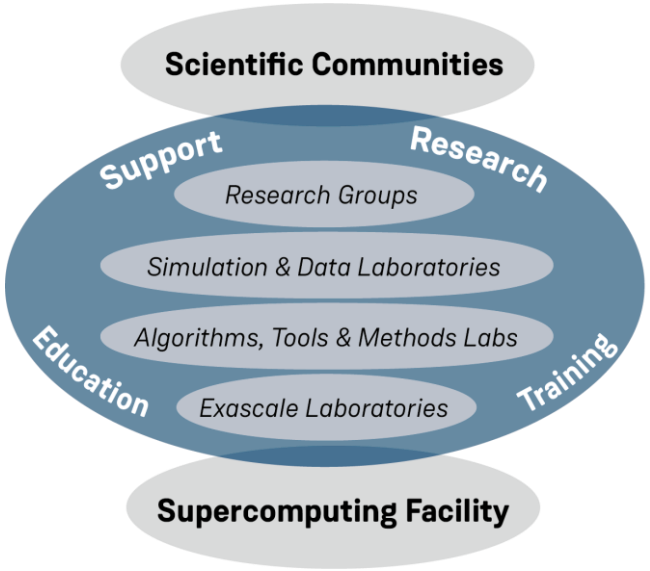
JÜLICH SUPERCOMPUTING CENTRE (JSC) INTRODUCTION

MAY 21, 2024 I BERND MOHR

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 + AI
  - Computer architectures, Co-Design, Modularity, Exascale Labs together with IBM, Intel, NVIDIA
- **Education and training**



DEEP

JÜLICH Forschungszentrum

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 partitions (HAICORE, HDFAI) (~2.5% of JUWELS Booster only)

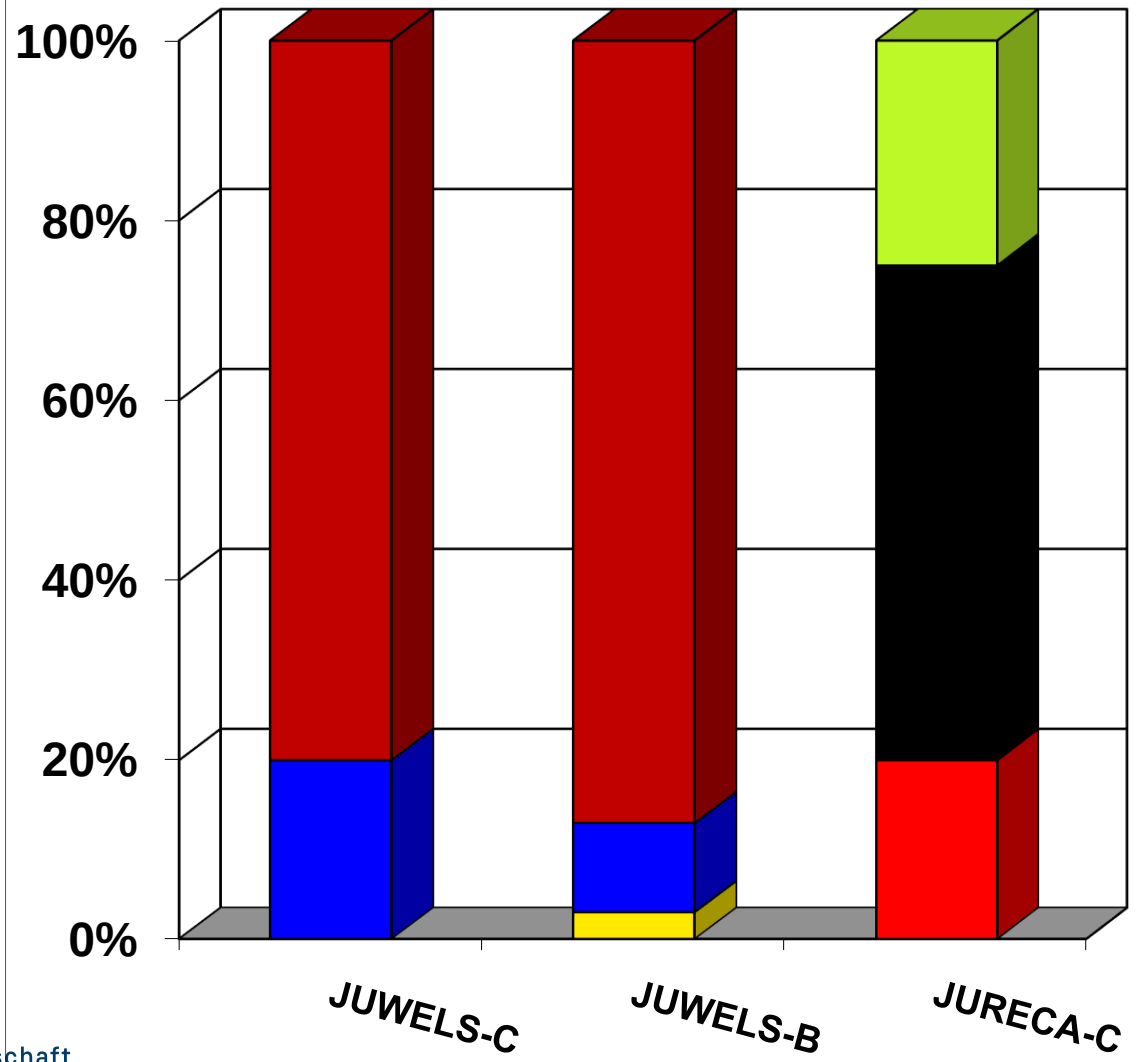
- **Access to JURECA-DC through biannual CfP via**
  - Kommission zur Vergabe von SC Resourcen (VSR) – Jülich internal

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

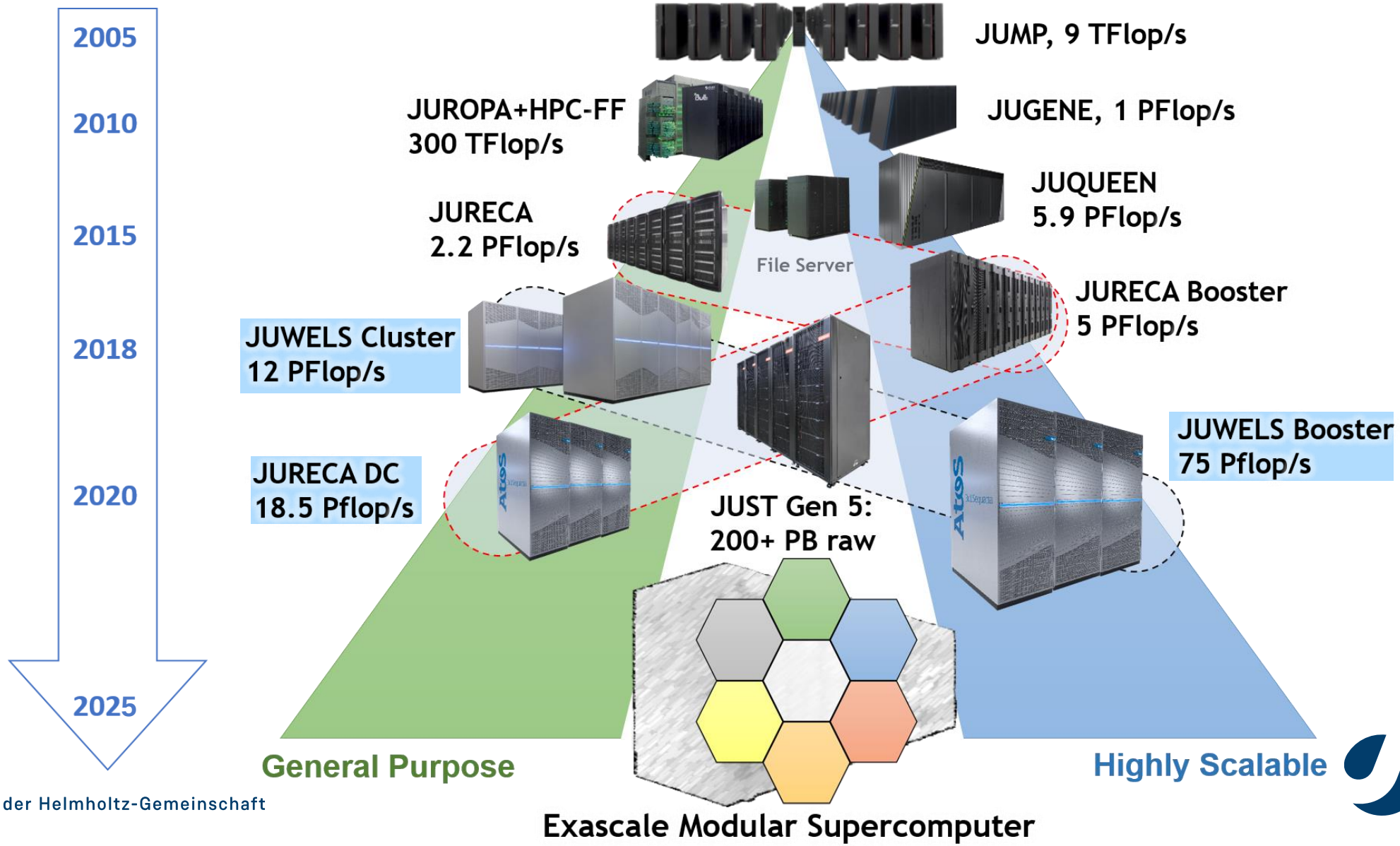
STAKEHOLDER‘S COMPUTE TIME SHARES



80% of the available time is being granted!

- FZJ obligations
- FZJ projects
- NIC (Germany)
- GCS/NIC (Germany)
- European share
- ESM partition
- HAICORE

(DUAL) HARDWARE STRATEGY AT JSC



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

GCS SYSTEM @ JÜLICH

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

JUWELS Cluster

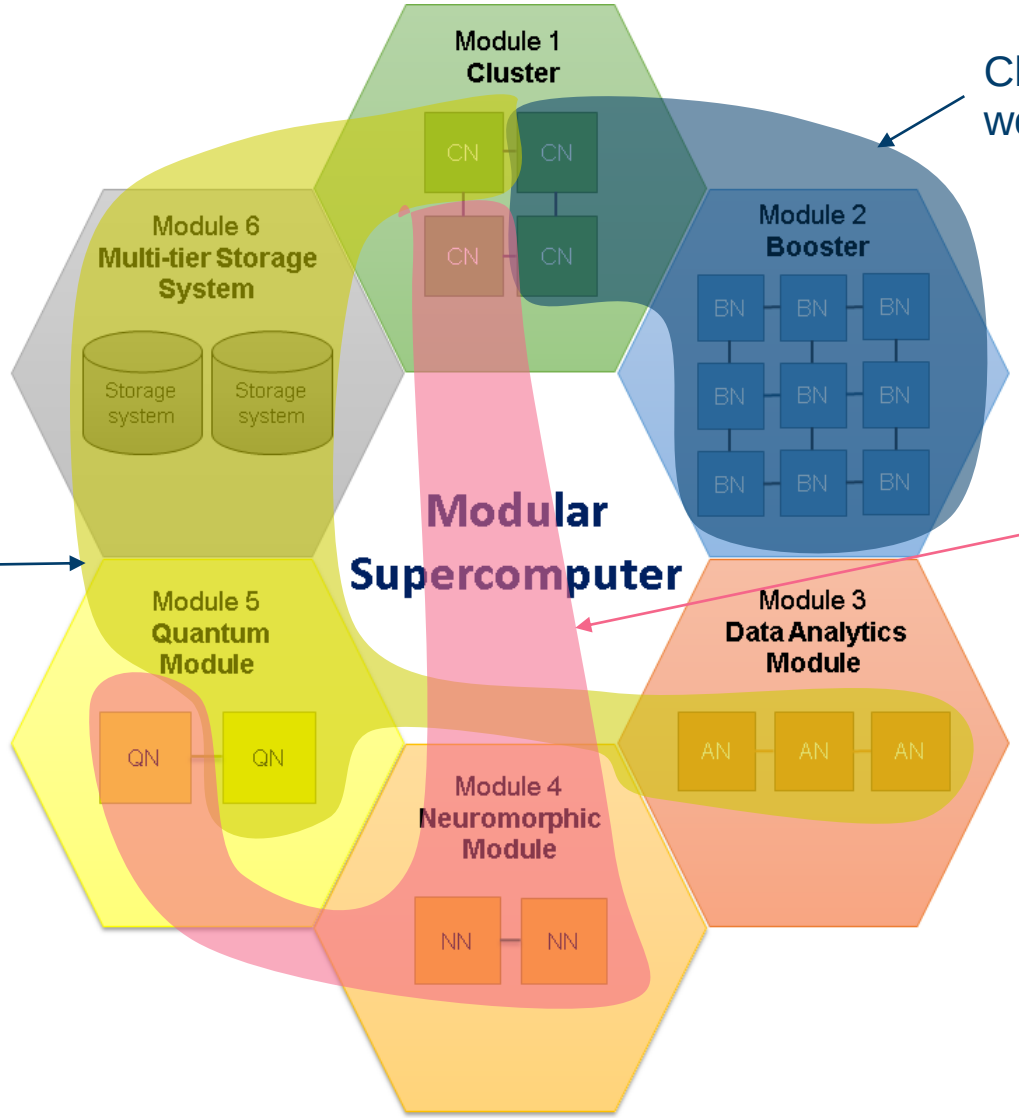
- Intel Skylake based system with **12 PF** peak (CPU:10.6 PF, GPU: 1.7 PF)
- 10 cells with altogether more than 2,500 nodes or 120,000 cores
- Mellanox InfiniBand EDR fat-tree network (2:1 pruning at leaf level)
- Entered #23 in Jun 2018 Top500

JUWELS Booster

- Nvidia A100 based system with **75 PF** peak (CPU: 2 PF, GPU 73 PF)
- 936 nodes with 4 Nvidia A100 graphics cards each
- Mellanox InfiniBand HDR DragonFly+ topology with 20 cells - 5 TB/s connection to Cluster
- 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

… AND EVOLUTION TO A MODULAR SUPERCOMPUTING ARCHITECTURE



Climatology workflow

HBP Data Analytics workflow

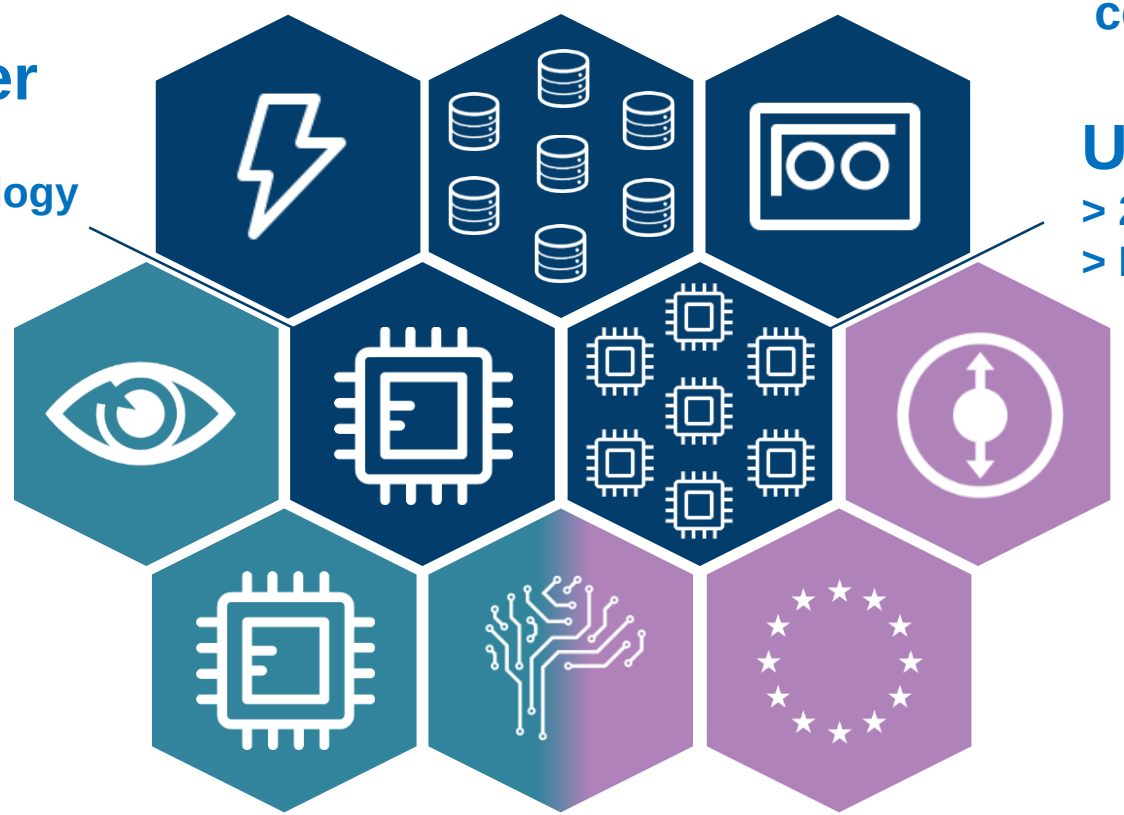
Deep Learning workflow

*Patents granted and pending

JUPITER – MODULAR EXASCALE COMPUTER

GPU Booster

- 1EF Linpack
- Nvidia technology



Target >20×

application performance
compared to JUWELS Booster

Universal Cluster

> 2025
> EPI Rhea

- **Basis Configuration**
- **Optional Modules**
- **Future Technology Modules**

Mitglied der Helmholtz-Gemeinschaft

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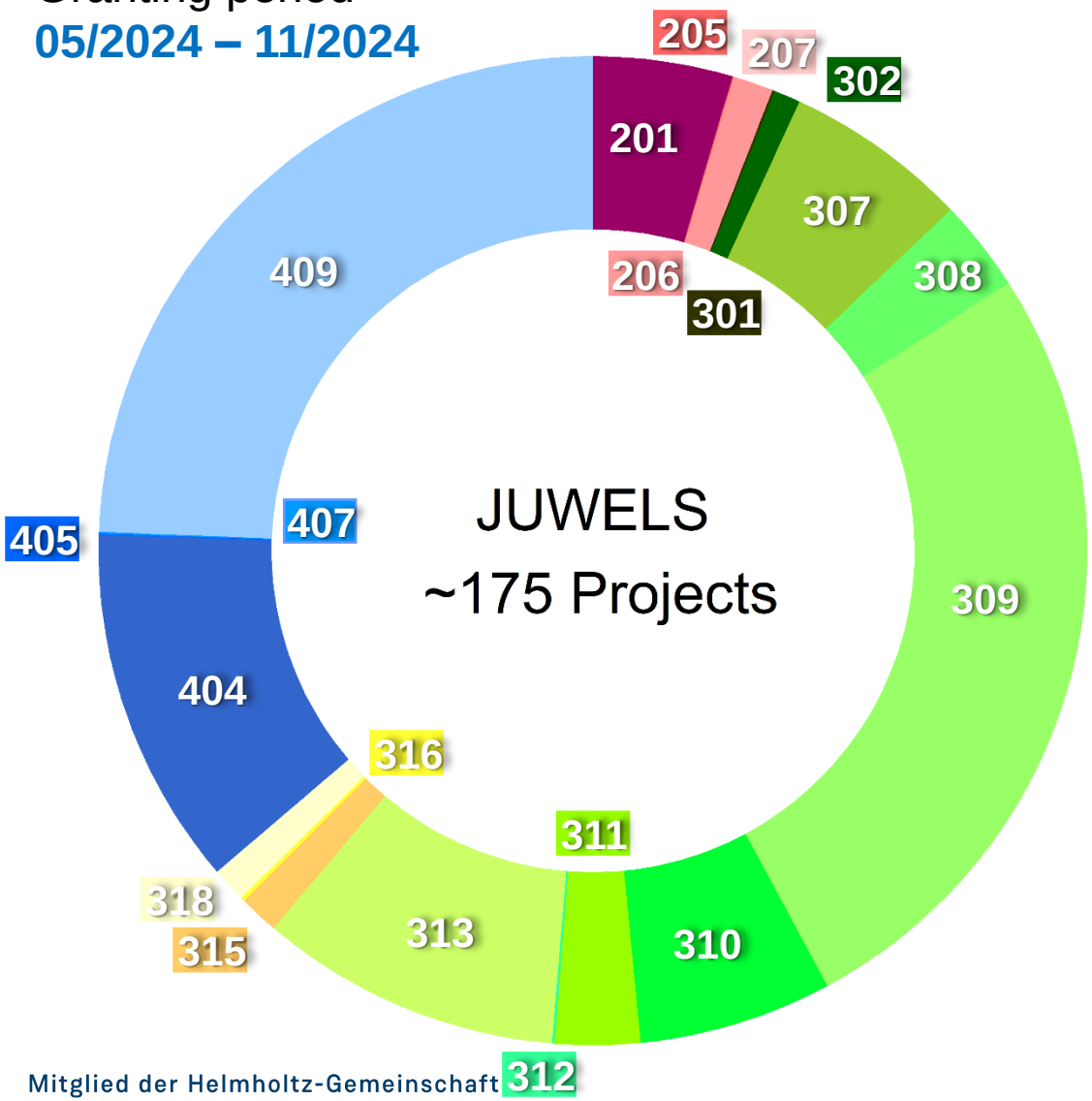
https://go.fzj.de/jupiter

JUWELS (CLUSTER + BOOSTER): GCS RESEARCH FIELDS

Granting period
05/2024 – 11/2024

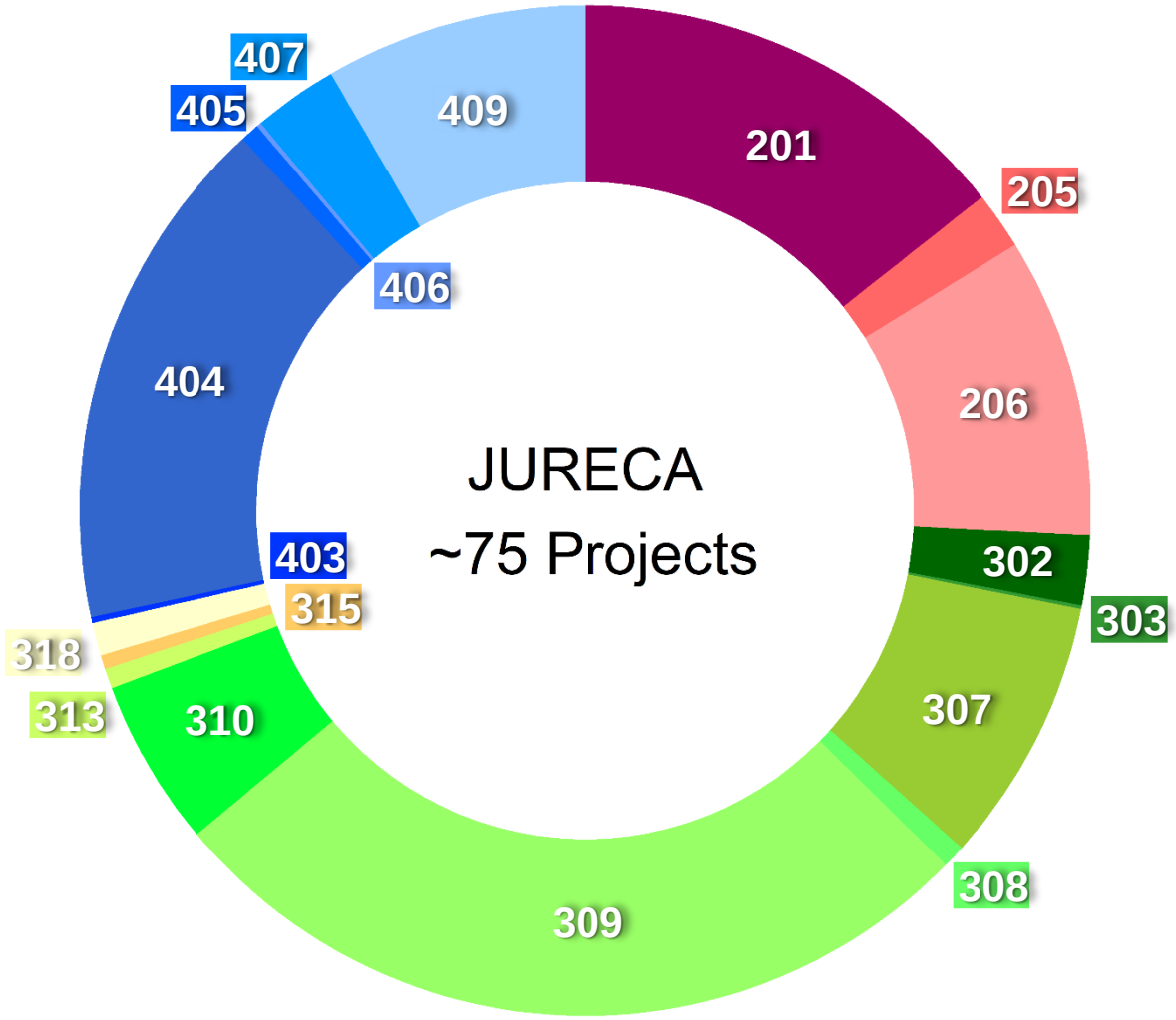


Reseach Fields

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
404	Heat Energy Technology, Thermal Machines, Fluid Mechanics
405	Materials Engineering
407	Systems Engineering
409	Computer Science

RESEARCH FIELDS ON JURECA (CLUSTER)

Granting period
05/2024 – 11/2024



Reseach Fields

- 201 Basic Biological and Medical Research
- 205 Medicine
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- 302 Chemical Solid State and Surface Research
- 303 Physical and Theoretical Chemistry
- 307 Condensed Matter Physics
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- 309 Particles, Nuclei and Fields
- 310 Statistical Physics, Soft Matter, Biological Physics, Nonlinear Dynamics
- 313 Atmospheric Science, Oceanography and Climate Research
- 315 Geophysics and Geodesy
- 318 Water Research
- 403 Process Engineering, Technical Chemistry
- 404 Heat Energy Technology, Thermal Machines, Fluid Mechanics
- 405 Materials Engineering
- 406 Materials Science
- 407 Systems Engineering
- 409 Computer Science

NATIONAL AND EUROPEAN USER GROUPS

- 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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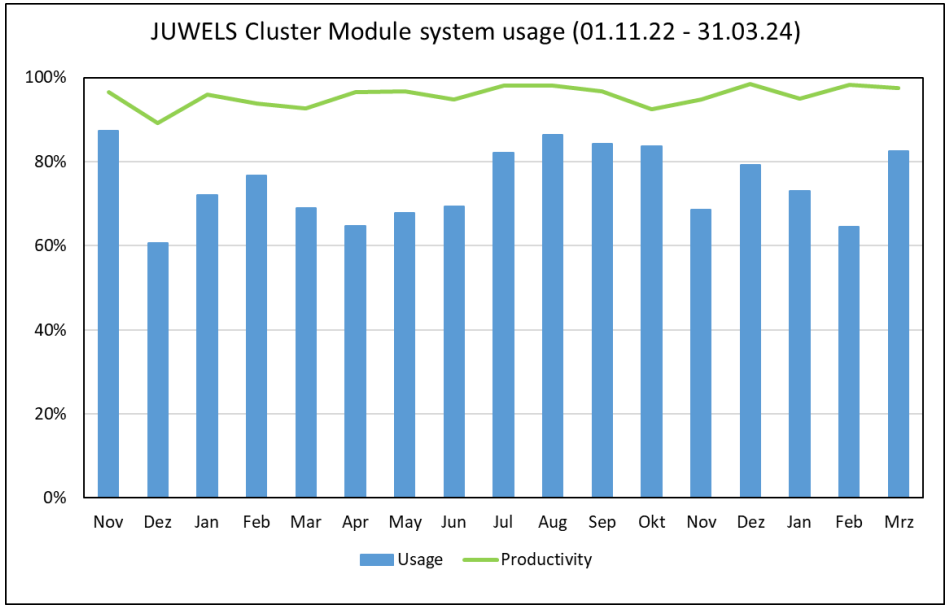
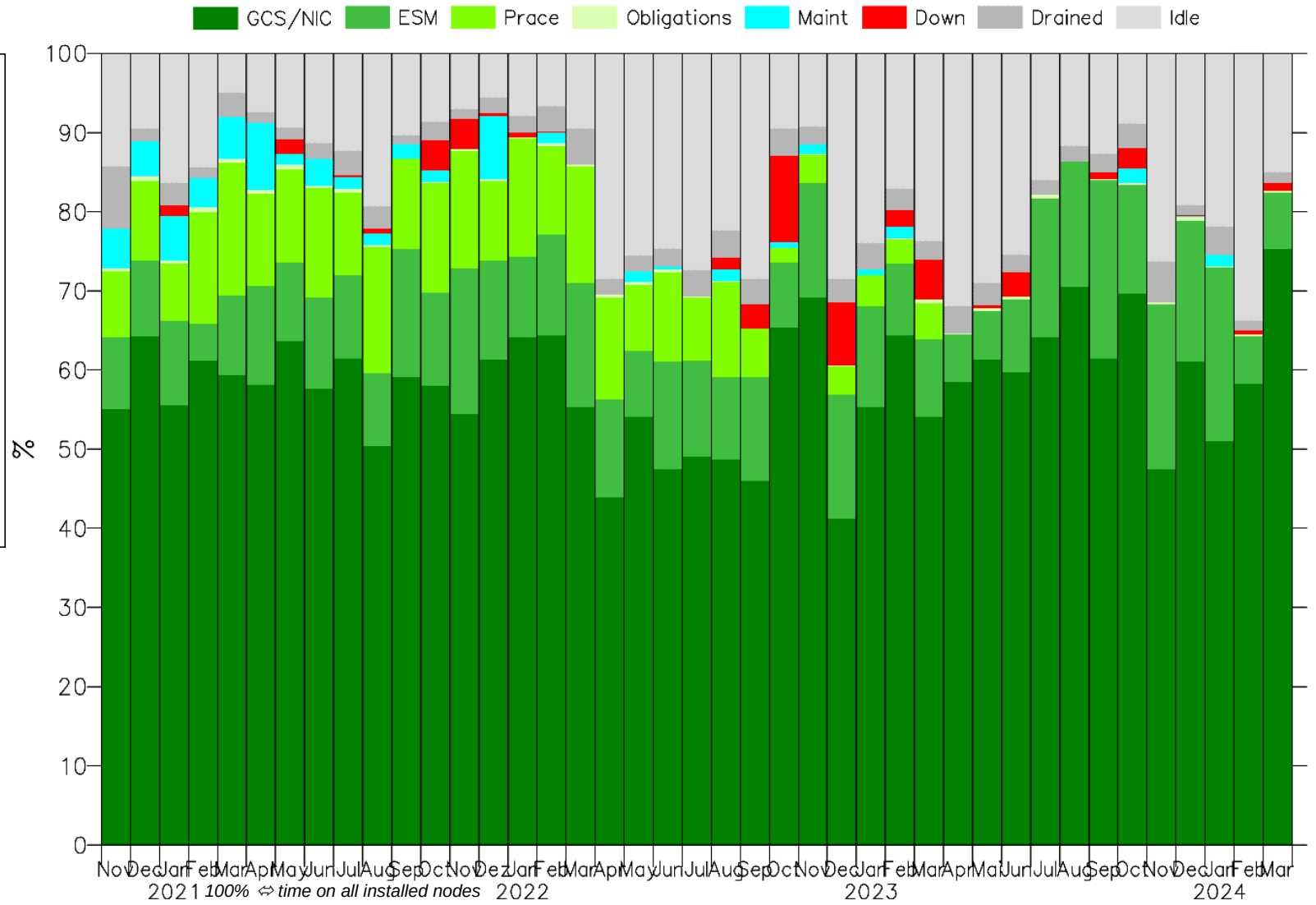
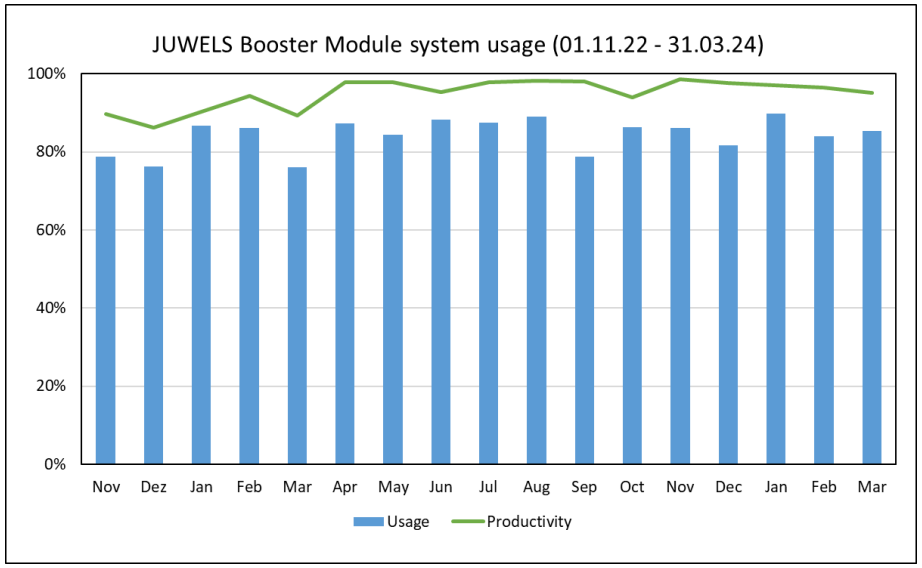
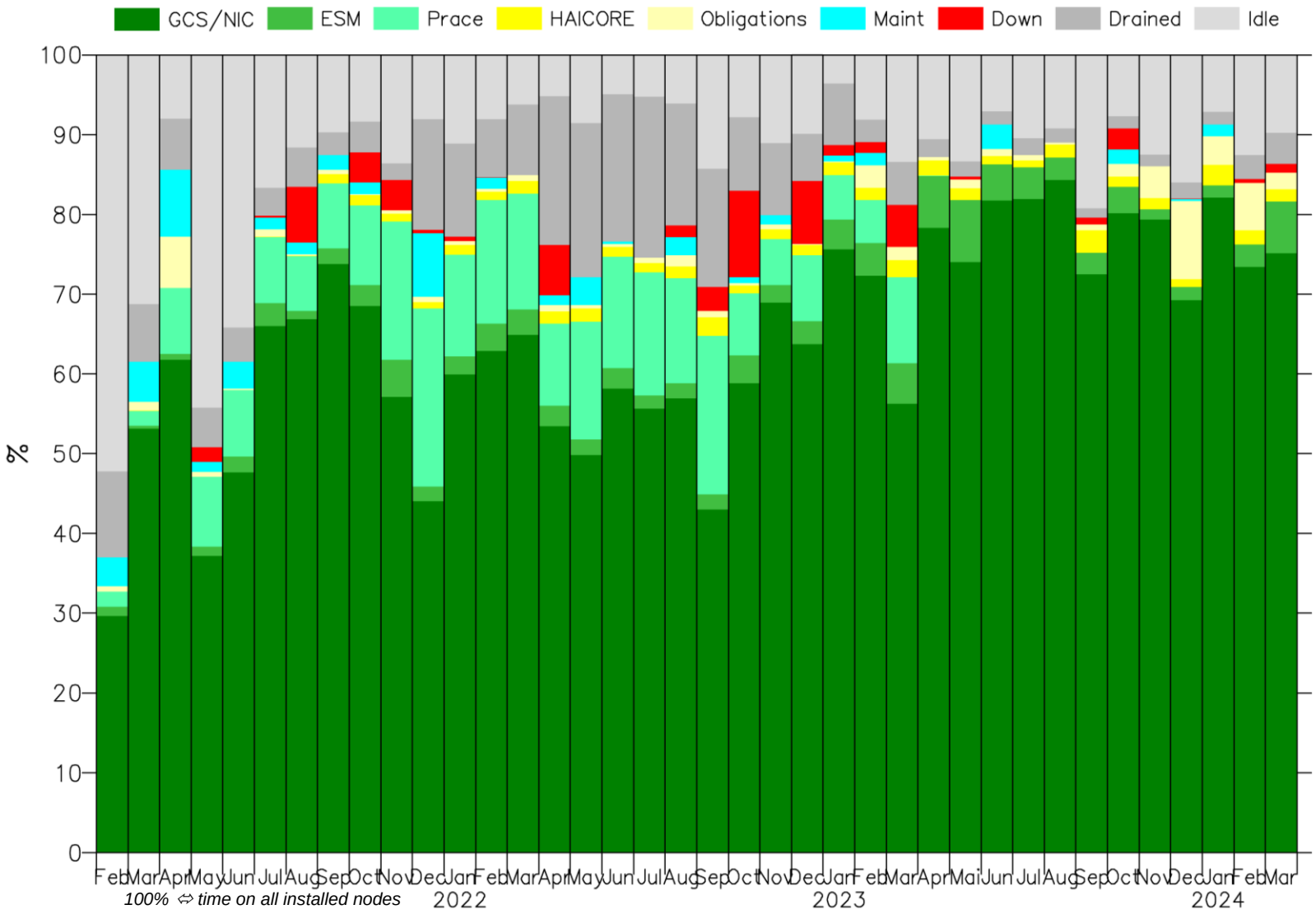
JUWELS CLUSTER USAGE



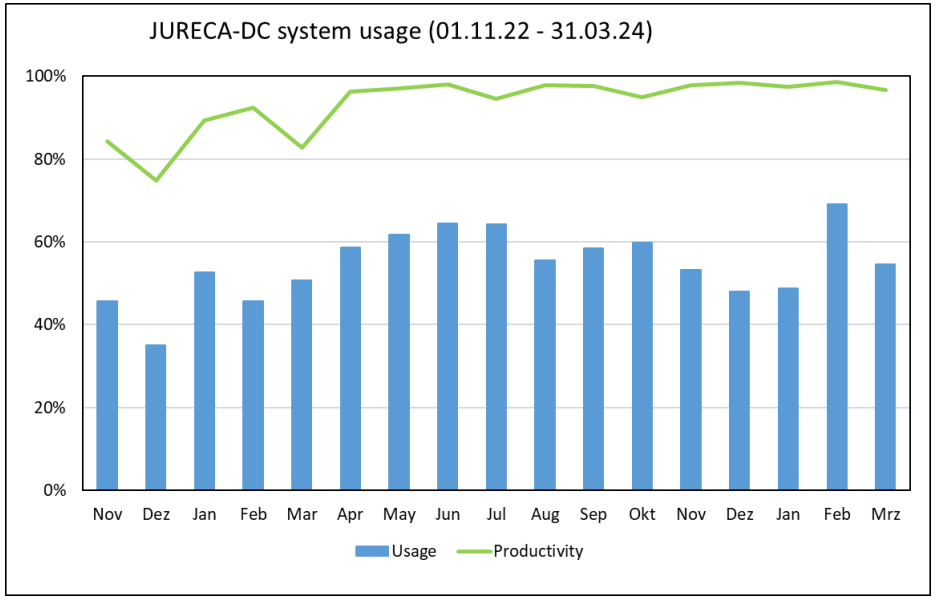


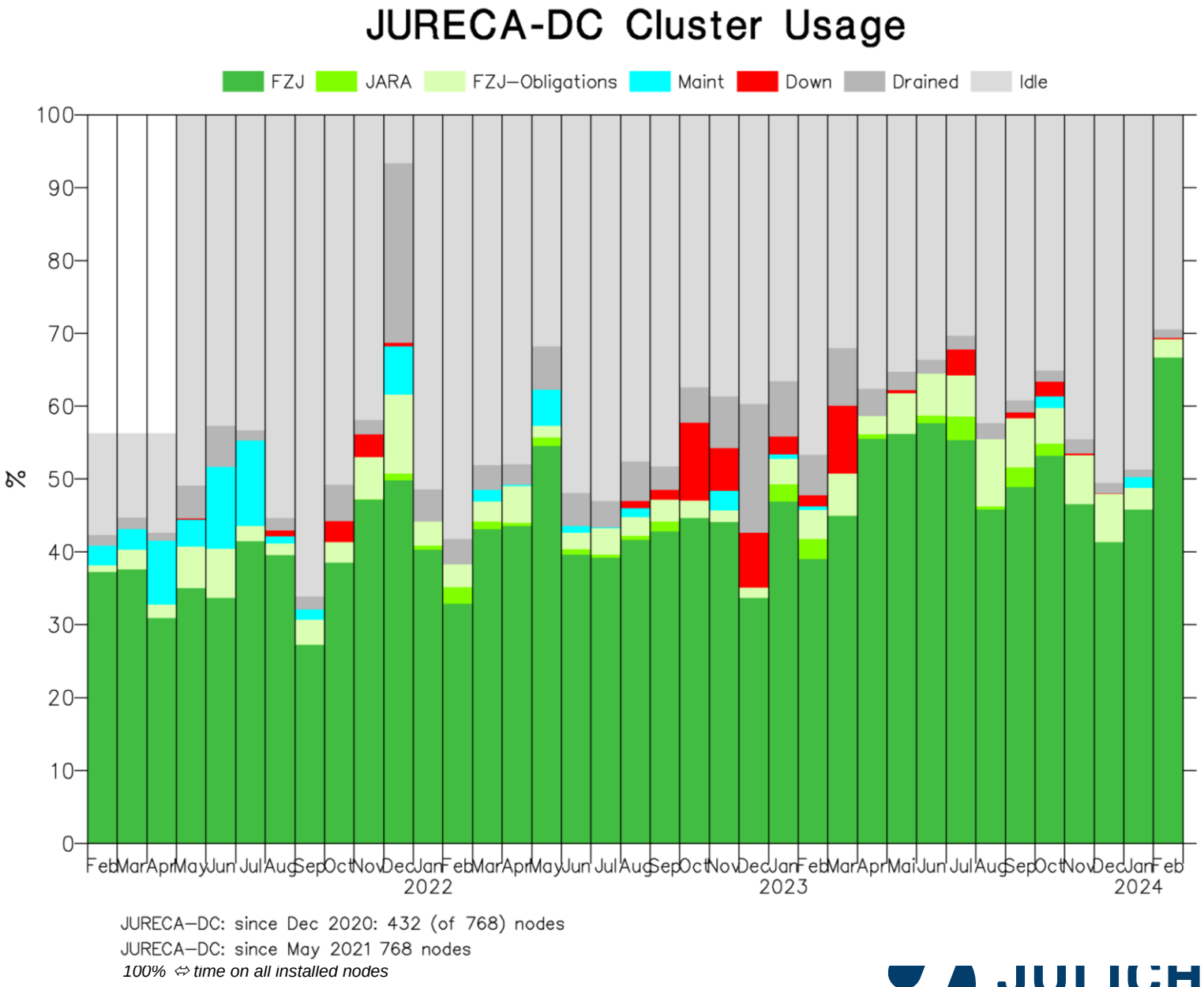
JUWELS BOOSTER USAGE





JURECA-DC USAGE

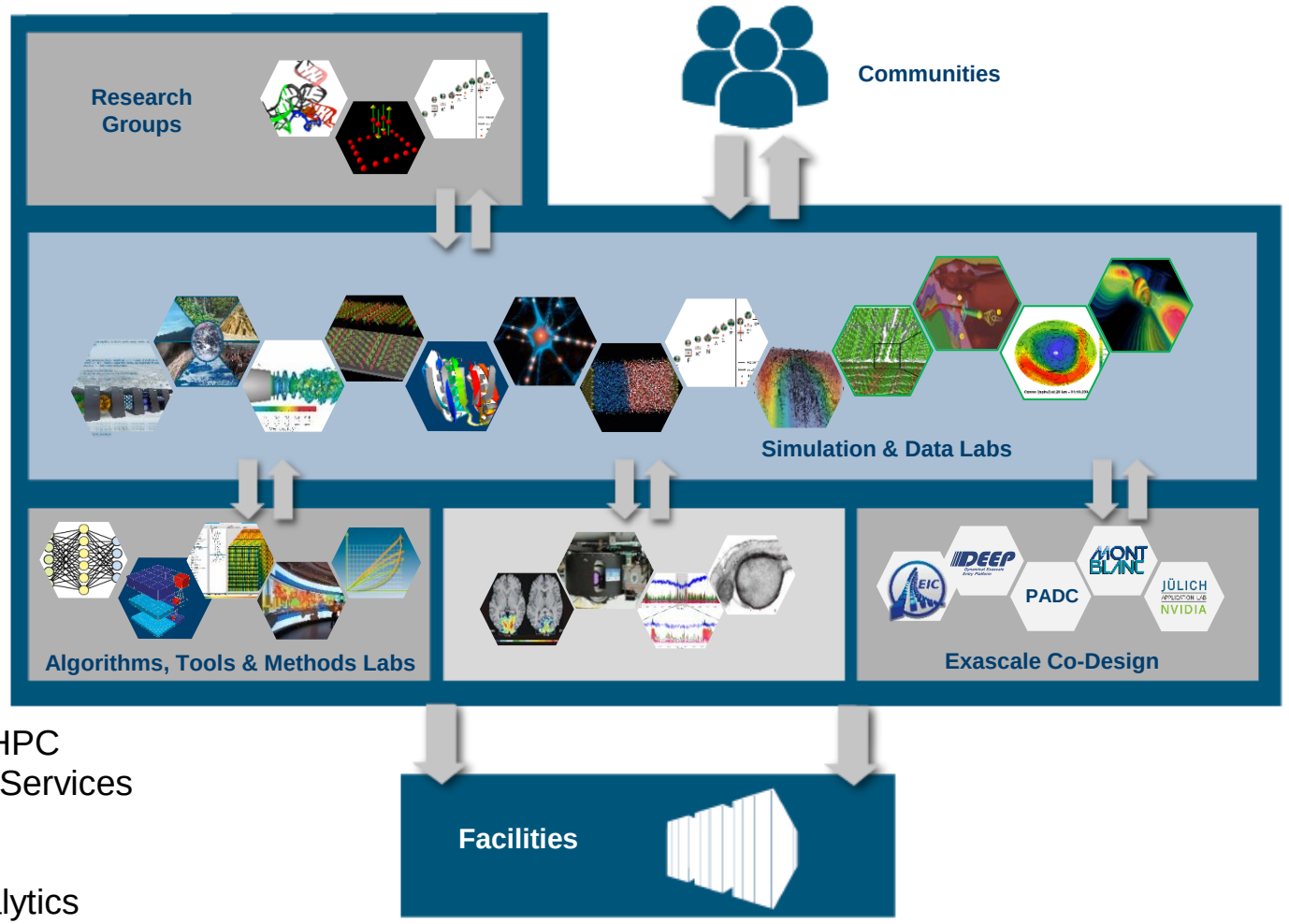




JURECA–DC: since Dec 2020: 432 (of 768) nodes
JURECA–DC: since May 2021 768 nodes
100% ⇔ time on all installed nodes

SUPPORT AND RESEARCH LANDSCAPE AT JSC

- Quantum Information Processing
- Earth System Data Exploration
- Computation Material Science
- Computational Structural Biology
- Next Generation Architectures
- Software for Modular
- Supercomputers
- RSE
- AI & ML for Healthcare

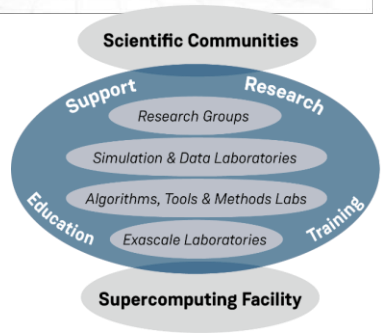


- Complex Particle Systems
- Quantum Materials
- Electrons and Neutrons
- Biology
- Neuroscience
- Fluids & Solids Engineering
- Plasma Physics
- Numerical Quantum Field Theory
- Astronomy & Astrophysics
- Climate Science
- Terrestrial Systems
- AI and ML for Remote Sensing

- Deep Learning
- Accelerating Devices
- Parallel Performance
- Application Optimization
- Applied Machine Learning
- Visualization & Interactive HPC
- Federation Technologies & Services
- Concurrency & Parallelism
- Advanced Time Integrators
- Data Management and Analytics
- Numerical & Statistical Methods

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



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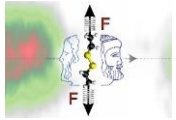

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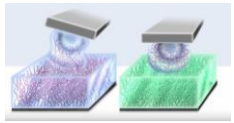

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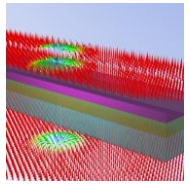

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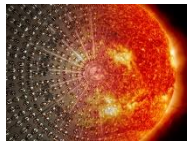

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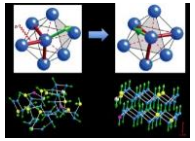

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