

INTRODUCTION TO THE PROGRAMMING AND USAGE OF THE SUPERCOMPUTING RESOURCES IN JÜLICH

ONLINE COURSE PROVIDED BY

JÜLICH
SUPERCOMPUTING
CENTRE

21.11.2022 | BERND MOHR



SCHEDULE MONDAY – NOVEMBER 21ST

12:30 - 12:50	Welcome and Introduction to JSC	Bernd Mohr (JSC)
12:50 - 13:30	HPC in a Nutshell	Ilya Zhukov (JSC)
13:30 - 14:20	User Portal and Job Monitoring	Jolanta Zjupa (JSC)
14:20 - 15:00	Break	
15:00 - 15:45	JupyterLab — Supercomputing in your Browser	Jens Henrik Göbbert (JSC)
15:50 - 16:25	JUST and IBM Spectrum Scale: Data management	Stephan Graf (JSC)
16:30 - 17:00	JSC Systems — JUWELS, JURECA & JUSUF	Damian Alvarez (JSC)

SCHEDULE TUESDAY – NOVEMBER 22ND

09:00 - 10:00	Hands-on I – Access	
10:00 - 11:00	Hands-on I – UNIX Shell Basics	
11:00 - 12:00	Hands-on I – Environment	
12:00 - 13:00	Lunch	
13:00 - 13:30	HPC Software - Modules, Libraries & Software	Ruth Schöbel (JSC)
13:35 - 14:20	Work load management with Slurm	Chrysovalantis Paschoulas (JSC)
14:20 - 15:00	Break	
15:00 - 16:20	HPC Software - Compiler and Tools	Michael Knobloch (JSC)
16:25 - 17:00	Uniform Resource Access, Data Access and Cloud Resources	Björn Hagemeier (JSC)

SCHEDULE WEDNESDAY – NOVEMBER 23RD

09:00 - 10:00	Hands-on II – Software Modules	
10:00 - 11:00	Hands-on II – Custom software	
11:00 - 12:00	Hands-on II – Accounting & Running Jobs	
12:00 - 13:00	Lunch	
13:00 - 14:20	JURECA and JUWELS –Tuning and Tweaks	Heinrich Bockhorst (Intel)
14:20 - 15:00	Break	
15:00 - 15:30	Proper Pinning Prevents Pretty Poor Performance	Thorsten Hater (JSC)
15:35 - 17:00	Using GPU accelerators on JURECA and JUWELS	Andreas Herten (JSC)

SCHEDULE THURSDAY - NOVEMBER 24TH

09:00 - 10:00	Hands-on III – CPU Affinity	
10:00 - 11:00	Hands-on III – Using GPUs	
11:00 - 12:00	Hands-on III – Remote Visualisation	Herwig Zilken (JSC)
12:00 - 13:00	Lunch	
13:00 - 13:40	Evolution of the Sequana System Architecture	Thomas Warschko (Atos)
13:45 - 14:30	ParTec Cluster Management	Patrick Küven (ParTec)
14:30 - 15:00	Break	
15:00 - 15:45	Deep Learning on Supercomputers	Alexandre Strube (JSC)
15:45 - 16:00	Closing Discussion	Jolanta Zjupa & Ilya Zhukov (JSC)

SCHEDULE FRIDAY - NOVEMBER 25TH (OPTIONAL)

09:00 - 12:00	Hands-on IV — Finish what you didn't manage & Bring your own code	Jolanta Zjupa & Ilya Zhukov (JSC)
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ORGANISATIONAL INFORMATION

- Certificates will be based on attendance of the hands-on component.
- Slides of selected talks are available after the course at <https://www.fz-juelich.de/en/ias/jsc/education/training-courses/training-materials>
- During a talk you can ask questions either in this Zoom chat or in the Slack chat.
- After a talk you can also ask questions verbally by turning on your microphone.
- For Hands-on questions please use only the Slack chat.
- Only screensharing will be recorded and published if allowed.
- More workshops and conferences on JSC website: <https://www.fz-juelich.de/en/ias/jsc/education/training-courses>
- Twitter: @fzj_jsc, @fzj_jscuser



JÜLICH SUPERCOMPUTING CENTRE (JSC) INTRODUCTION

NOVEMBER 21, 2022 | 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 – PRACE (+ EuroHPC JU), EU projects

- **Application support**

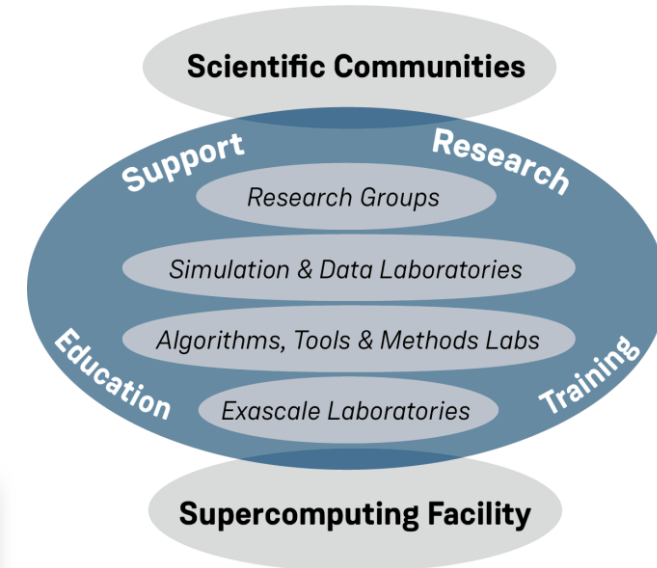
- Unique support & research environment at JSC
- Peer review support and coordination

- **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



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)
 - European Research Infrastructure PRACE
 - Project Access: Biannual CfPs since June 2010 up to March 2022
 - Call for preparatory access open, no closing dates
 - ESM partition for Earth System scientists only (20% of JUWELS Cluster and 10% of JUWELS Booster)
 - AI partition ($\sim 2\%$ 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)

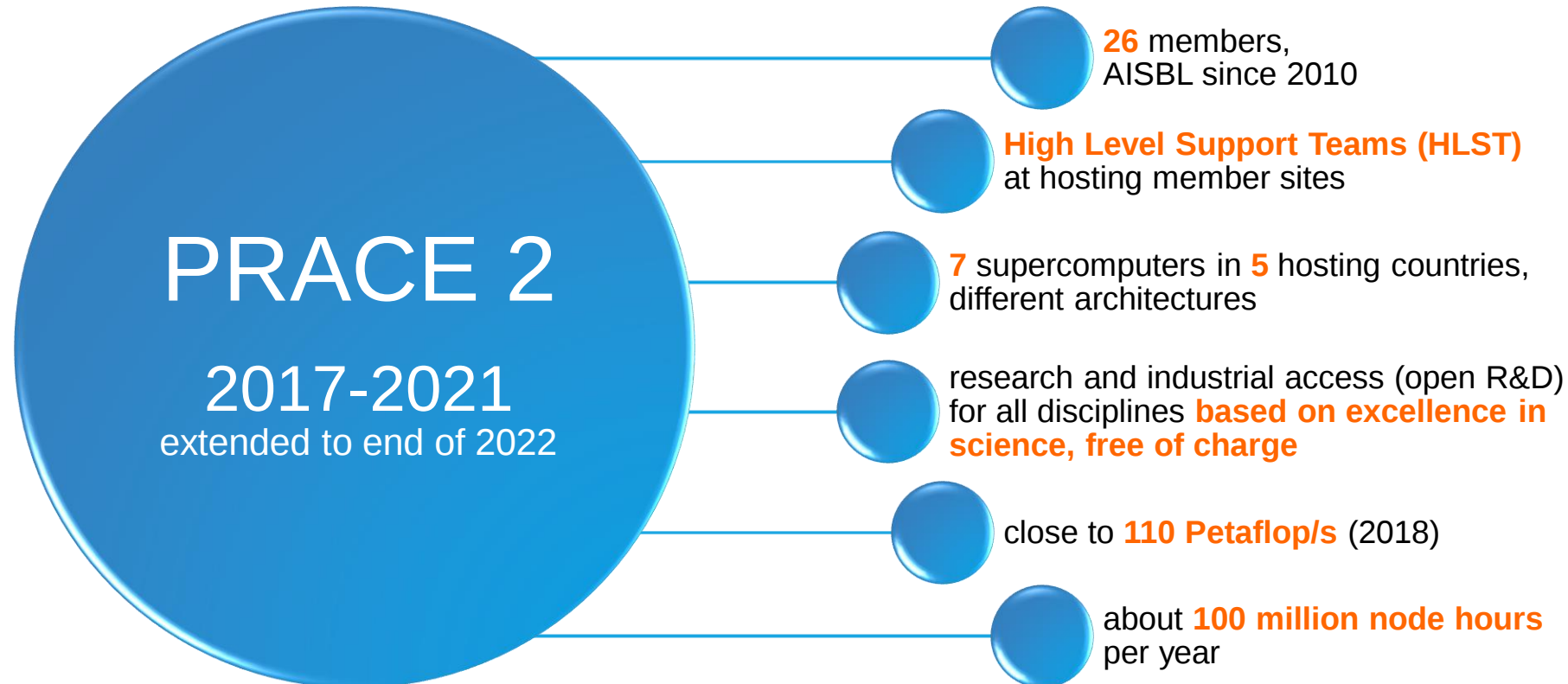
GAUSS CENTRE FOR SUPERCOMPUTING (GCS)

- **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

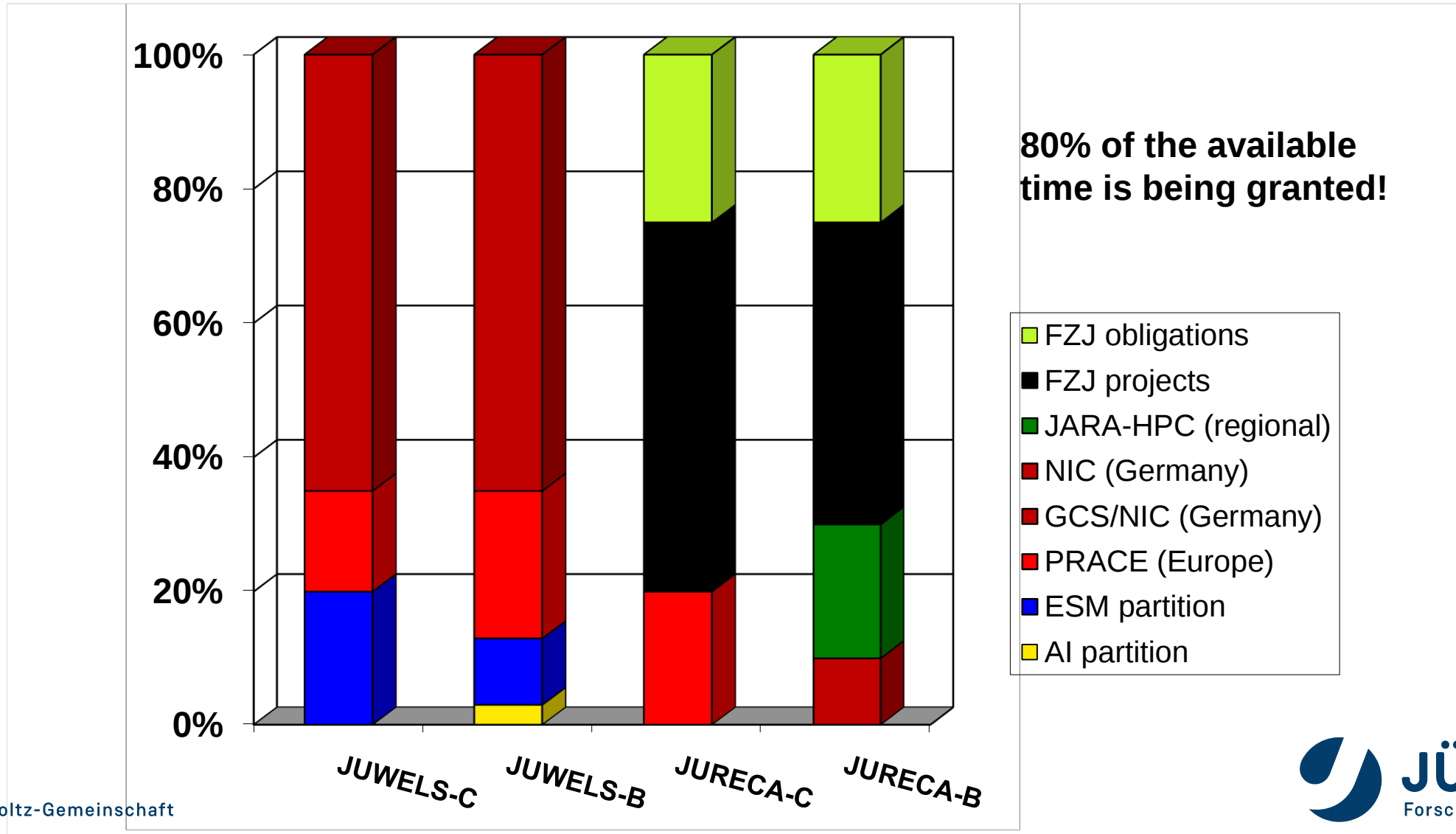


PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

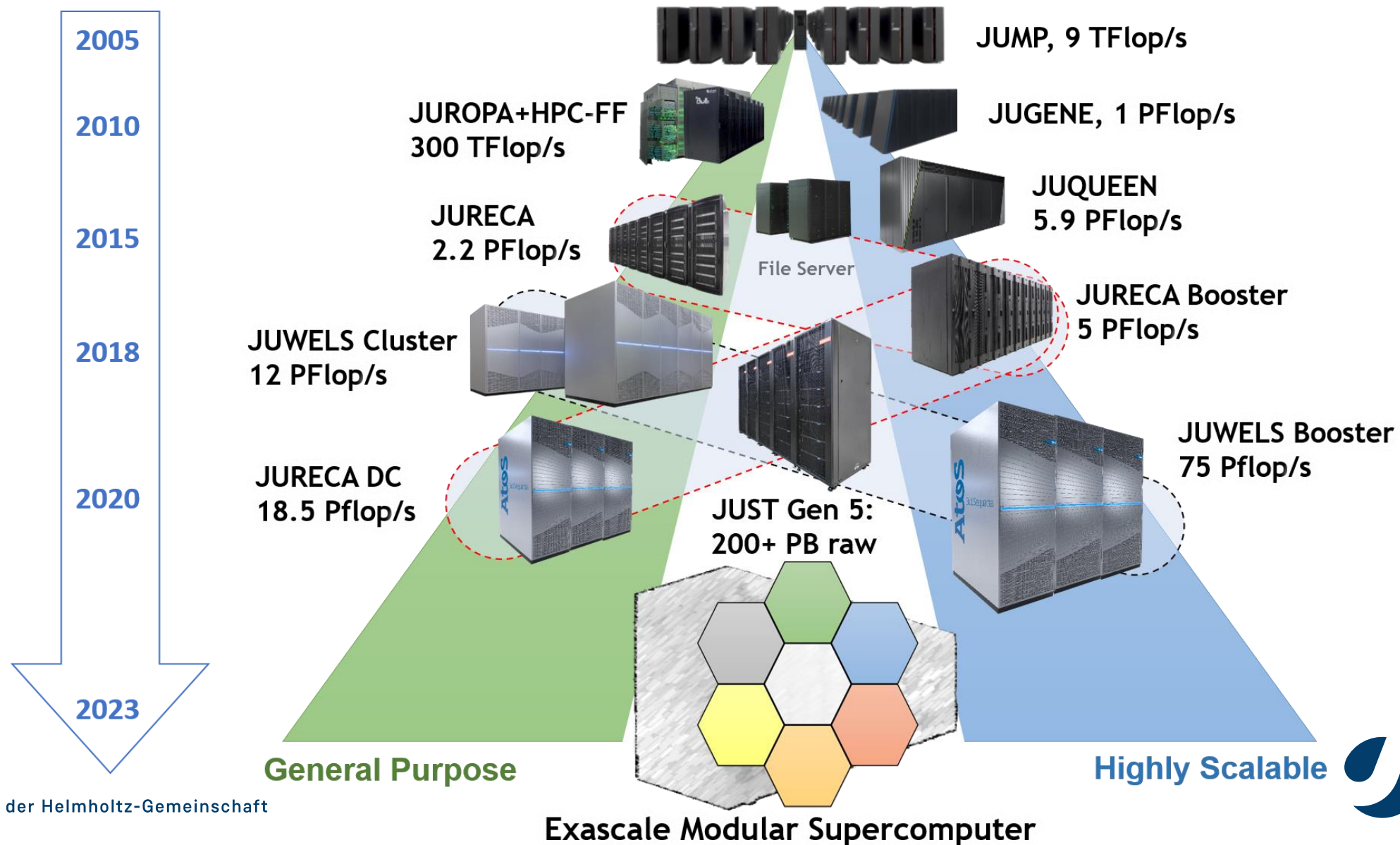
The European HPC e-infrastructure (ESFRI)



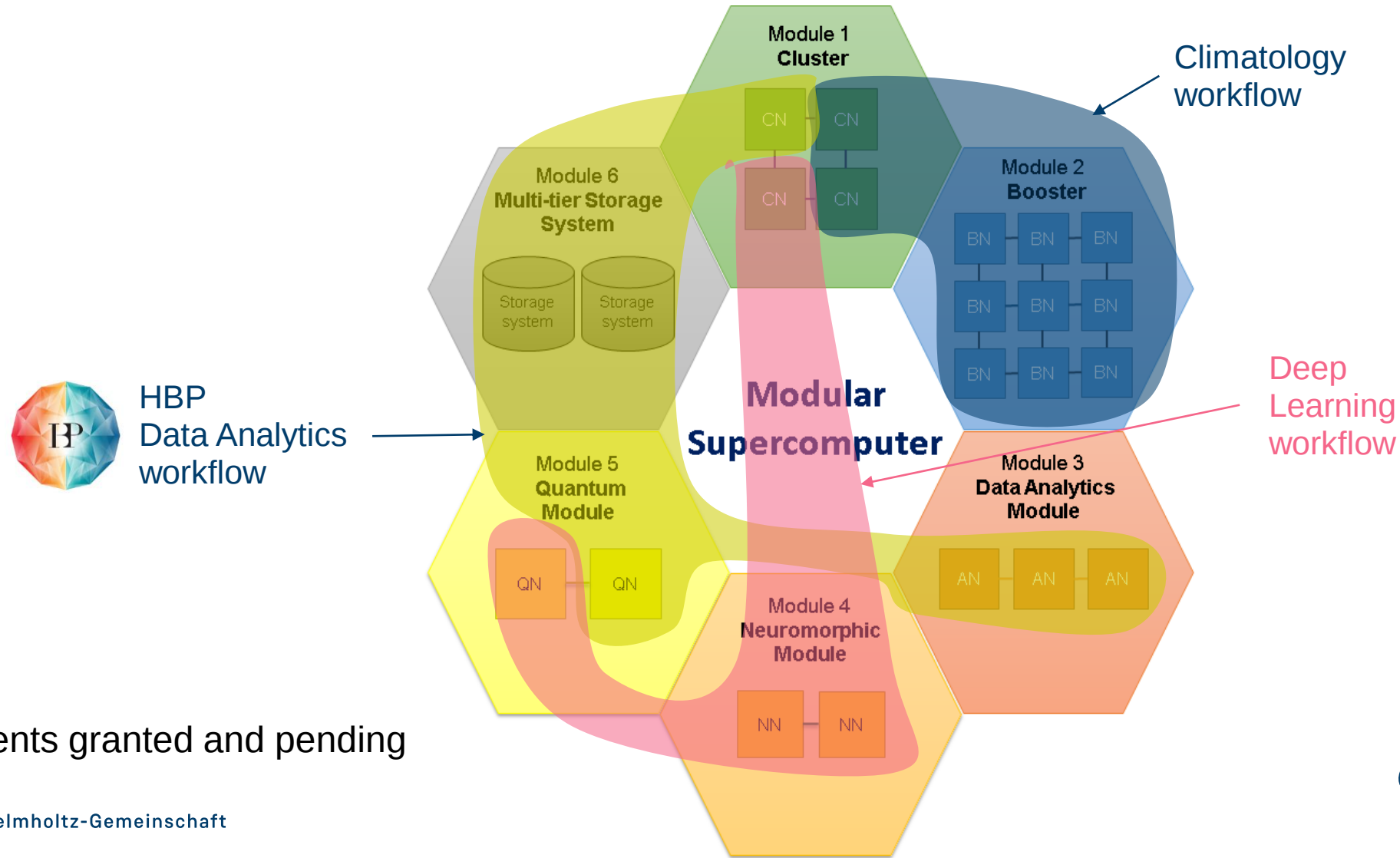
STAKEHOLDER'S COMPUTE TIME SHARES



(DUAL) HARDWARE STRATEGY AT JSC

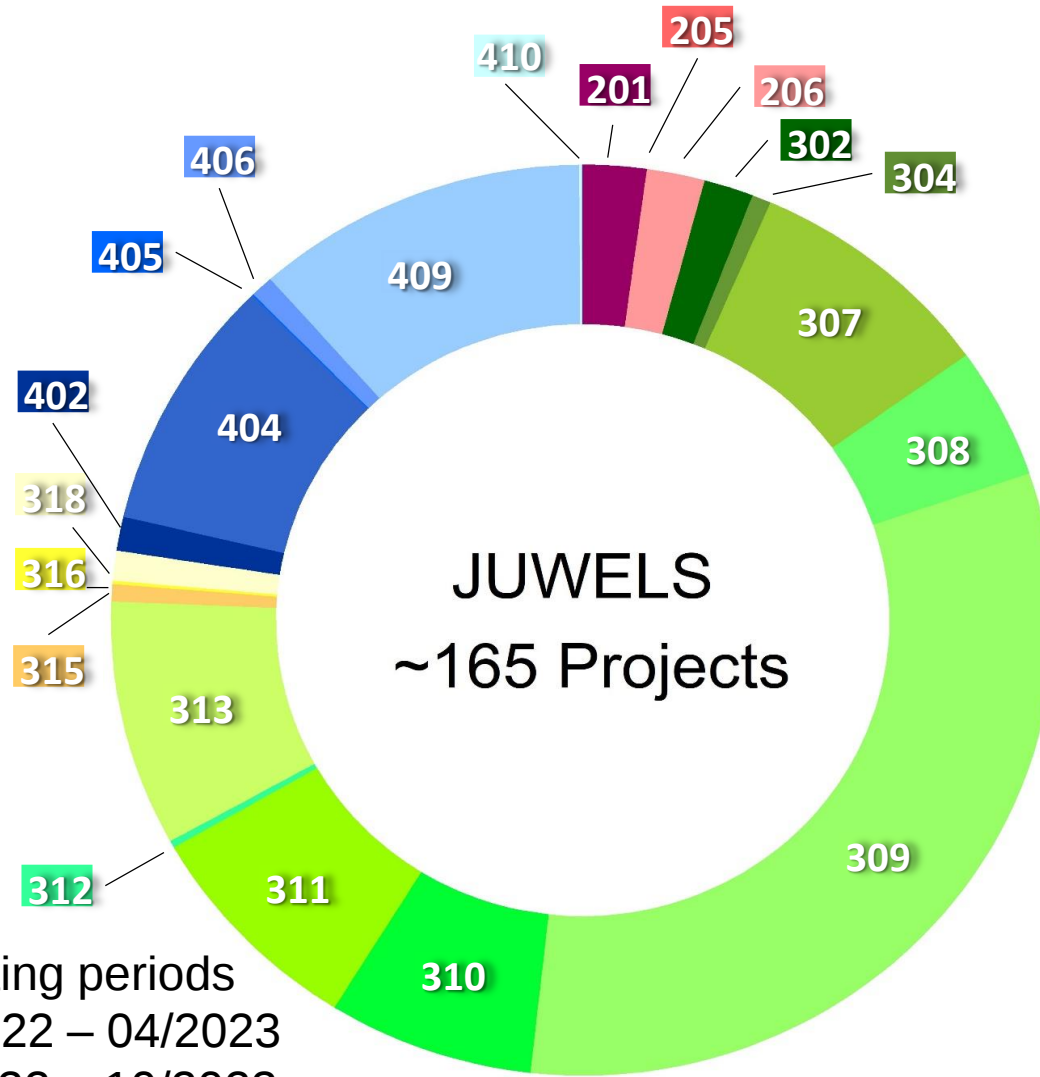


... AND EVOLUTION TO A MODULAR SUPERCOMPUTING ARCHITECTURE



*Patents granted and pending

RESEARCH FIELDS ON JUWELS (CLUSTER + BOOSTER)

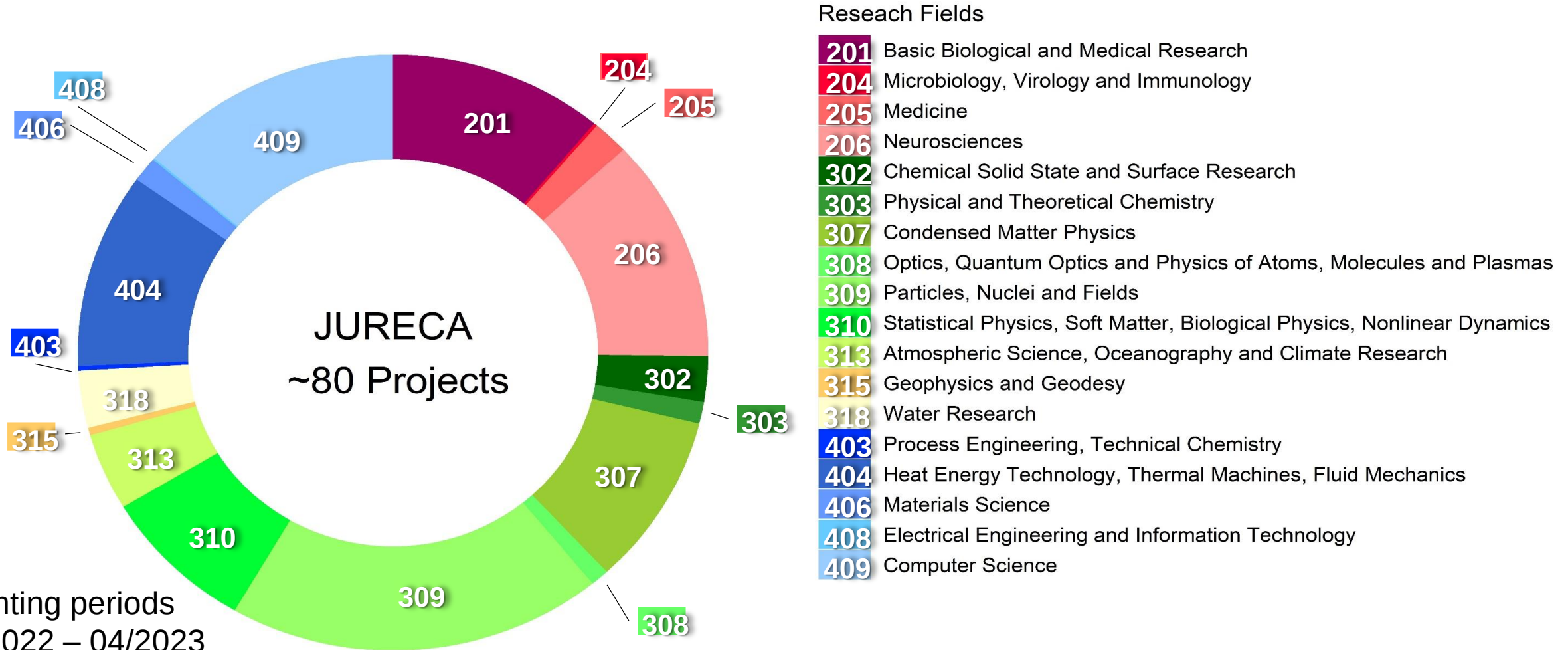


Research Fields

- 201 Basic Biological and Medical Research
- 205 Medicine
- 206 Neurosciences
- 302 Chemical Solid State and Surface Research
- 304 Analytical Chemistry, Method Development (Chemistry)
- 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
- 409 Computer Science
- 410 Construction Engineering and Architecture

Granting periods
05/2022 – 04/2023
11/2022 – 10/2023

RESEARCH FIELDS ON JURECA (CLUSTER + BOOSTER)

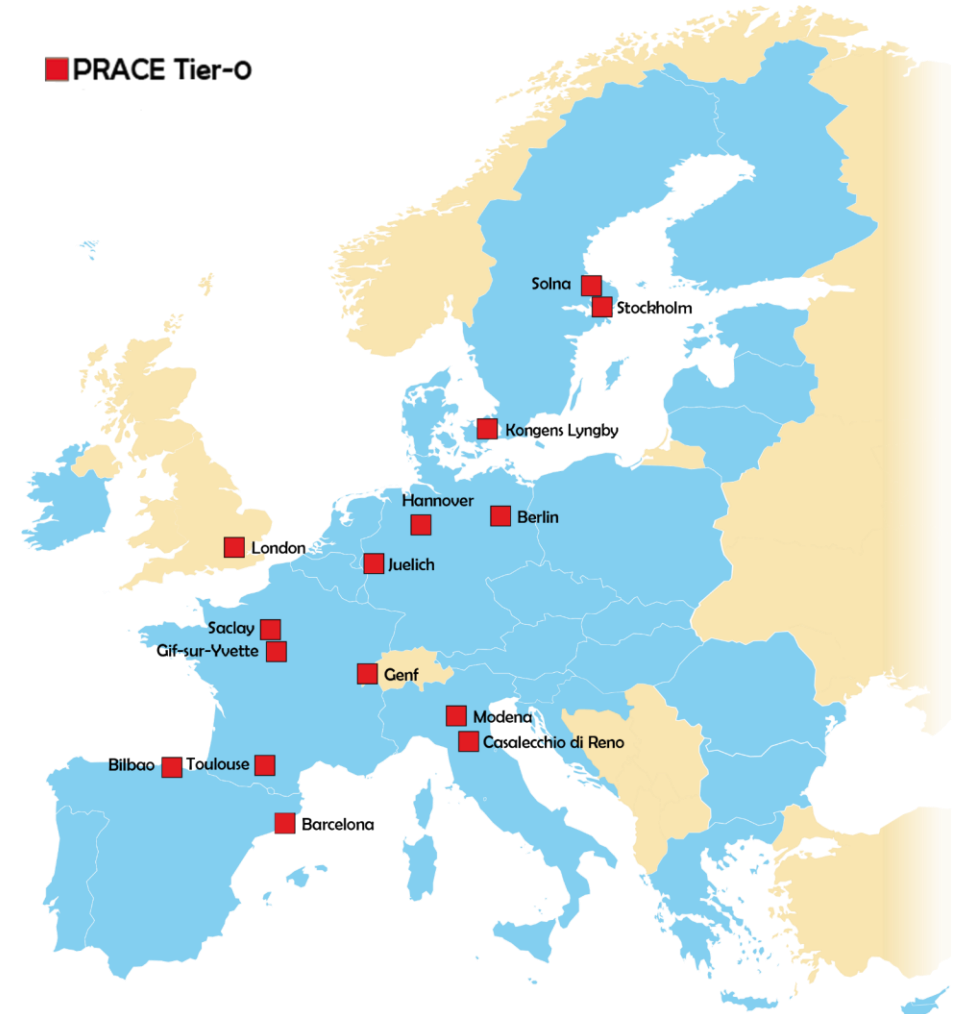


Granting periods
05/2022 – 04/2023
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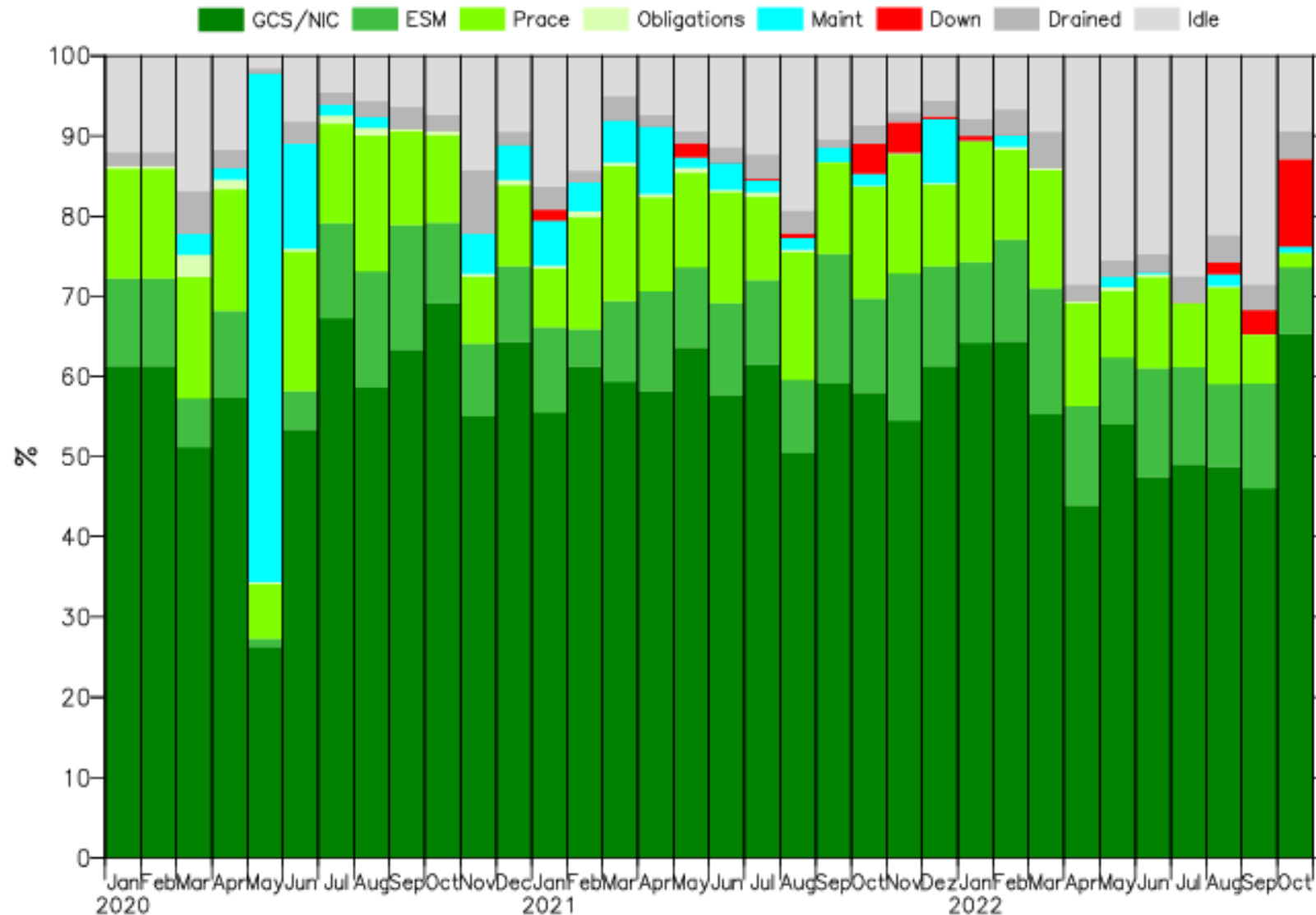
NATIONAL AND EUROPEAN USER GROUPS



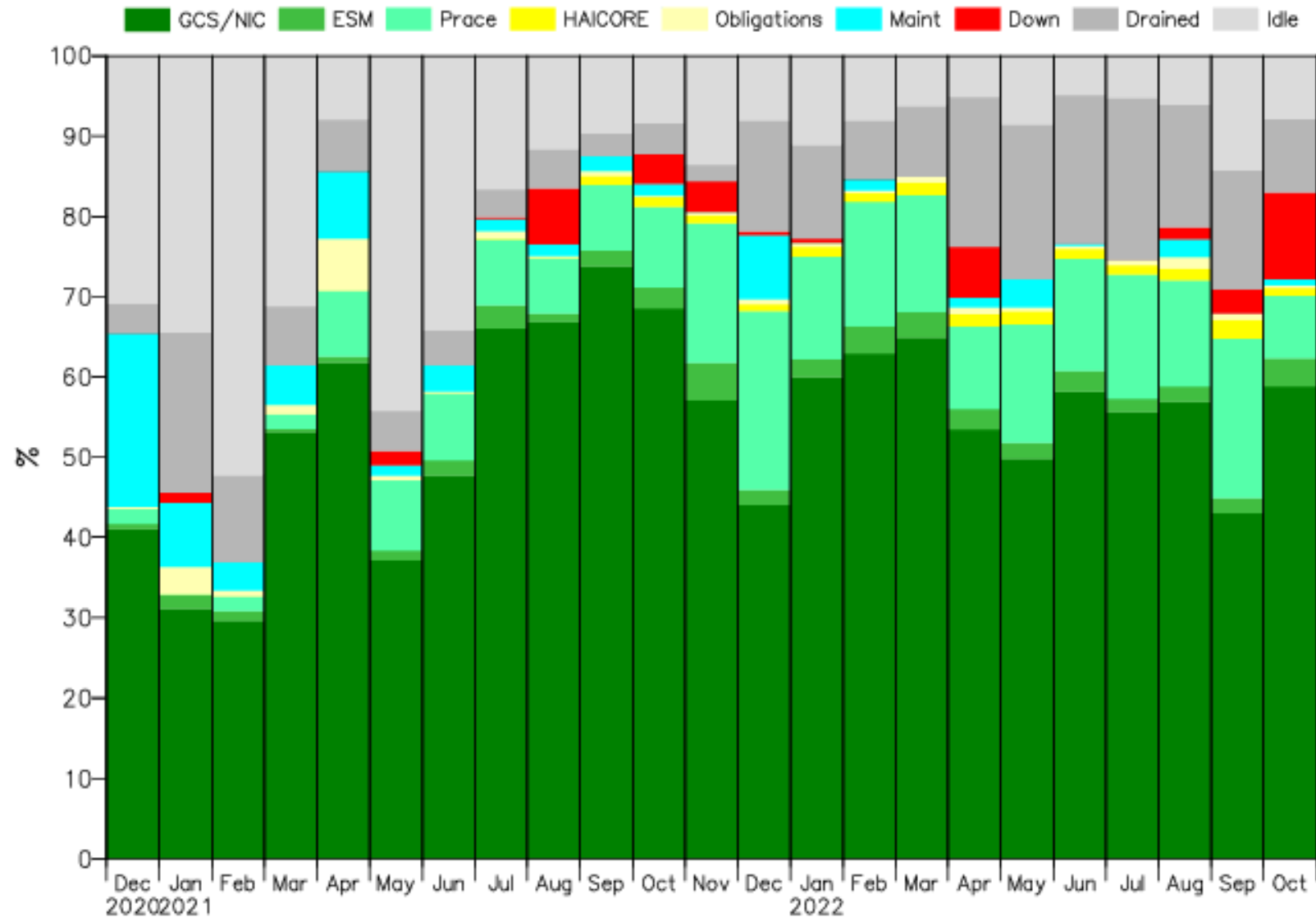
- Proposals for computer time accepted from Germany and Europe
- Peer review by international referees
- CPU time is granted by independent Scientific Councils



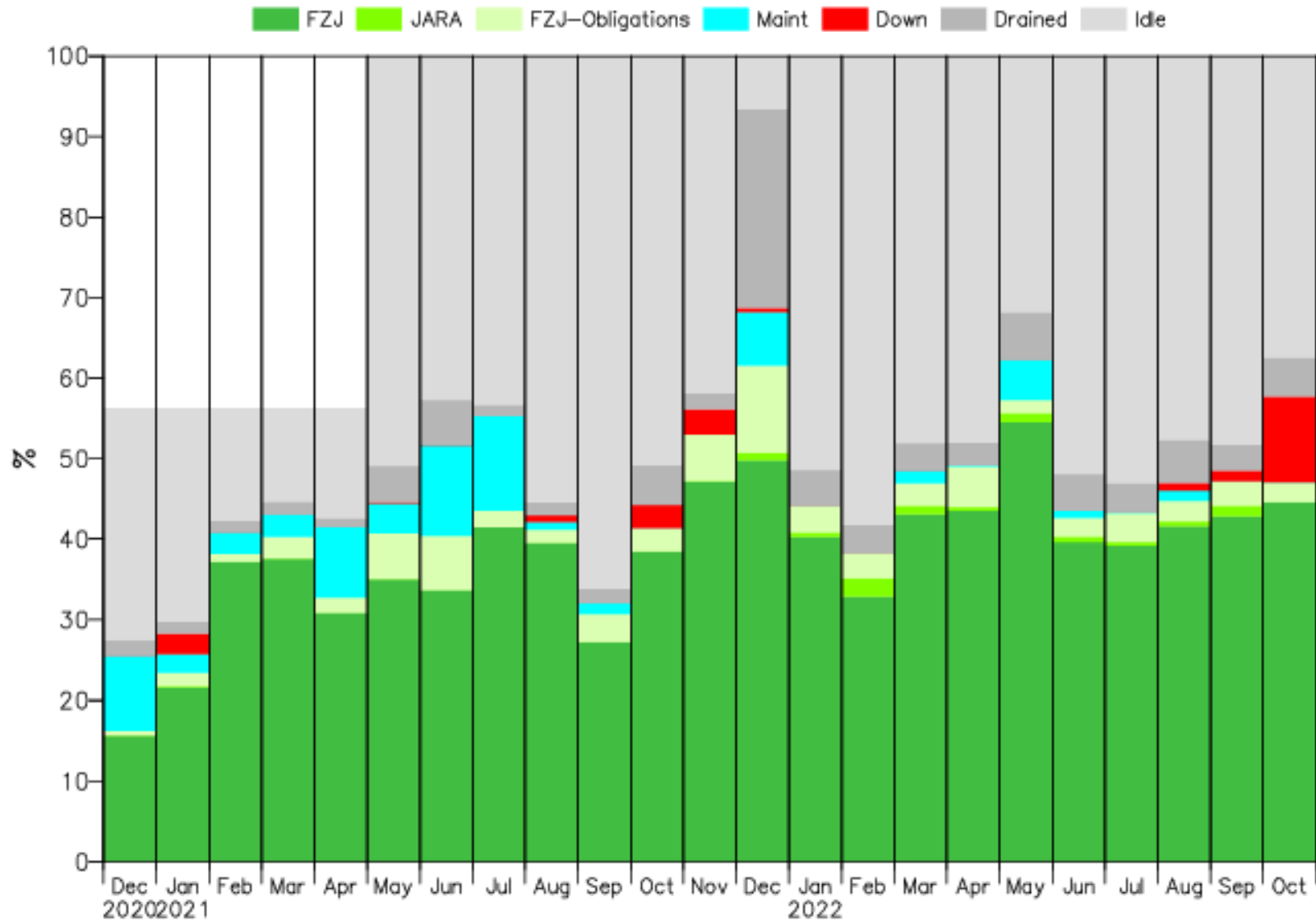
JUWELS CLUSTER USAGE



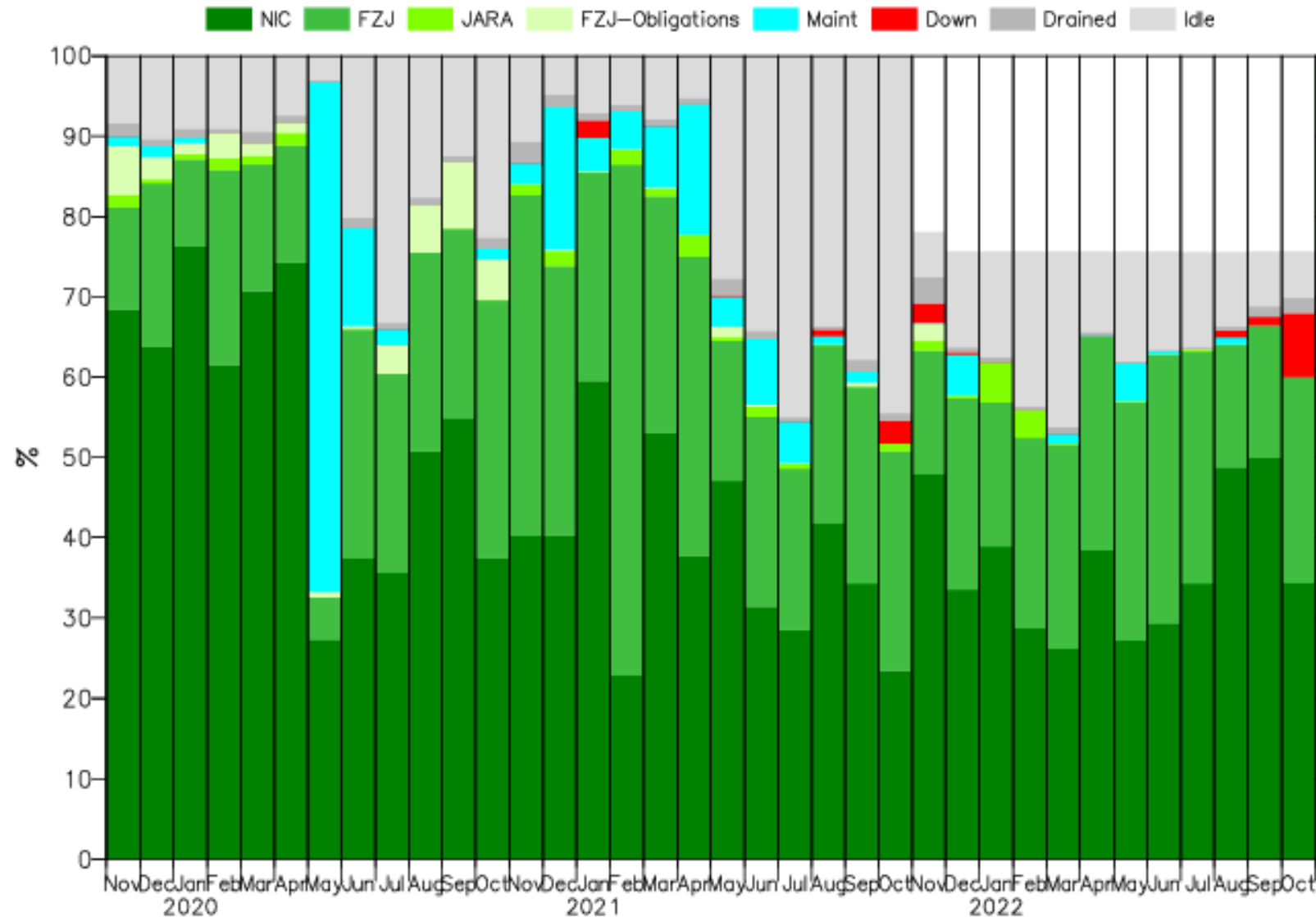
JUWELS BOOSTER USAGE



JURECA-DC USAGE

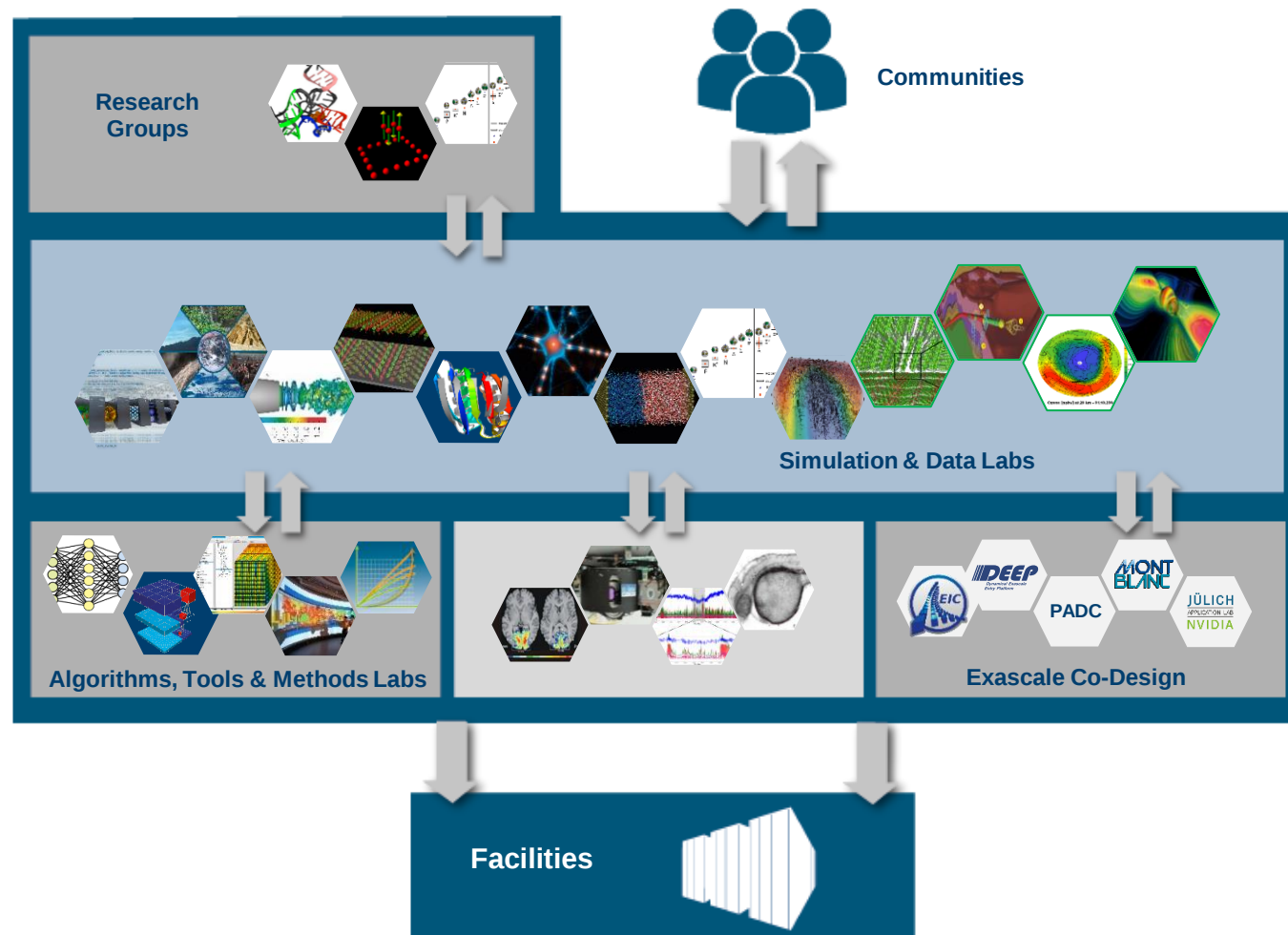


JURECA BOOSTER USAGE



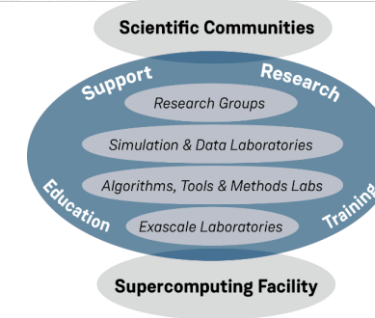
JURECA-Booster: since Nov 4th, 2021: 1240 (of 1640) nodes

SUPPORT AND RESEARCH LANDSCAPE AT JSC



SUMMARY

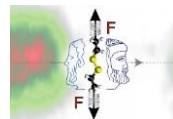
- The Jülich Supercomputing Centre (JSC) provides
 - Tier-0/1 HPC resources of the highest perf. class
 - high-end primary and domain-specific user support
 - ...
- JSC expects to see
 - breakthrough science
 - parallel applications, using efficient and optimized algorithms & programs on a substantial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



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



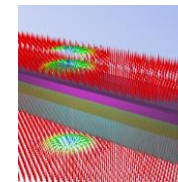
Sz. Borsanyi, Z. Fodor et al.,
Nature **593** (2021) 51



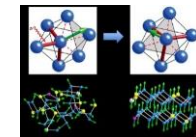
D. Marx et al.,
Nature Chemistry **5** (2013) 685



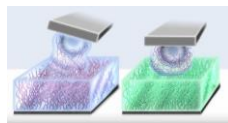
M. Lezaic et al.,
Nature Materials **9** (2010) 649



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