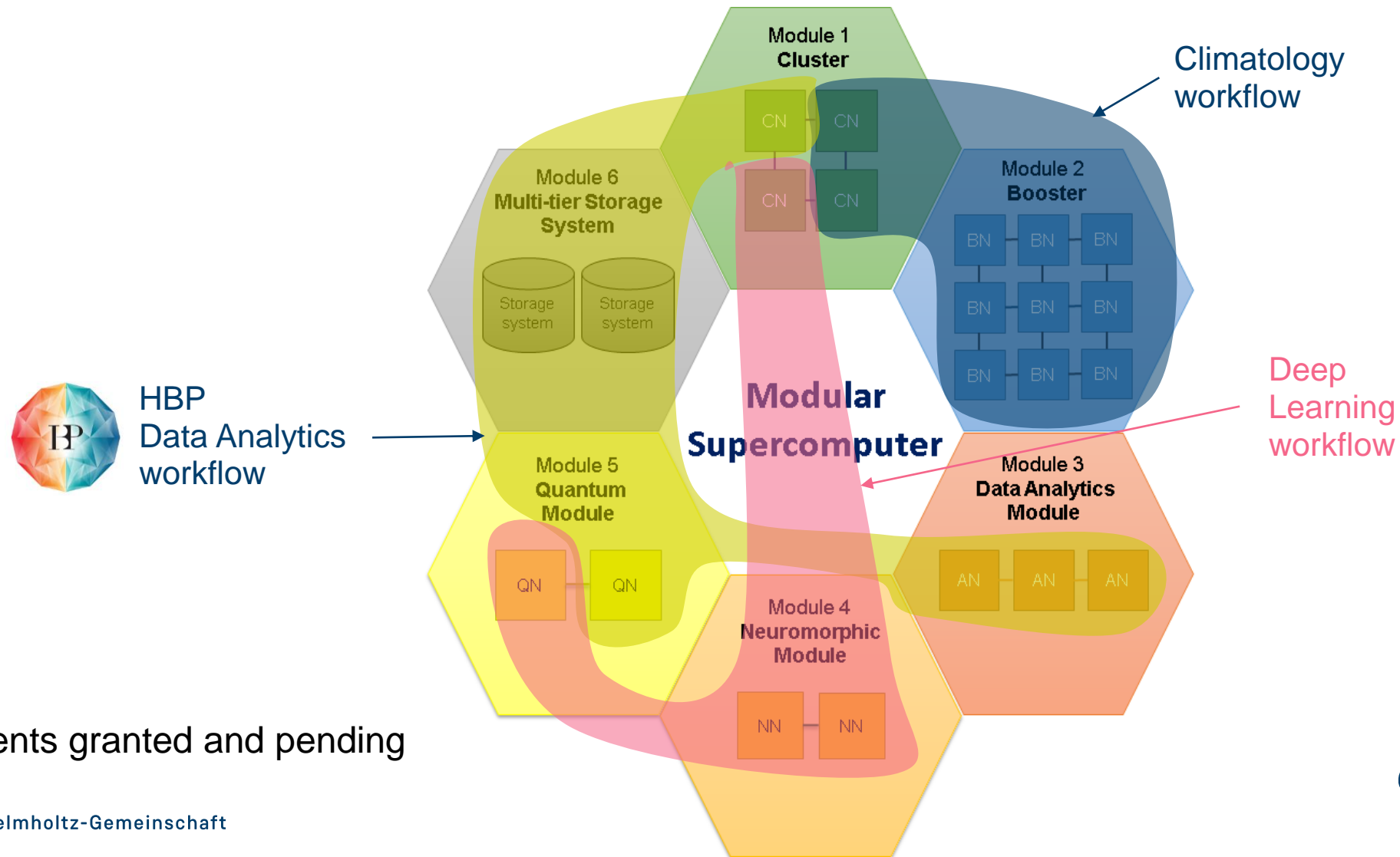 - Extensive know-how in key scientific fields

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STAKEHOLDER'S COMPUTE TIME SHARES

80% of the available time is being granted!

Legend:
- FZJ obligations
- FZJ projects
- JARA-HPC (regional)
- NIC (Germany)
- GCS/NIC (Germany)
- PRACE (Europe)
- ESM partition
- AI partition

Categories: JUWELS-C, JUWELS-B, JURECA-C, JURECA-B

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(DUAL) HARDWARE STRATEGY AT JSC

Exascale Modular Supercomputer

General Purpose

Highly Scalable

2005 — JUMP, 9 TFlop/s

2010 — JUROPA+HPC-FF 300 TFlop/s — JUGENE, 1 PFlop/s

2015 — JURECA 2.2 PFlop/s — JUQUEEN 5.9 PFlop/s

File Server

JUWELS Cluster 12 PFlop/s — JURECA Booster 5 PFlop/s

2018

2020 — JURECA DC 18.5 Pflop/s — JUST Gen 5: 200+ PB raw — JUWELS Booster 75 Pflop/s

2023

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JUWELS @ FZJ/JSC:
CLUSTER AND BOOSTER MODULE IN PRODUCTION

… AND EVOLUTION TO A
MODULAR SUPERCOMPUTING ARCHITECTURE

Module 1
Cluster

CN   CN
CN   CN

Climatology
workflow

Module 6
Multi-tier Storage
System

Storage
system
Storage
system

Module 2
Booster

BN   BN   BN
BN   BN   BN
BN   BN   BN

HBP
Data Analytics
workflow

Modular
Supercomputer

Deep
Learning
workflow

Module 5
Quantum
Module

QN   QN

Module 3
Data Analytics
Module

AN   AN   AN

Module 4
Neuromorphic
Module

NN   NN

*Patents granted and pending

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RESEARCH FIELDS ON JUWELS (CLUSTER + BOOSTER)
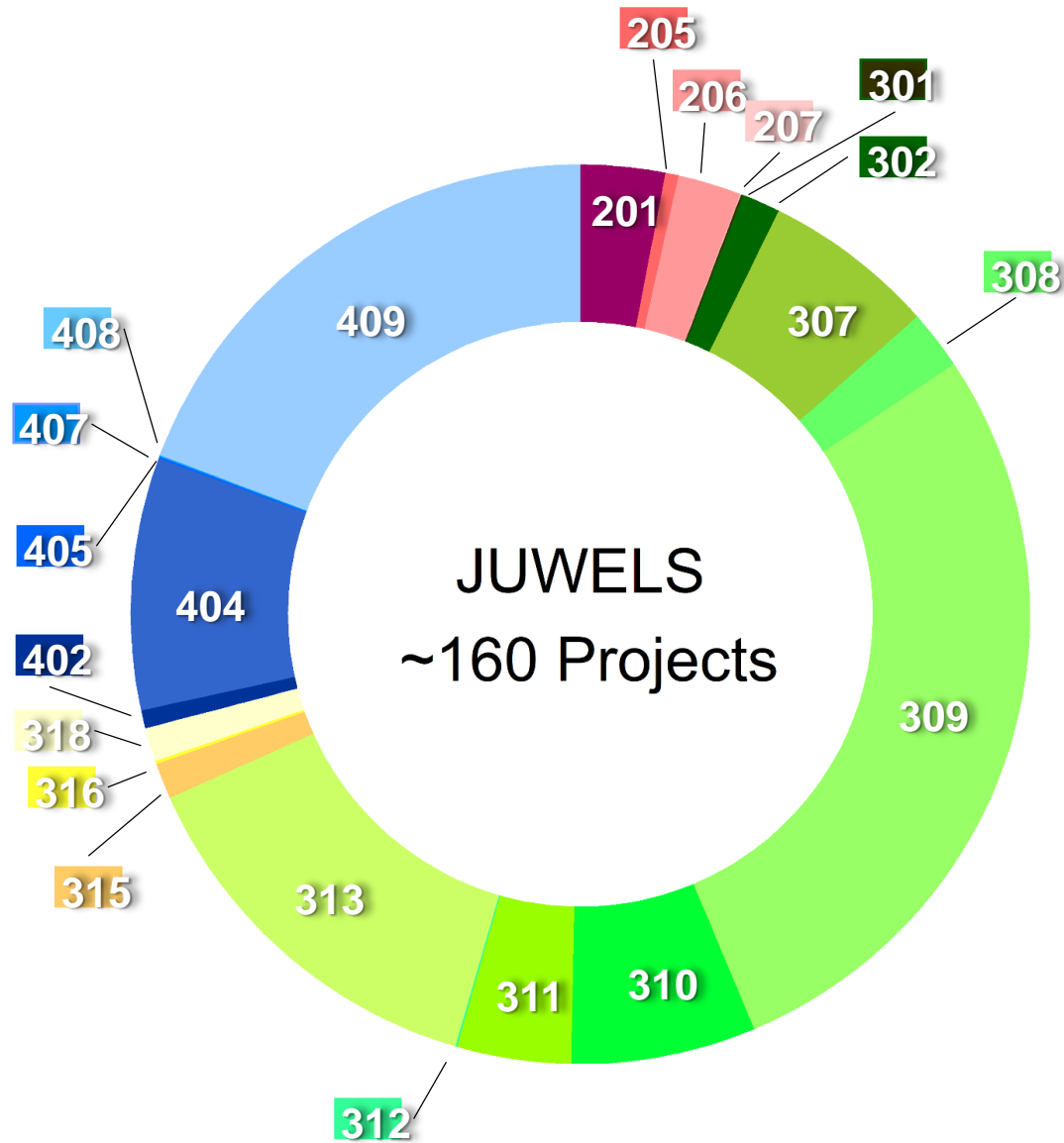
Reseach Fields

201	Basic Biological and Medical Research
205	Medicine
206	Neurosciences
207	Agriculture, Forestry and Veterinary Medicine
301	Molecular Chemistry
302	Chemical Solid State and Surface Research
307	Condensed Matter Physics
308	Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
309	Particles, Nuclei and Fields
310	Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
311	Astrophysics and Astronomy
312	Mathematics
313	Atmospheric Science, Oceanography and Climate Research
315	Geophysics and Geodesy
316	Geochemistry, Mineralogy and Crystallography
318	Water Research
402	Mechanics and Constructive Mechanical Engineering
404	Heat Energy Technology, Thermal Machines, Fluid Mechanics
405	Materials Engineering
407	Systems Engineering
408	Electrical Engineering and Information Technology
409	Computer Science

JUWELS
~160 Projects

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RESEARCH FIELDS ON JURECA (CLUSTER)

JURECA
~75 Projects
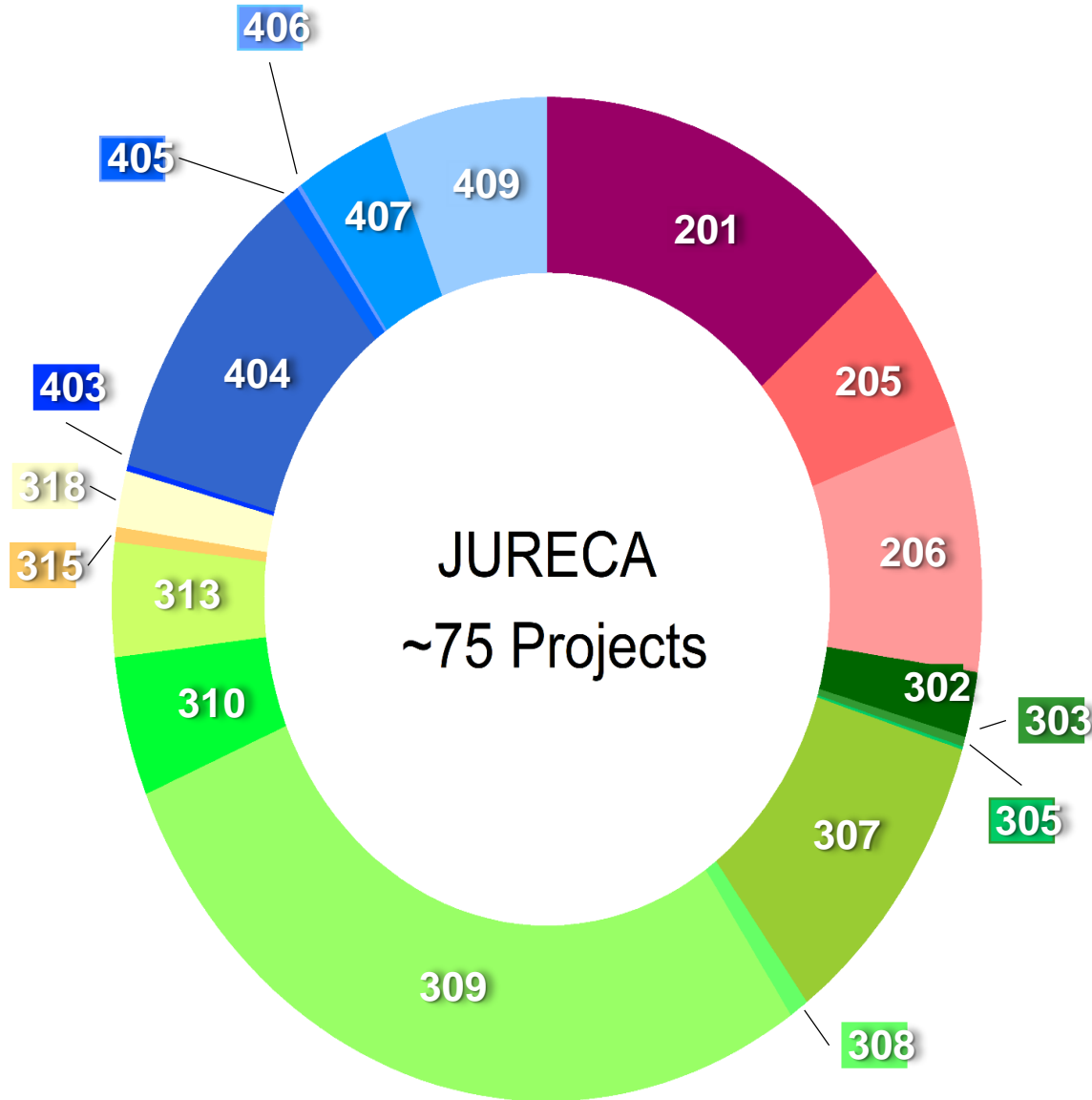
Research Fields

20	Basic Biological and Medical Research
20	Medicine
20	Neurosciences
60	Chemical Solid State and Surface Research
30	Physical and Theoretical Chemistry
30	Biological Chemistry and Food Chemistry
50	Condensed Matter Physics
30	Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
80	Particles, Nuclei and Fields
91	Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
61	Atmospheric Science, Oceanography and Climate Research
31	Geophysics and Geodesy
51	Water Research
40	Process Engineering, Technical Chemistry
30	Heat Energy Technology, Thermal Machines, Fluid Mechanics
40	Materials Engineering
40	Materials Science
60	Systems Engineering
40	Computer Science

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Mitglied der Helmholtz-Gemeinschaft

NATIONAL AND EUROPEAN USER GROUPS

Legend:
- Biology
- Medicine
- Agriculture, Forestry and Veterinary Medicine
- Chemistry
- Physics
- Mathematics
- Geosciences
- Mechanical and Industrial Engineering
- Thermal Engineering/Process Engineering
- Materials Science and Engineering
- Computer Science, System and Electrical Engineering
- Construction Engineering and Architecture

ICEI/Fenix RI

- Proposals for computer time accepted from Germany and Europe
- Peer review by international referees
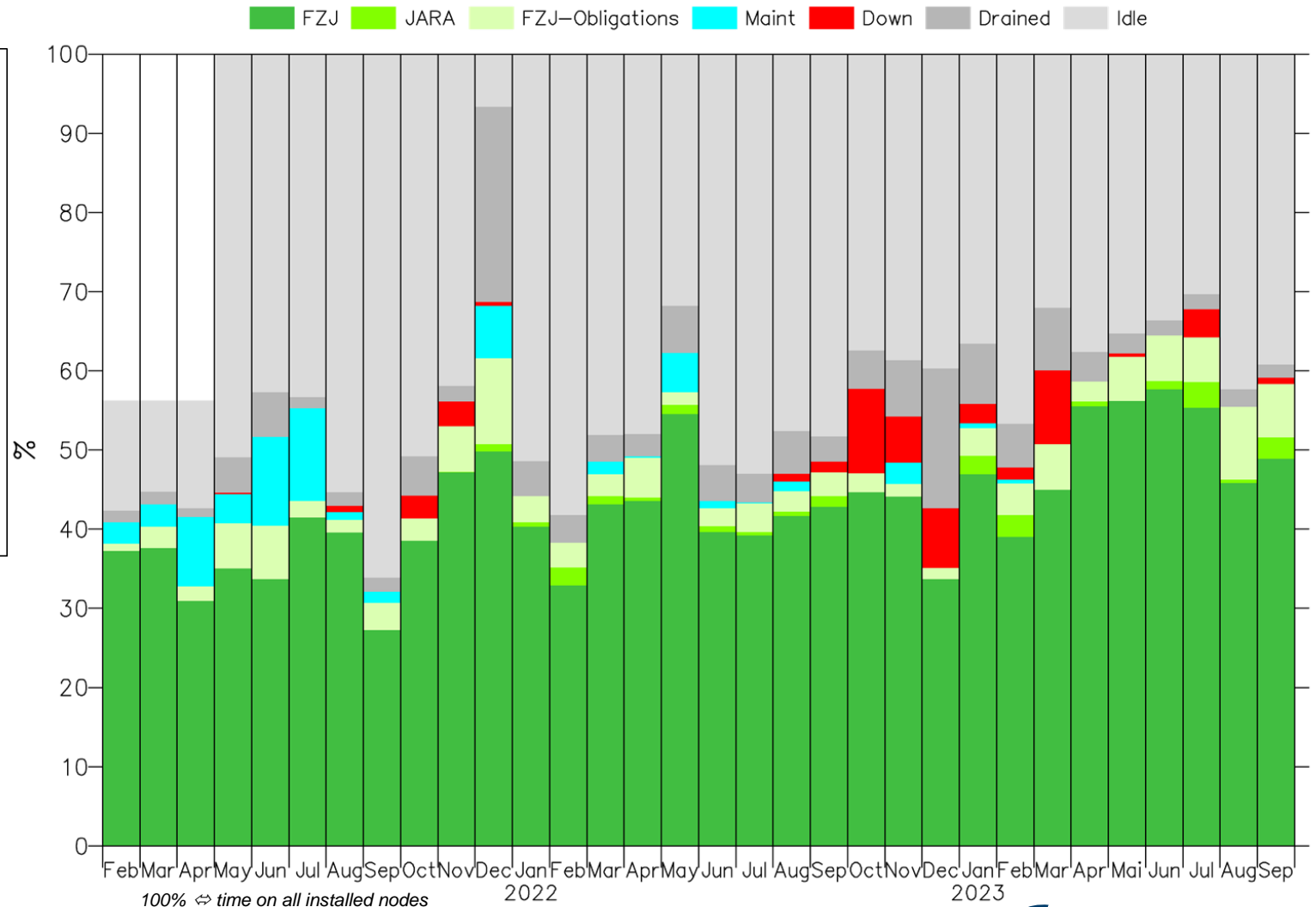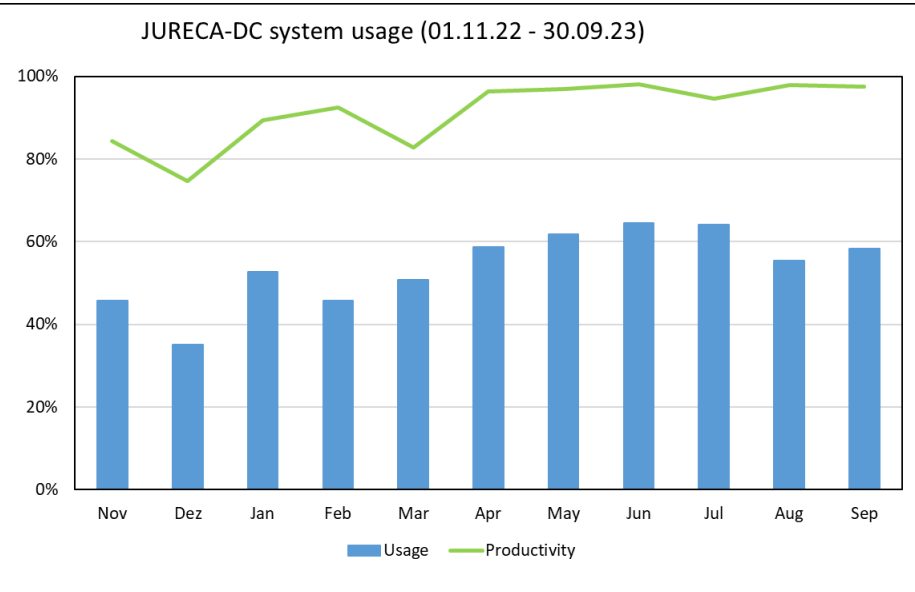- CPU time is granted by independent Scientific Councils

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JUWELS CLUSTER USAGE
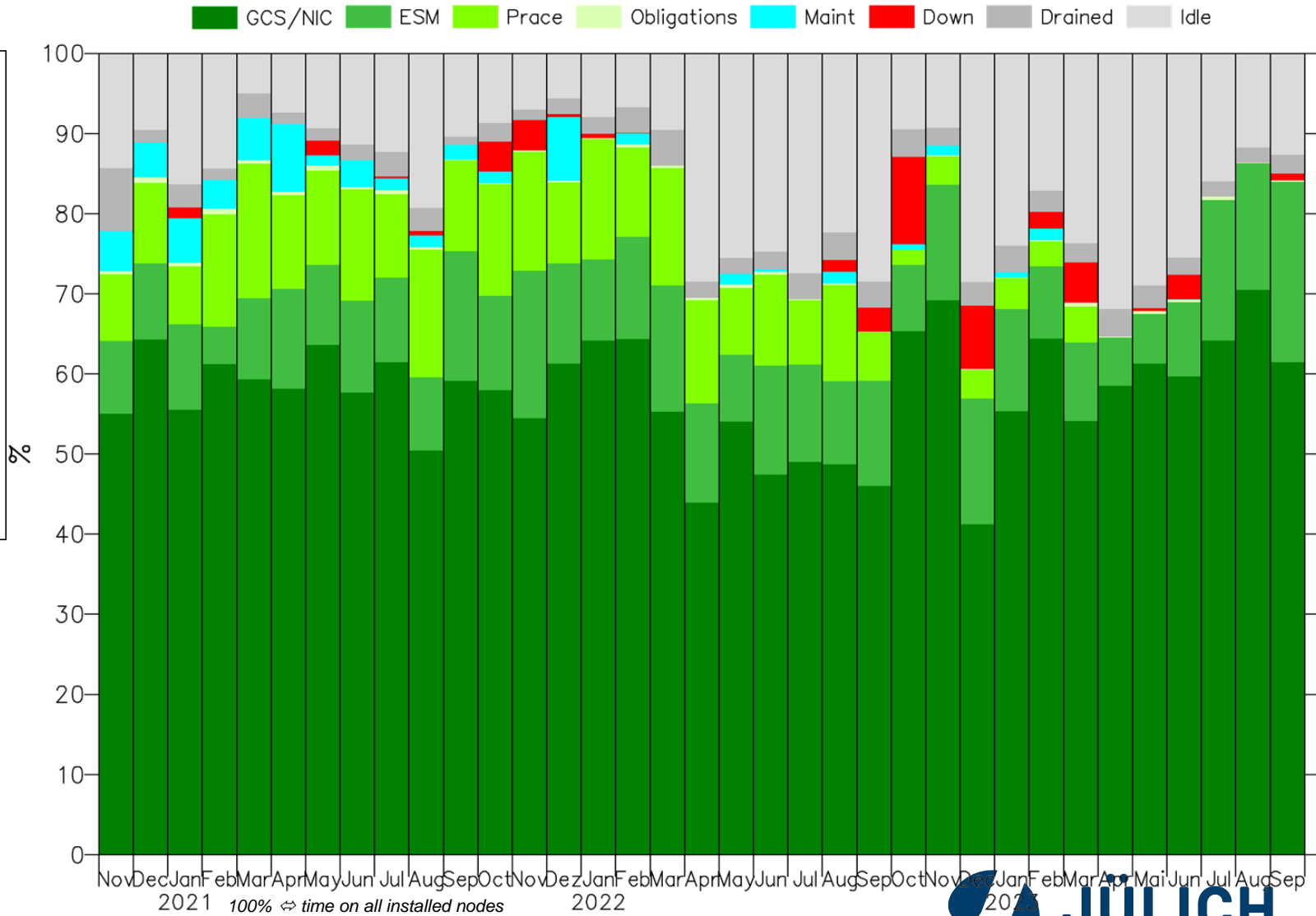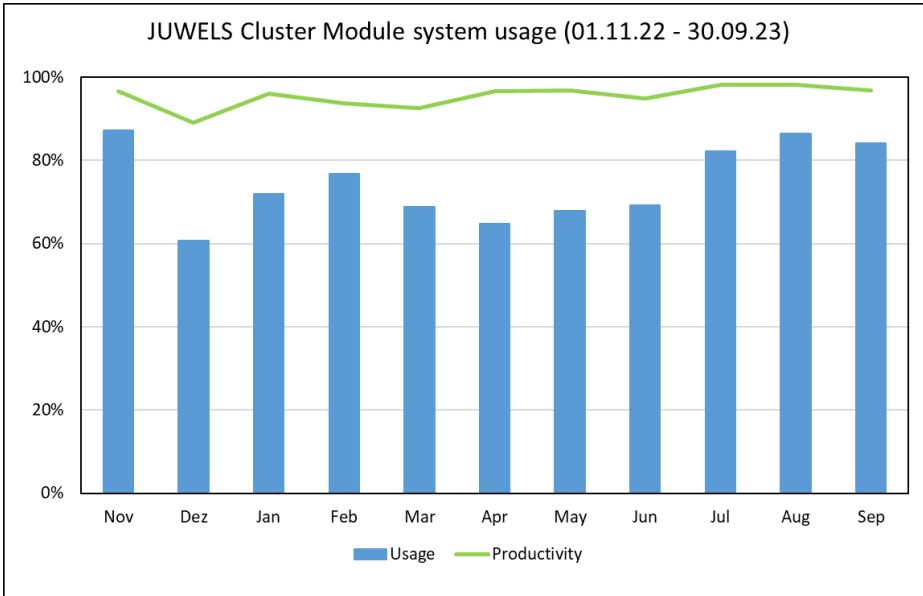
JUWELS BOOSTER USAGE
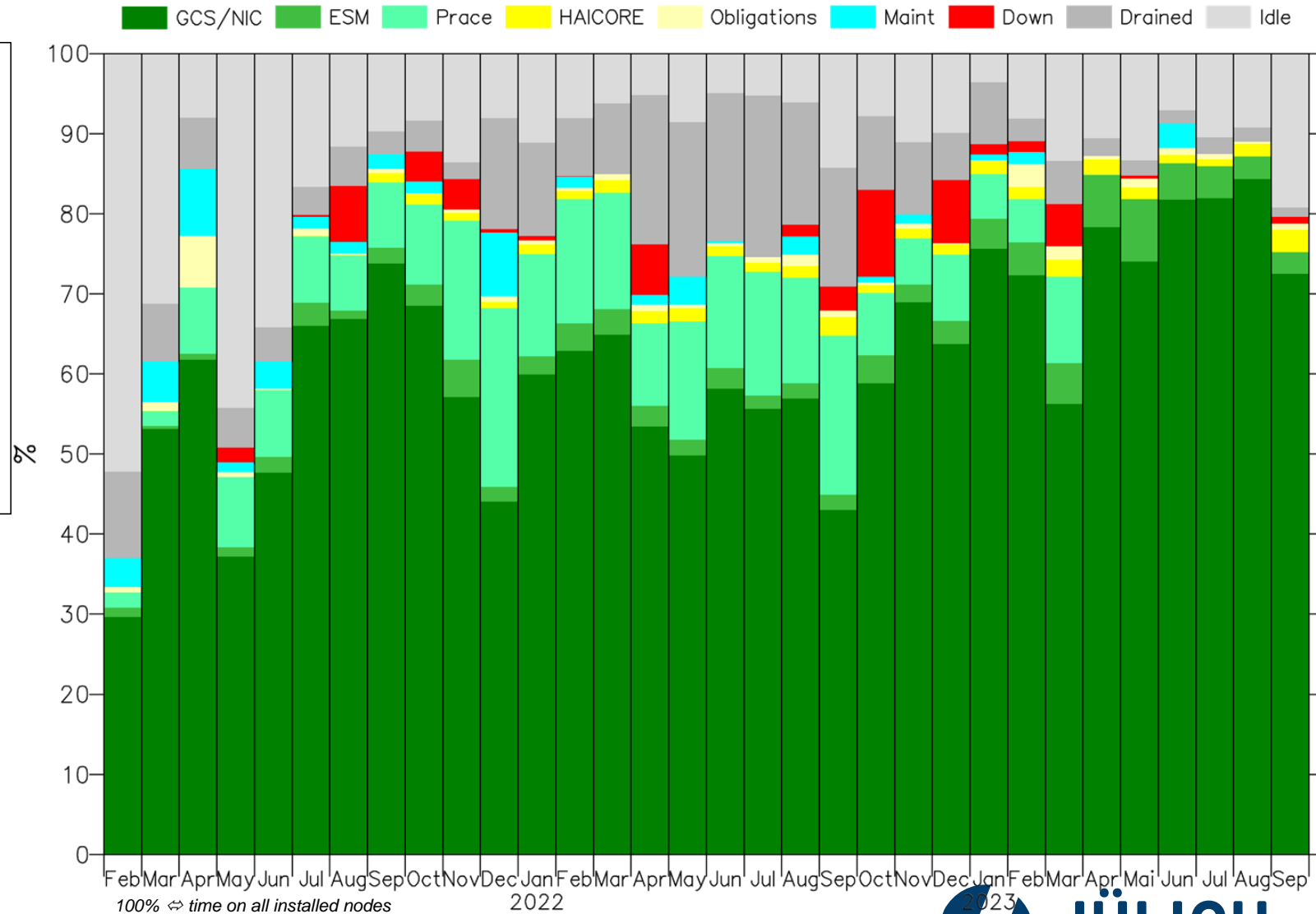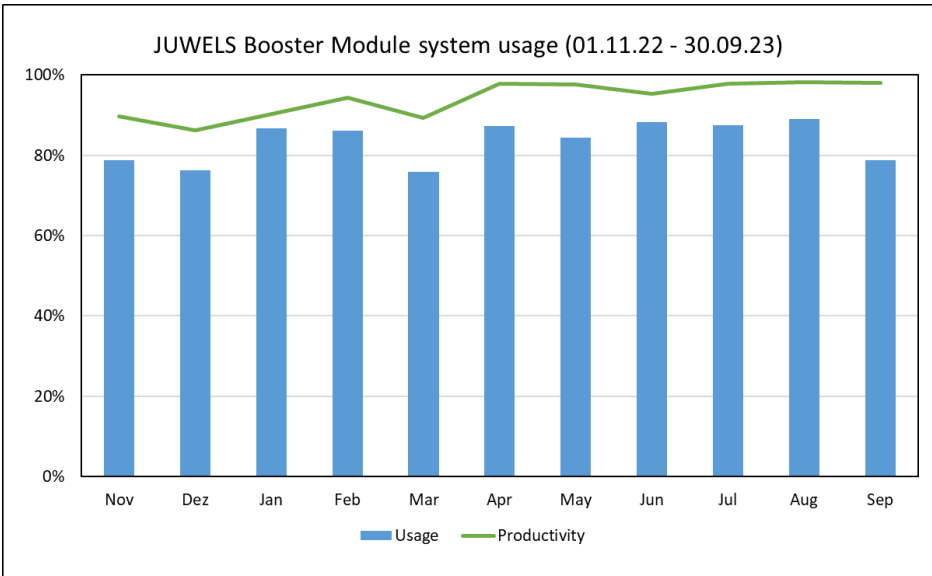
JURECA-DC USAGE

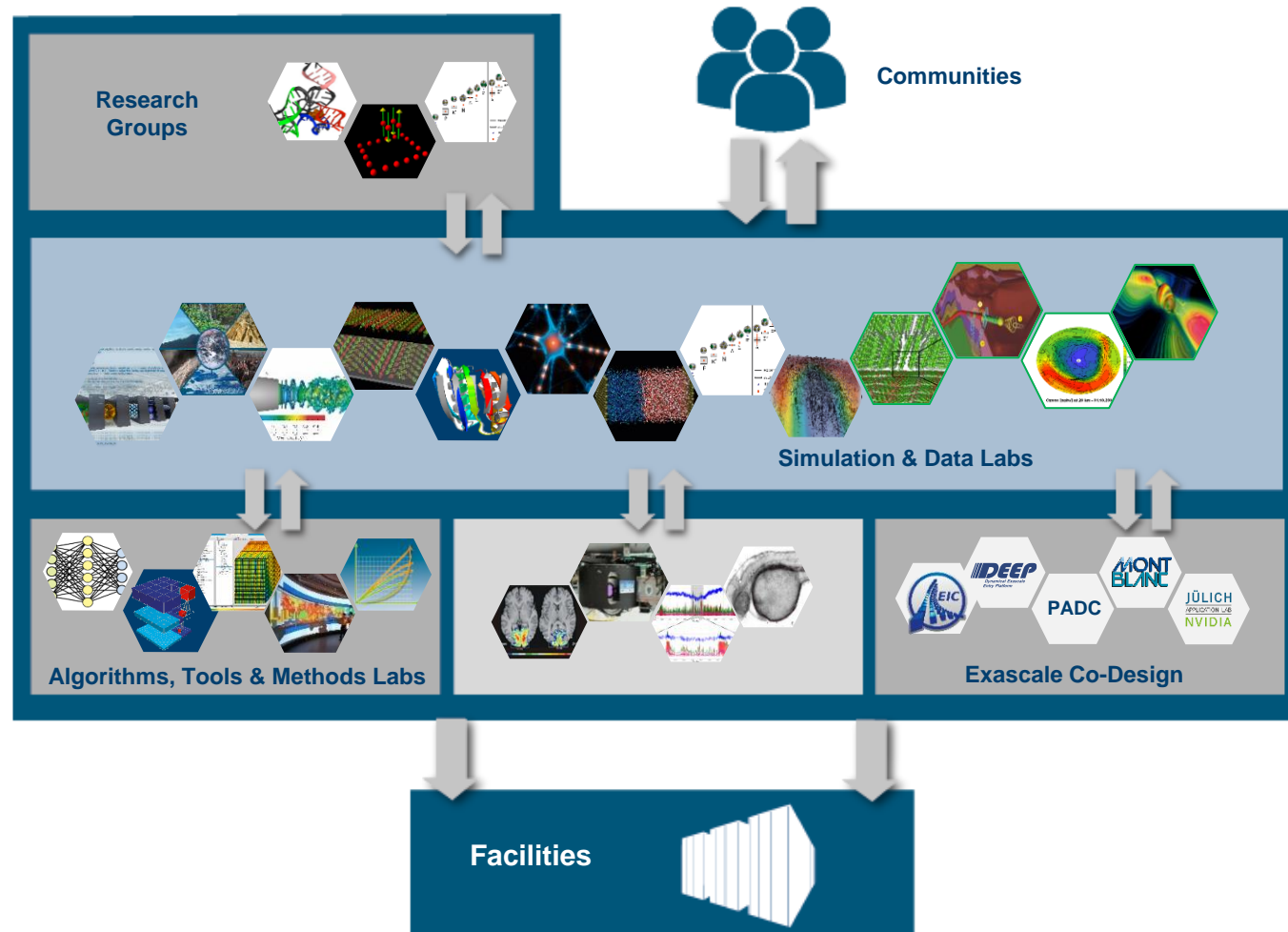JURECA-DC system usage (01.11.22 - 30.09.23)

100% ⇔ time on all installed nodes

JURECA-DC: since Dec 2020: 432 (of 768) nodes
JURECA-DC: since May 2021 768 nodes

SUPPORT AND RESEARCH LANDSCAPE AT JSC

SUMMARY

- **The Jülich Supercomputing Centre (JSC) provides**
  - Tier-0/1 HPC resources of the highest perf. class
  - high-end primary and domain-specific user support
  - …

- **JSC expects to see**
  - breakthrough science
  - parallel applications, using efficient and optimized algorithms & programs on a substantial number of processors simultaneously
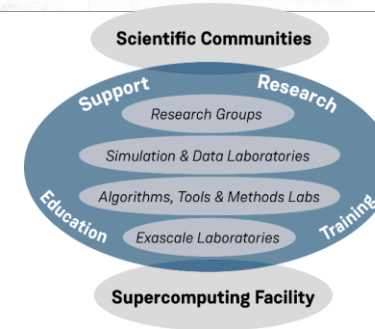
Sz. Borsanyi et al.,
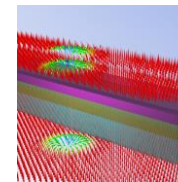Science **347** (2015) 6229
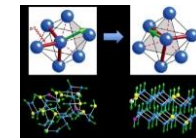
Sz. Borsanyi, Z. Fodor et al.,
Nature **593** (2021) 51
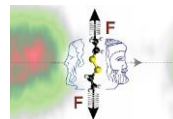
D. Marx et al.,
Nature Chemistry **5** (2013) 685

S. de Beer, M. Müser
Nature Communications **5** (2013)
doi 10.1038/ncomms4781
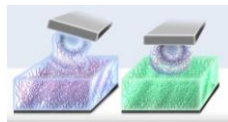
U. Meissner et al.,
Nature **528** (2015) 111

M. Lezaic et al.,
Nature Materials **9** (2010) 649

S. Blügel et al.,
Nature Communications **7** (2016)
doi 10.1038/ncomms11779

D. Bravo et al.,
Nature **562** (2018) 505

R.O. Jones et al.,
Nature Materials **10** (2011) 129

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BACKUP

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GCS SYSTEM @ JÜLICH

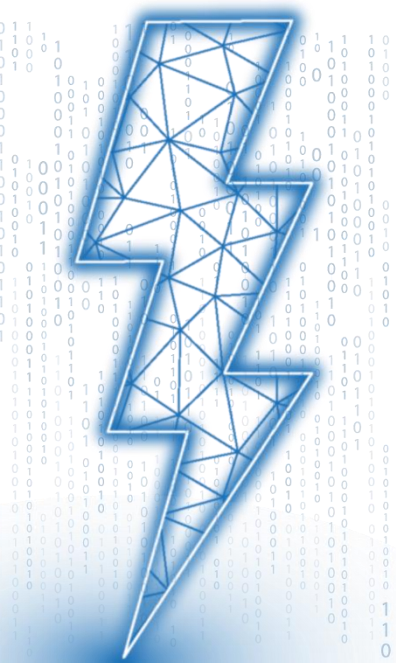**JUWELS (Jülich Wizard for European Leadership Science): Modular Supercomputer**

- **JUWELS Cluster:** Intel Skylake based system with 12 PF (10.6 CPU + (1.7 GPU)) peak performance
  - 10 cells with altogether more than 2,500 nodes or 120,000 cores
    80% funded by GCS → **GCS System@Jülich**
    20% funded by Helmholtz for Earth System Modelling (ESM)
  - Entered #23 in Jun 2018 Top500

- **JUWELS Booster:** Nvidia A100 based system with 75 PF ((2 CPU) + 73 GPU) peak performance
  - 936 nodes with 4 Nvidia A100 graphics cards each
    87,5% funded by GCS (including resources for PRACE) → **GCS System@Jülich**
    10,0% funded by Helmholtz for Earth System Modelling (ESM)
    2,5% funded by Helmholtz for AI applications (HAICORE)
  - Entered #7 in Nov 2020 Top500, #1 in Europe, #1 in Green250

- Connected to file server **JUST** with about **100 PB disk** capacity and more than **300 PB tape** capacity

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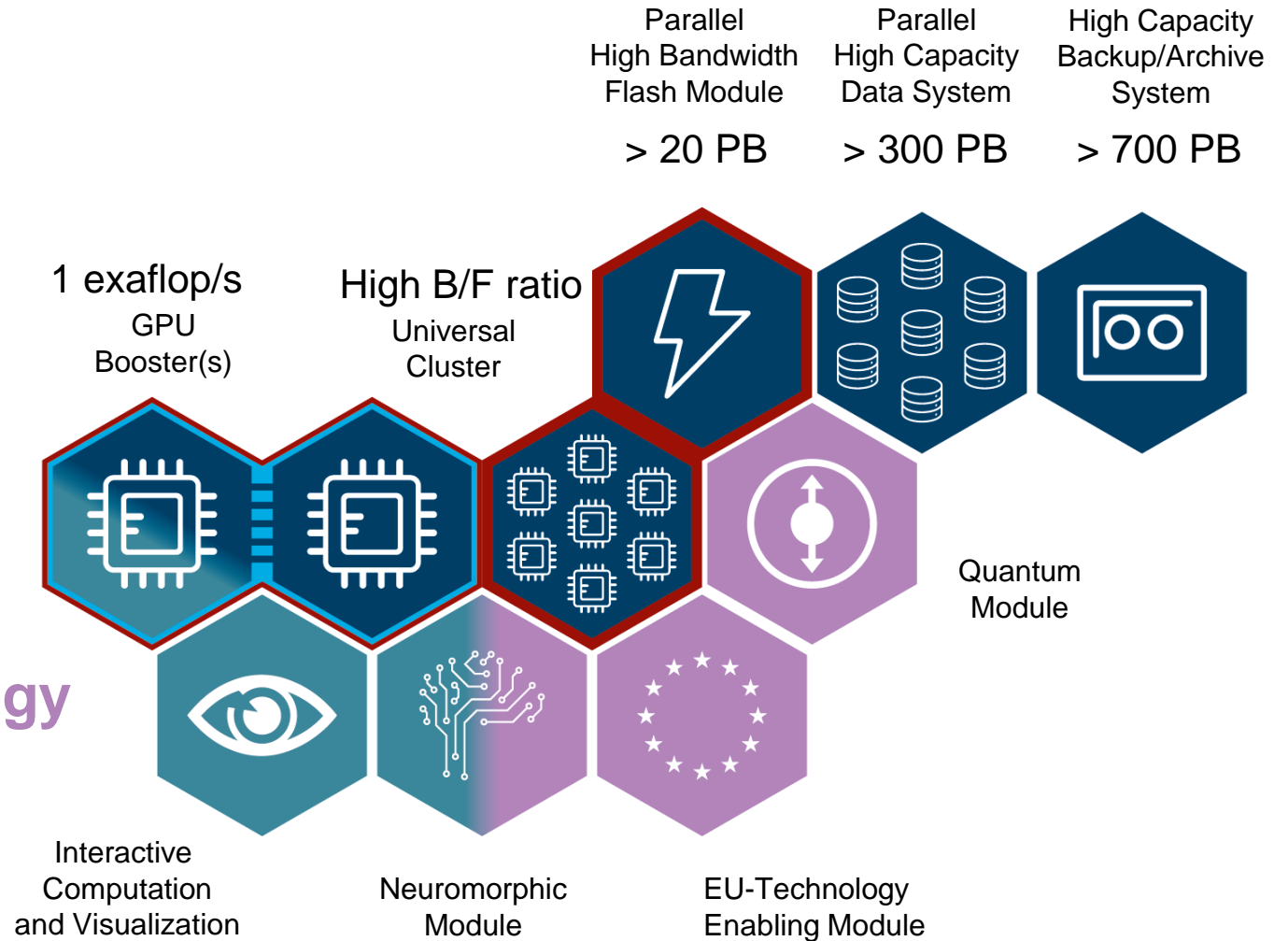# Measures to Reduce Energy Consumption

Funding agencies require energy savings

1. Free cooling systems replace the cold water cooling

   since May 2022: Juwels-Booster

   since Nov 2022: Jureca-DC

2. Switch-off of non-used nodes by the Slurm scheduler

   enabled on JURECA-DC, JUSUF (Oct/Nov 2022)

JUPITER - High level architecture

Basic Configuration

Optional Modules

Future Technology Modules

Parallel High Bandwidth Flash Module
> 20 PB

Parallel High Capacity Data System
> 300 PB

High Capacity Backup/Archive System
> 700 PB

1 exaflop/s
GPU Booster(s)

High B/F ratio
Universal Cluster

Quantum Module

Interactive Computation and Visualization

Neuromorphic Module

EU-Technology Enabling Module

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JÜLICH SUPERCOMPUTING CENTRE

JUWELS vs. JUPITER

	JUWELS	JUPITER
Cluster	**CPU:** Intel Xeon Platinum 8168 **GPU:** NVIDIA V100 **Peak:** 10 PFlop/s	**CPU:** SiPearl Rhea **GPU: none** **Focus:** High Byte/Flop
Booster	**CPU:** AMD Epyc Rome **GPU:** 4× NVIDIA A100 GPUs **Peak:** 70 PFlop/s	**CPU:** Nvidia Grace **GPU:** Nvidia Hopper H100 **Rmax: >1 EFlop/s**
Network topology	Fat tree and DragonFly+	Some kind of DragonFly
System access	GCS or PRACE proposals	GCS and EuroHPC proposals
User support	HLST, SDL, ATML, training courses, targeted early access program	**same**