



# JÜLICH SUPERCOMPUTING CENTRE (JSC) INTRODUCTION

MAY 30, 2023 | 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**

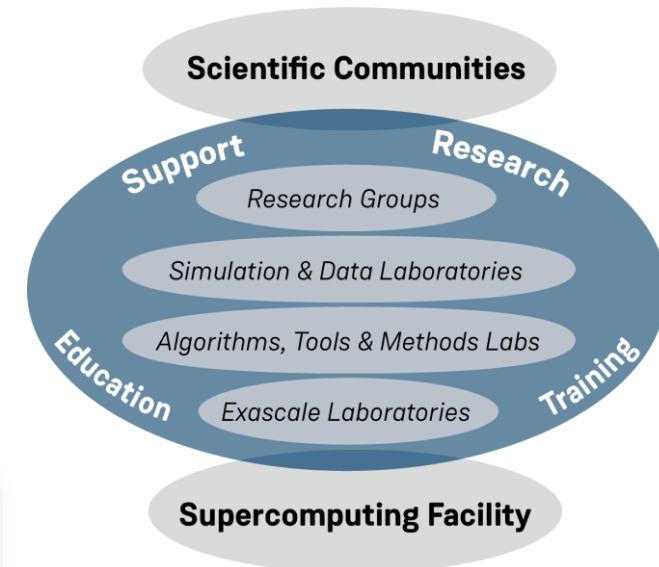
- Unique support & research environment at JSC
- Peer review support and coordination

- **R&D work**

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

- **Education and training**

Mitglied der Helmholtz-Gemeinschaft



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:  $\geq 2\%$  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)

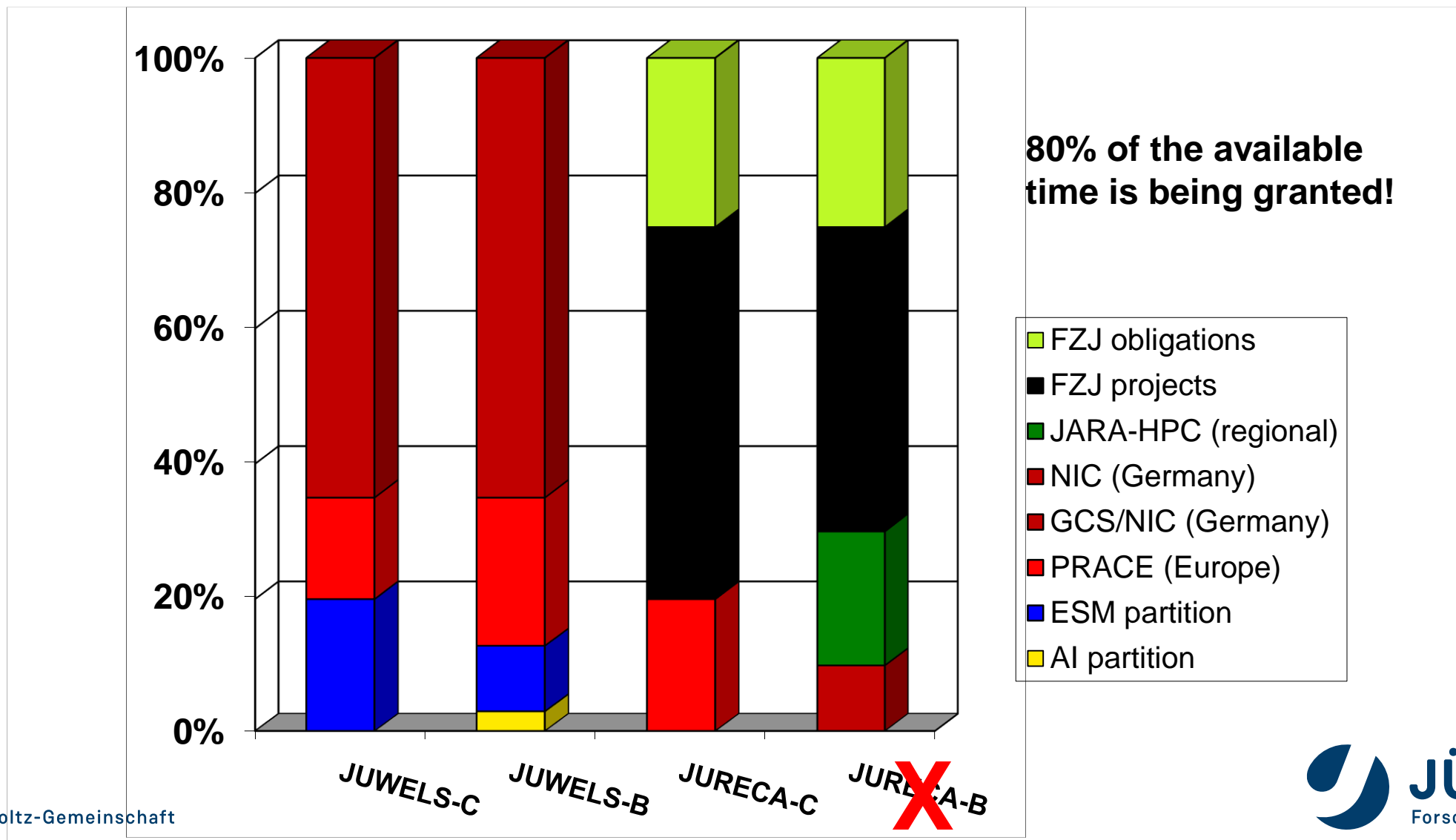


# GAUSS CENTRE FOR SUPERCOMPUTING (GCS)

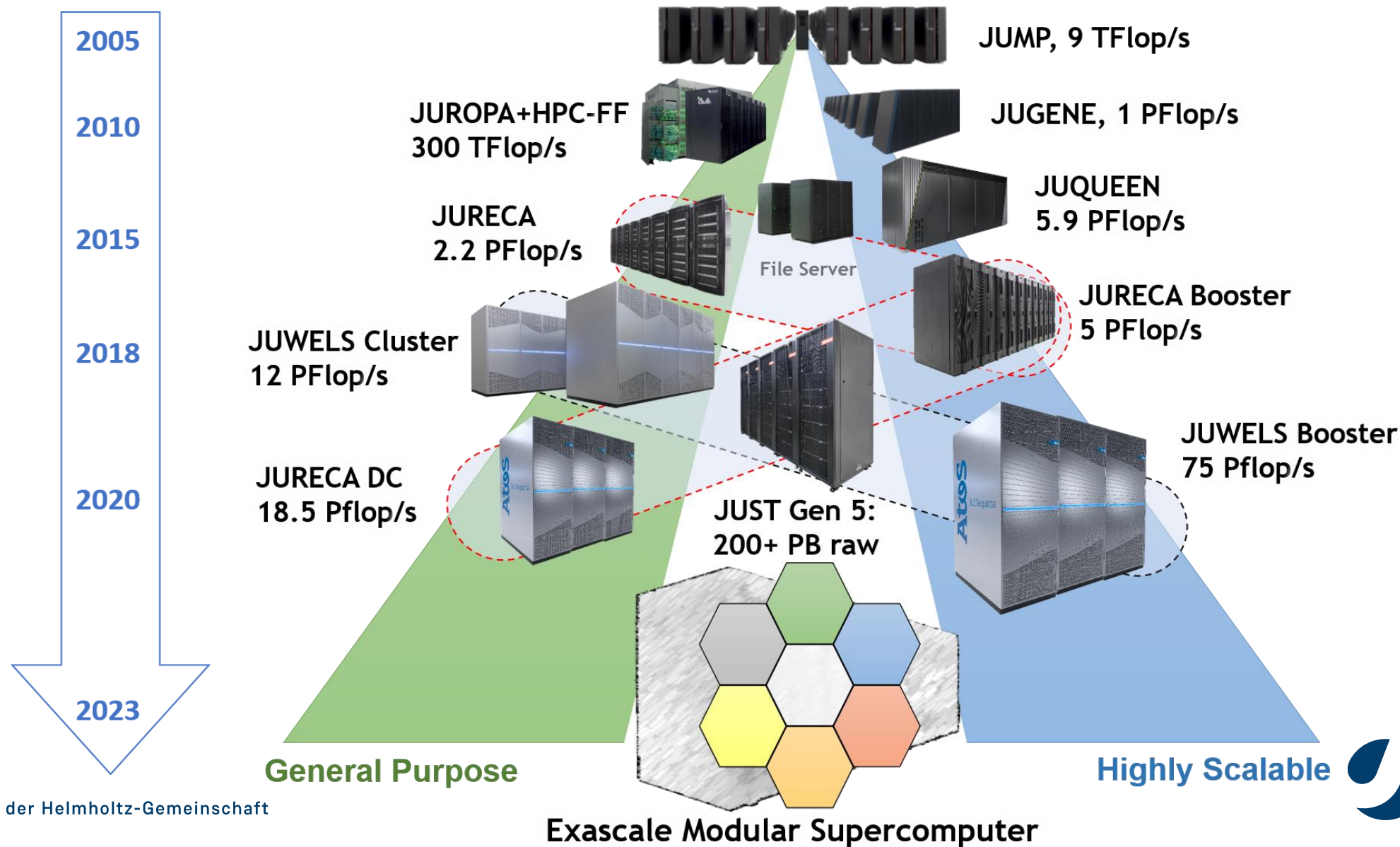
- **GCS is the leading Tier-0 HPC centre in Europe**
  - Alliance of the three German Tier-1 centres
  - High Performance Computing Centre Stuttgart (HLRS)
  - Jülich Supercomputing Centre (JSC)
  - Leibniz Rechenzentrum (LRZ), Garching
- **Key facts**
  - To date in sum more than 140 Petaflops (continuously expanding)
  - 600 people for operation, HPC R&D, services, training
  - Extensive know-how in key scientific fields



# STAKEHOLDER'S COMPUTE TIME SHARES



# (DUAL) HARDWARE STRATEGY AT JSC

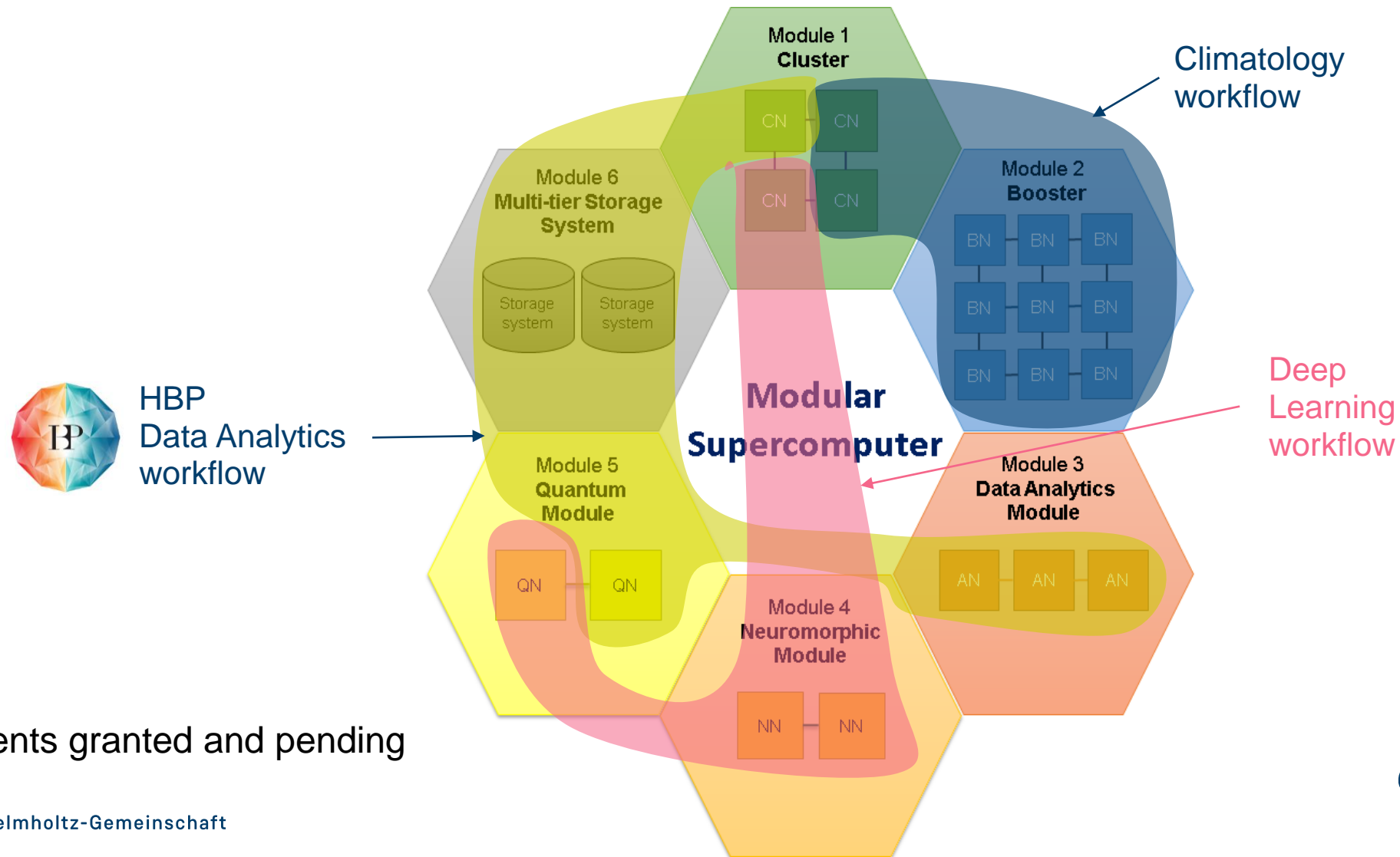




# JUWELS @ FZJ/JSC: CLUSTER AND BOOSTER MODULE IN PRODUCTION



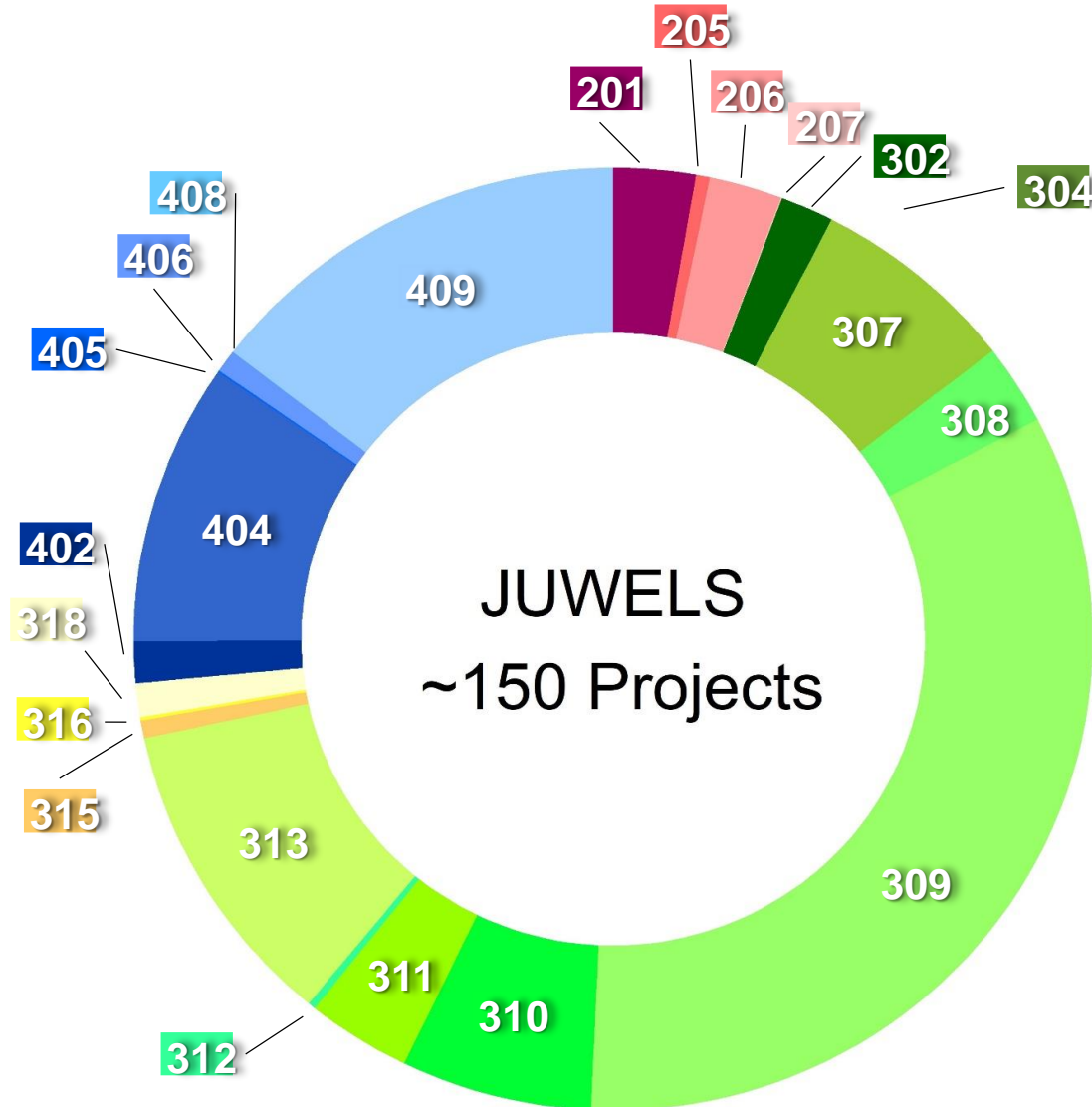
# ... AND EVOLUTION TO A MODULAR SUPERCOMPUTING ARCHITECTURE



\*Patents granted and pending



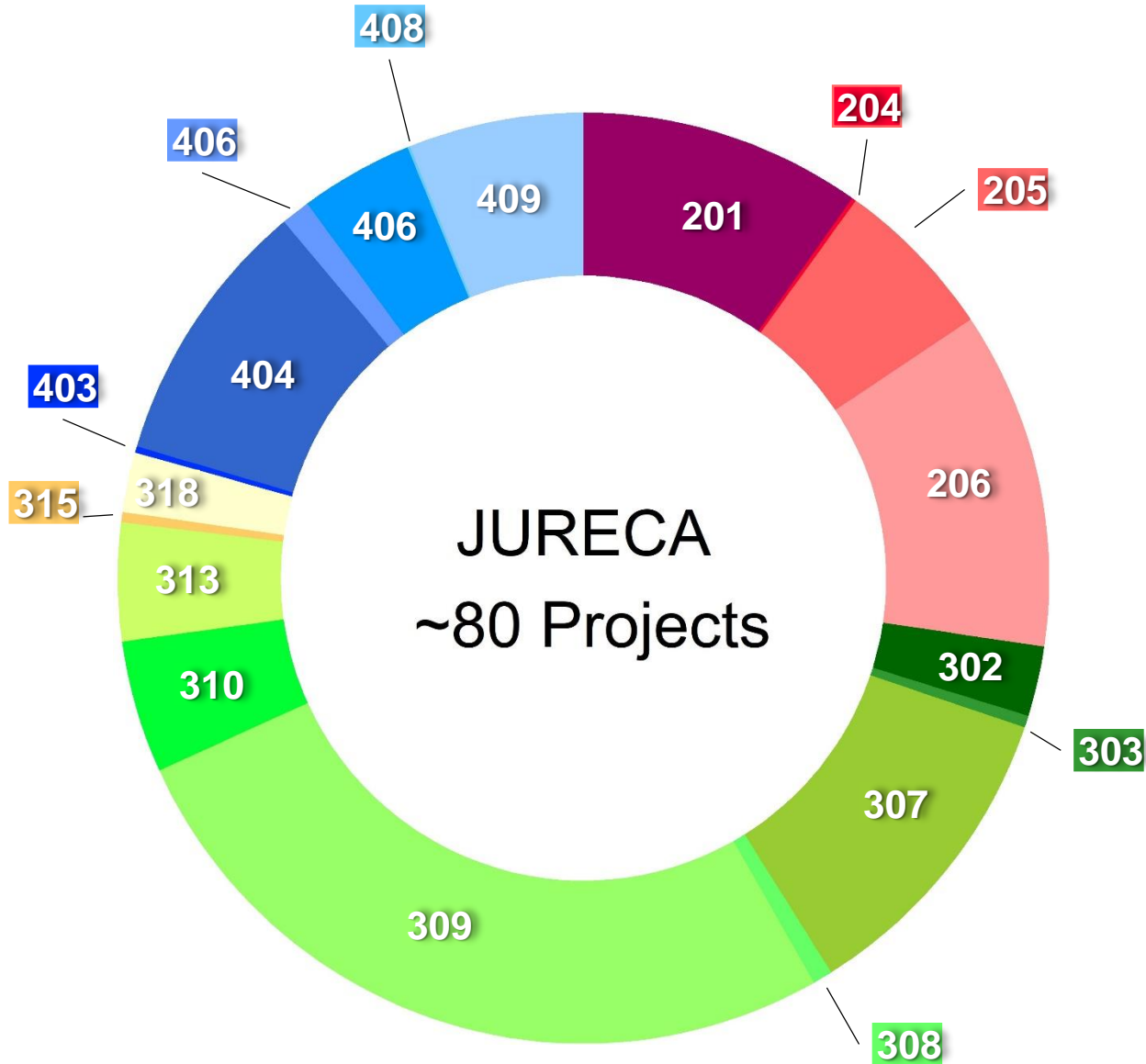
# RESEARCH FIELDS ON JUWELS (CLUSTER + BOOSTER)



## Research Fields

- 201** Basic Biological and Medical Research
- 205** Medicine
- 206** Neurosciences
- 207** Agriculture, Forestry and Veterinary Medicine
- 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
- 406** Materials Science
- 408** Electrical Engineering and Information Technology
- 409** Computer Science

# RESEARCH FIELDS ON JURECA (CLUSTER + BOOSTER)



## Research Fields

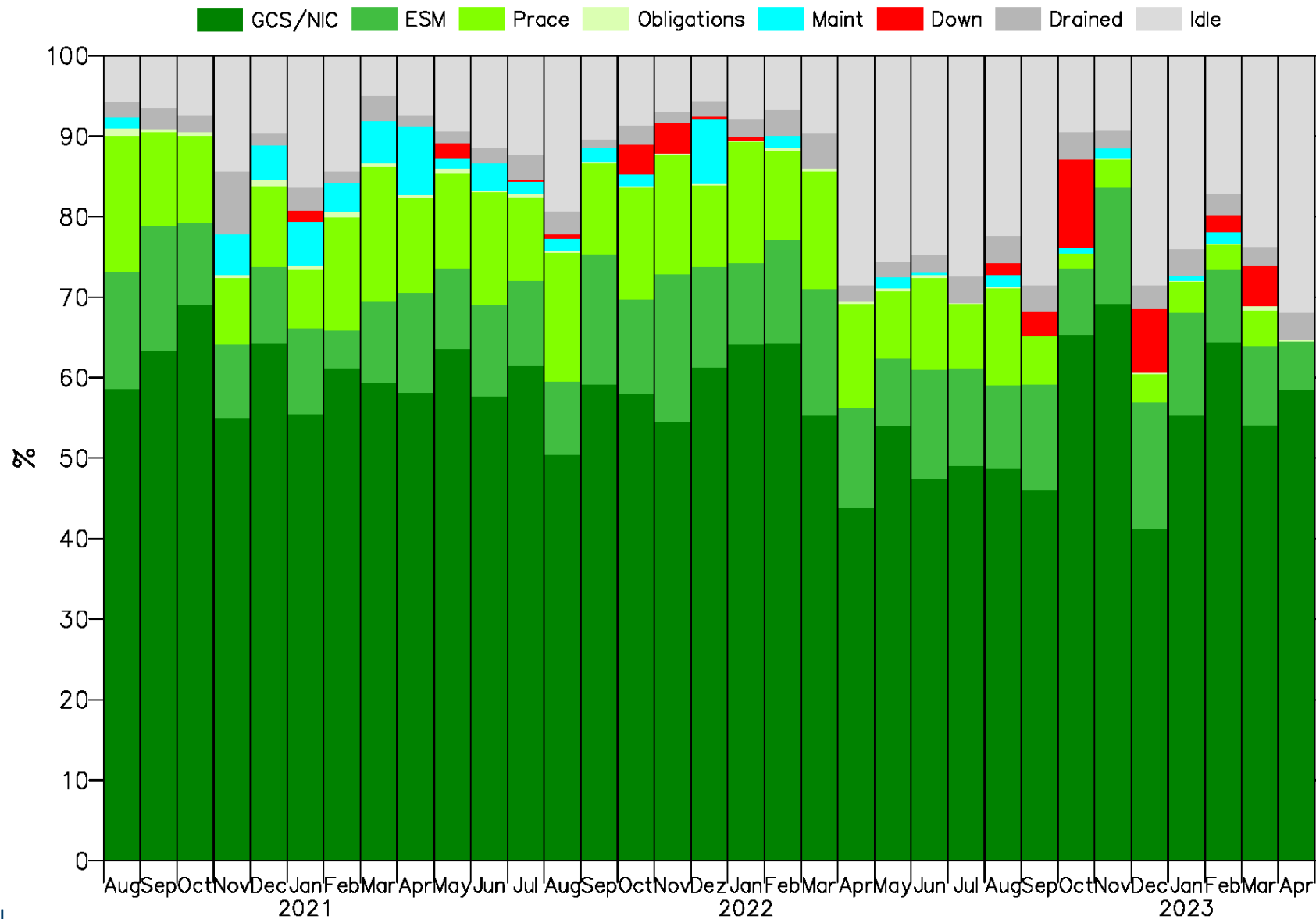
- 201** Basic Biological and Medical Research
- 204** Microbiology, Virology and Immunology
- 205** Medicine
- 206** Neurosciences
- 302** Particles, Nuclei and Fields
- 303** Chemical Solid State and Surface Research
- 307** Physical and Theoretical Chemistry
- 308** Condensed Matter Physics
- 309** Optics, Quantum Optics and Physics of Atoms, Molecules and Plasmas
- 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
- 406** Materials Science
- 407** Systems Engineering
- 408** Electrical Engineering and Information Technology
- 409** Computer Science

# NATIONAL AND EUROPEAN USER GROUPS



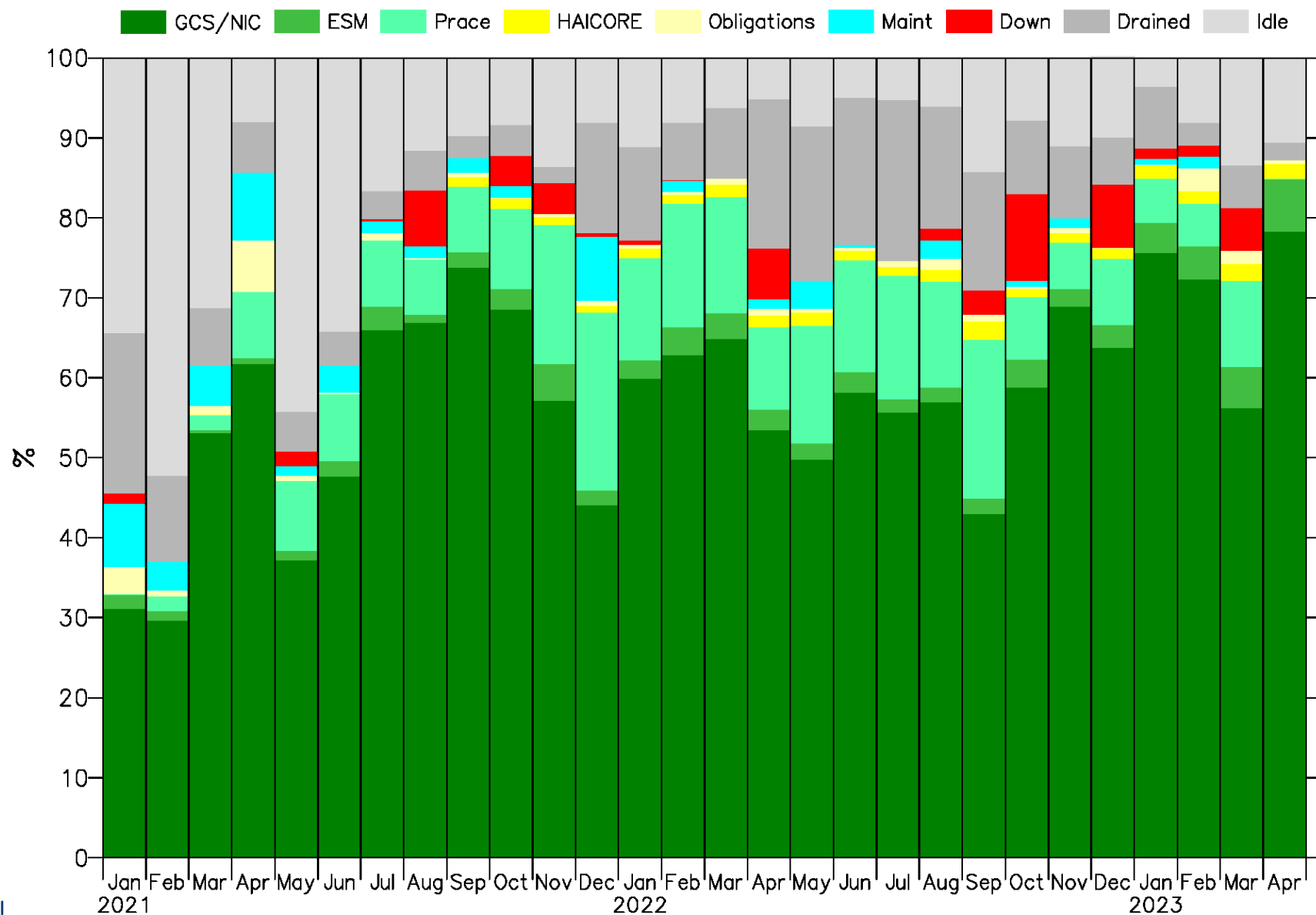
- Proposals for computer time accepted from Germany and Europe
- Peer review by international referees
- CPU time is granted by independent Scientific Councils

# JUWELS CLUSTER USAGE

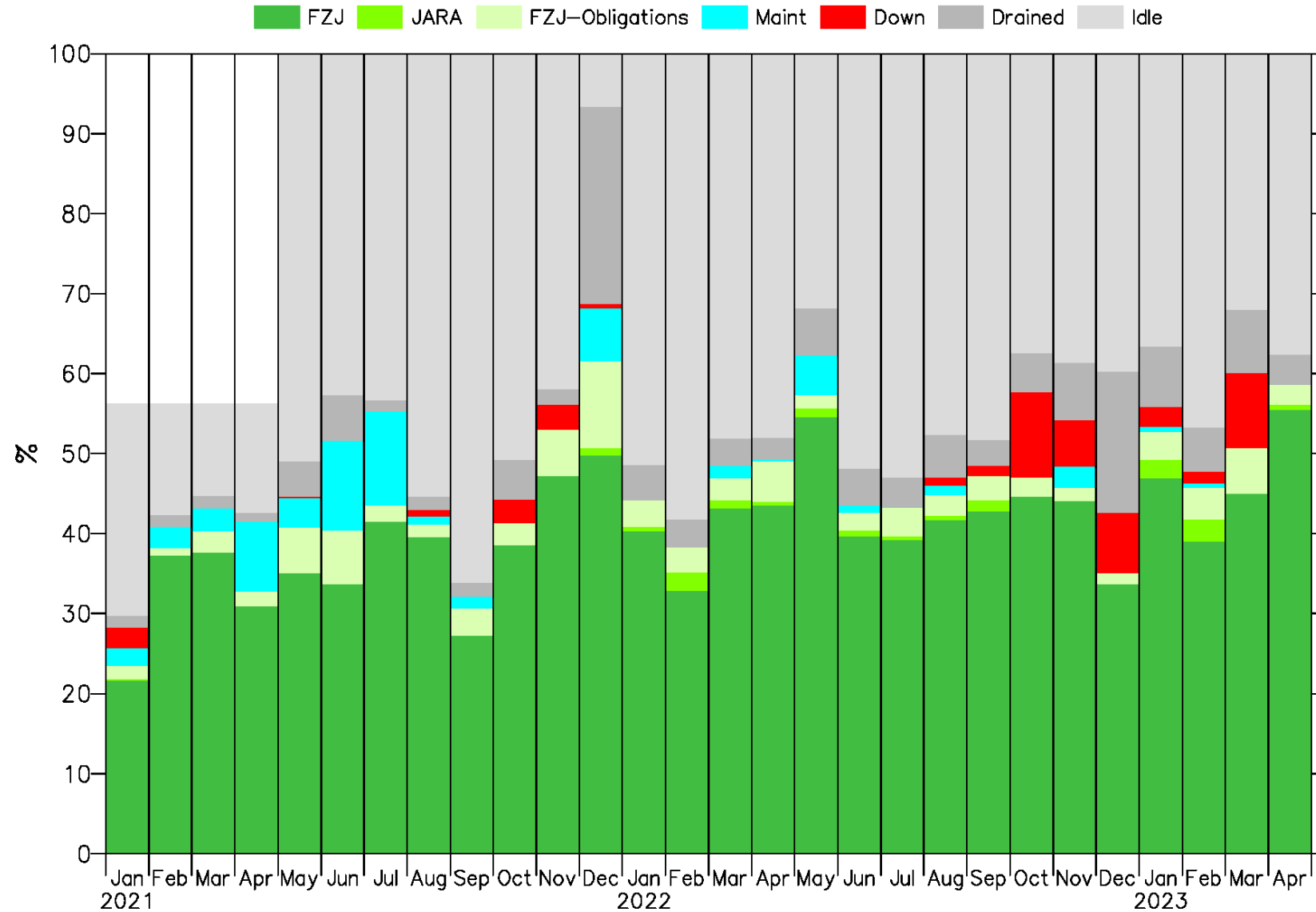




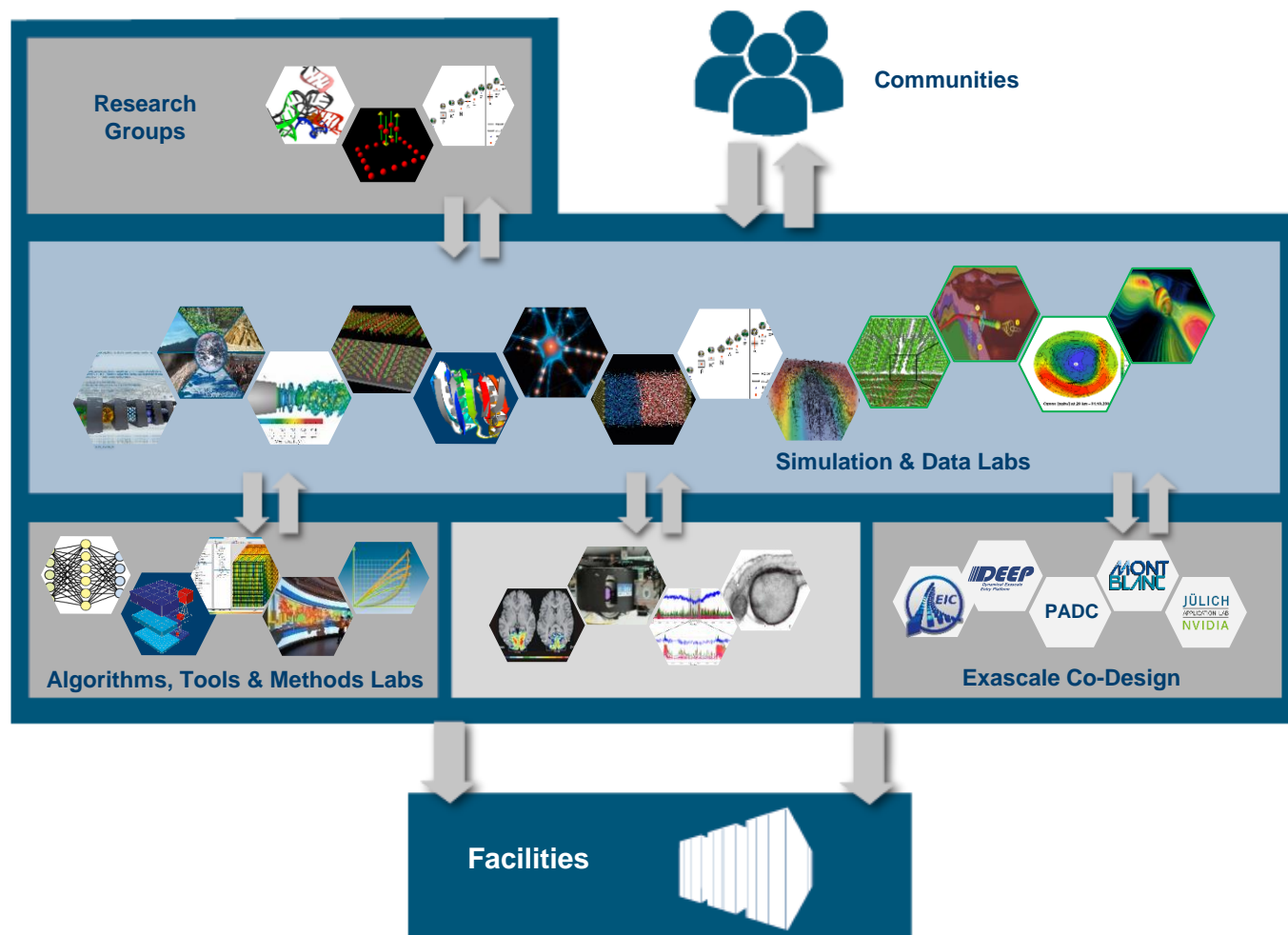
# JUWELS BOOSTER USAGE



# JURECA-DC USAGE

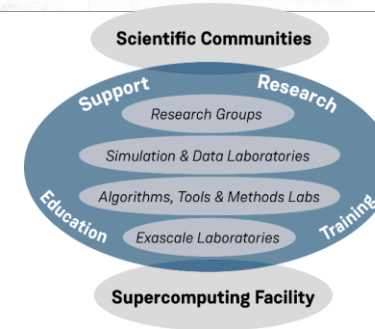


# SUPPORT AND RESEARCH LANDSCAPE AT JSC



# SUMMARY

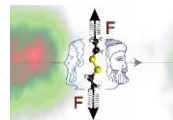
- **The Jülich Supercomputing Centre (JSC) provides**
  - Tier-0/1 HPC resources of the highest perf. class
  - high-end primary and domain-specific user support
  - ...
- **JSC expects to see**
  - breakthrough science
  - parallel applications, using efficient and optimized algorithms & programs on a substantial number of processors simultaneously



Sz. Borsanyi et al.,  
Science **347** (2015) 6229



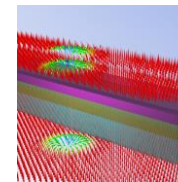
Sz. Borsanyi, Z. Fodor et al.,  
Nature **593** (2021) 51



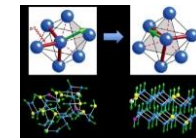
D. Marx et al.,  
Nature Chemistry **5** (2013) 685



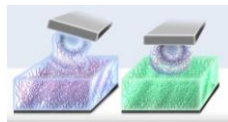
M. Lezaic et al.,  
Nature Materials **9** (2010) 649



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



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



S. de Beer, M. Müser  
Nature Communications **5** (2013)  
doi 10.1038/ncomms4781



U. Meissner et al.,  
Nature **528** (2015) 111



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



# BACKUP

# 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

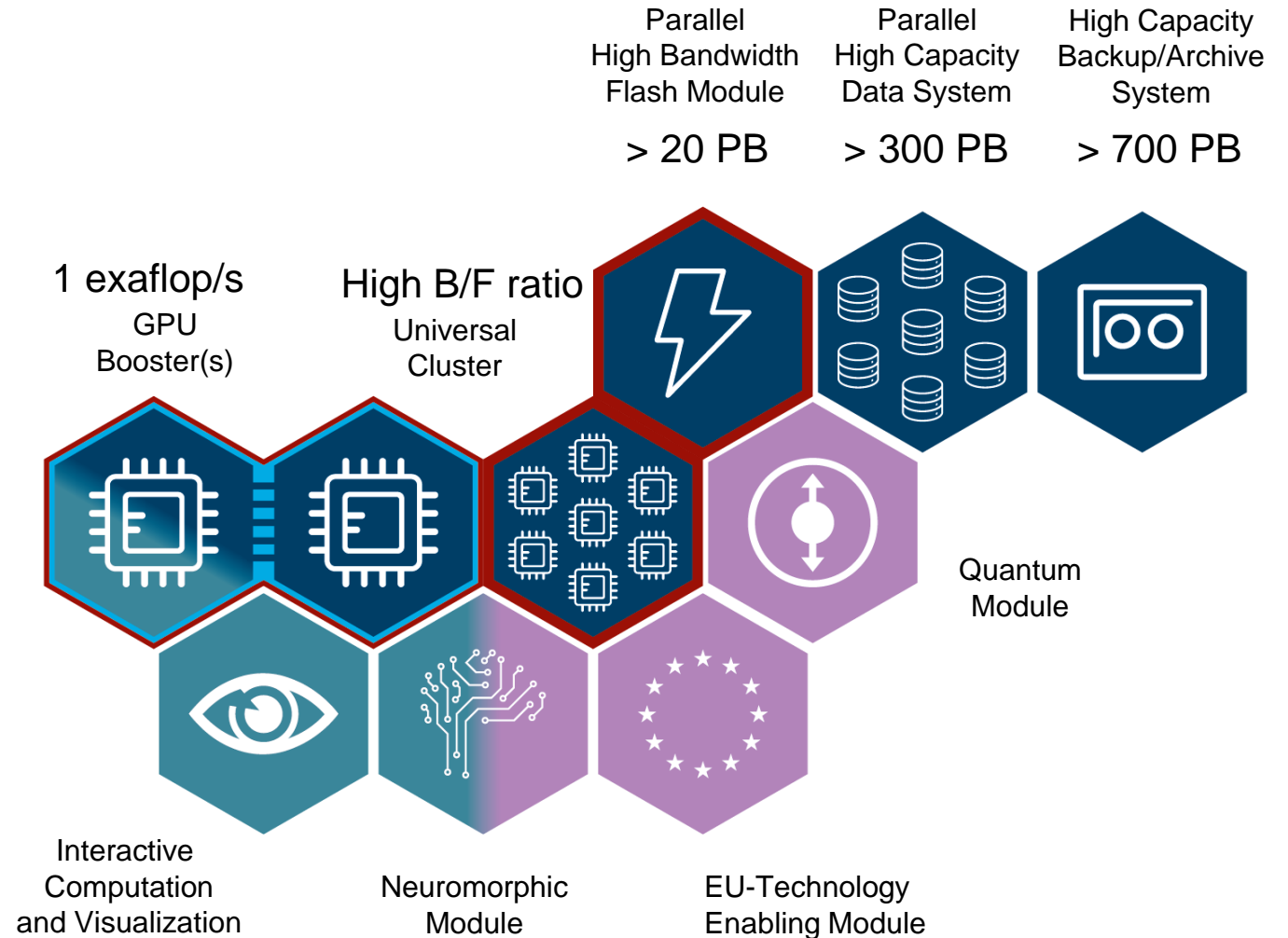
# Measures to Reduce Energy Consumption

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**





# JUWELS vs. JUPITER

	JUWELS	JUPITER
Cluster	<b>CPU:</b> Intel Xeon Platinum 8168 <b>GPU:</b> NVIDIA V100 <b>Peak:</b> 10 PFlop/s	<b>CPU:</b> ? (AMD, Arm, Intel,...) <b>GPU:</b> none <b>Focus:</b> High Byte/Flop
Booster	<b>CPU:</b> AMD Epyc Rome <b>GPU:</b> 4x NVIDIA A100 GPUs <b>Peak:</b> 70 PFlop/s	<b>CPU:</b> ? (AMD, Arm, Intel,...) <b>GPU:</b> ? (AMD, Intel, NVIDIA) <b>Rmax:</b> >1 EFlop/s
Network topology	Fat tree and DragonFly+	? (likely 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