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

ONLINE COURSE PROVIDED BY

JÜLICH SUPERCOMPUTING CENTRE

16.05.2022 I BERND MOHR

SCHEDULE MONDAY – MAY 16TH

13:00 - 13:20	Welcome and Introduction to JSC	Bernd Mohr (JSC)
13:20 - 13:40	HPC in a Nutshell	Ilya Zhukov
13:45 - 14:30	Job Monitoring and User Portal	Max Holicki (JSC)
14:30 - 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 – MAY 17TH

09:00 - 10:00	Hands-on I – Access	
10:00 - 11:00	Hands-on II – UNIX Shell Basics	
11:00 - 12:00	Hands-on III – 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 24TH

09:00 - 10:00	Hands-on I – Software Modules	
10:00 - 11:00	Hands-on II – Custom software	
11:00 - 12:00	Hands-on III – 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 25TH

09:00 - 10:00	Hands-on I – CPU Affinity	
10:00 - 11:00	Hands-on II – Using GPUs	
11:00 - 12:00	Hands-on III – Remote Visualisation	Herwig Zilken(JSC)
12:00 - 13:00	Lunch	
13:00 - 13:45	Evolution of the Sequana System Architecture	Thomas Warschko (Atos)
13:50 - 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	Max Holicki & Ilya Zhukov (JSC)

ORGANISATIONAL INFORMATION

- Certificates will be based on attendance of the hands-on component.

- Slides of select talks are available after the course at
  - http://www.fz-juelich.de/jsc (English)
    Expertise - Services - Documentation – Presentations

- You can ask questions either in this Zoom chat or in the Slack Chat.
- After a talk you can verbally ask questions by turning on your microphone.
- Hands-on questions please only in Slack Chat.

- More workshops and conferences on JSC website: www.fz-juelich.de/ias/jsc/events

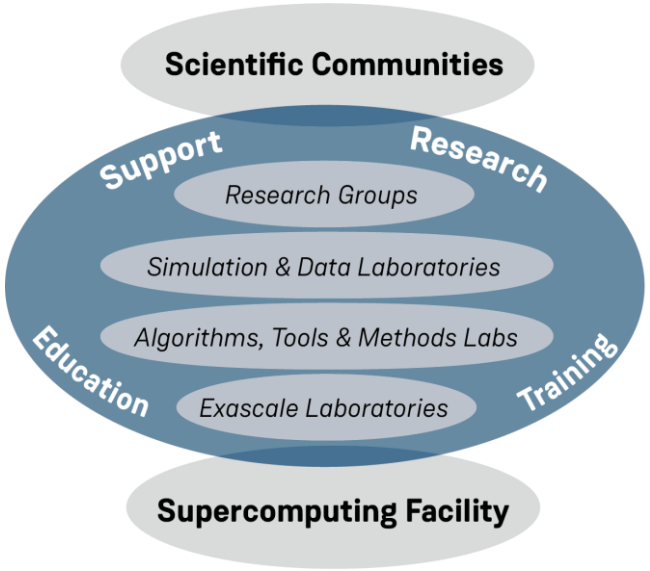
- Twitter: @fzj_jsc, @fzj_jscuser

JÜLICH SUPERCOMPUTING CENTRE (JSC) INTRODUCTION

MAY 16, 2022 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 – 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**



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)
  - 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 (~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)

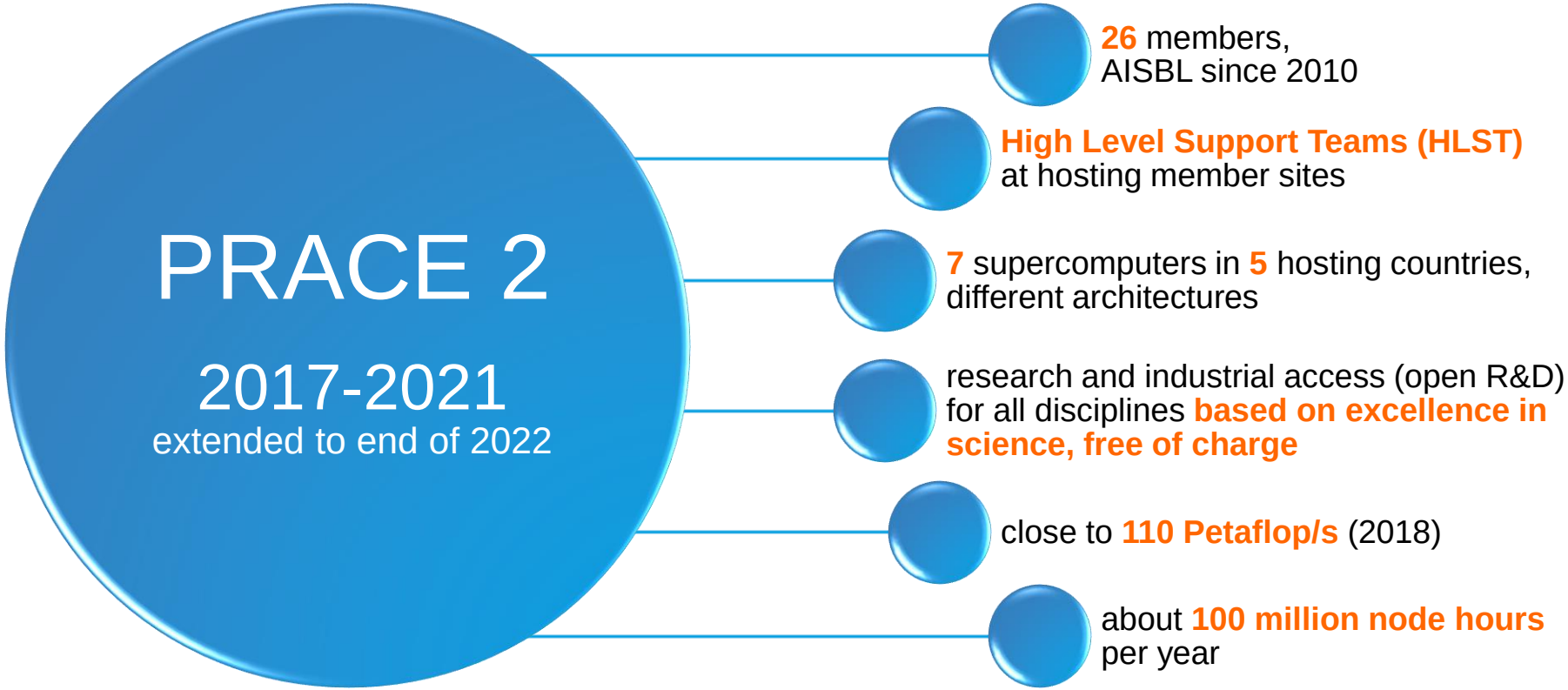
GAUSS CENTRE FOR SUPERCOMPUTING (GCS)

- **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

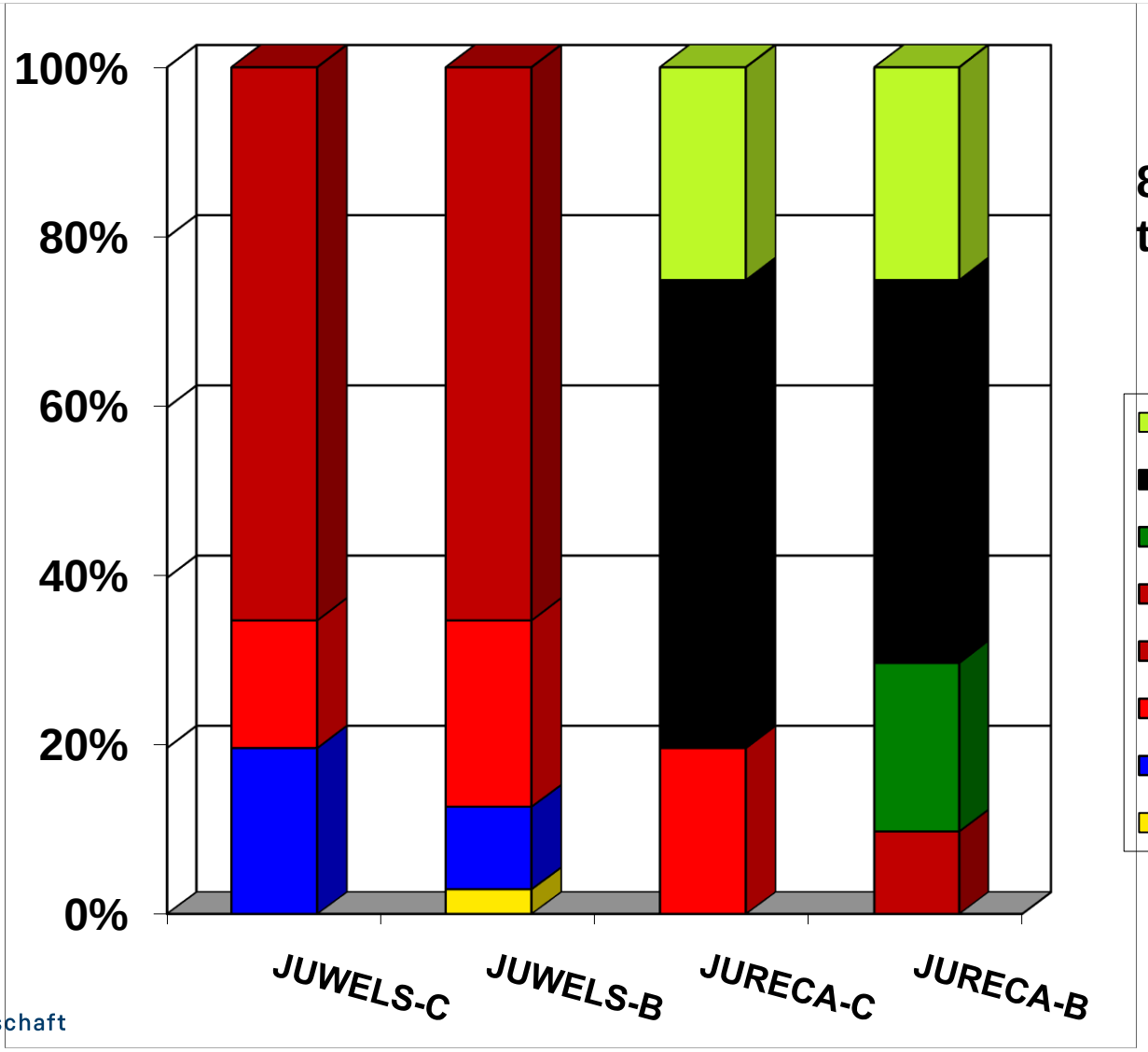
- **Key facts**
  - To date in sum more than 140 Petaflops (continuously expanding)
  - 600 people for operation, HPC R&D, services, training
  - Extensive know-how in key scientific fields

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

The European HPC e-infrastructure (ESFRI)

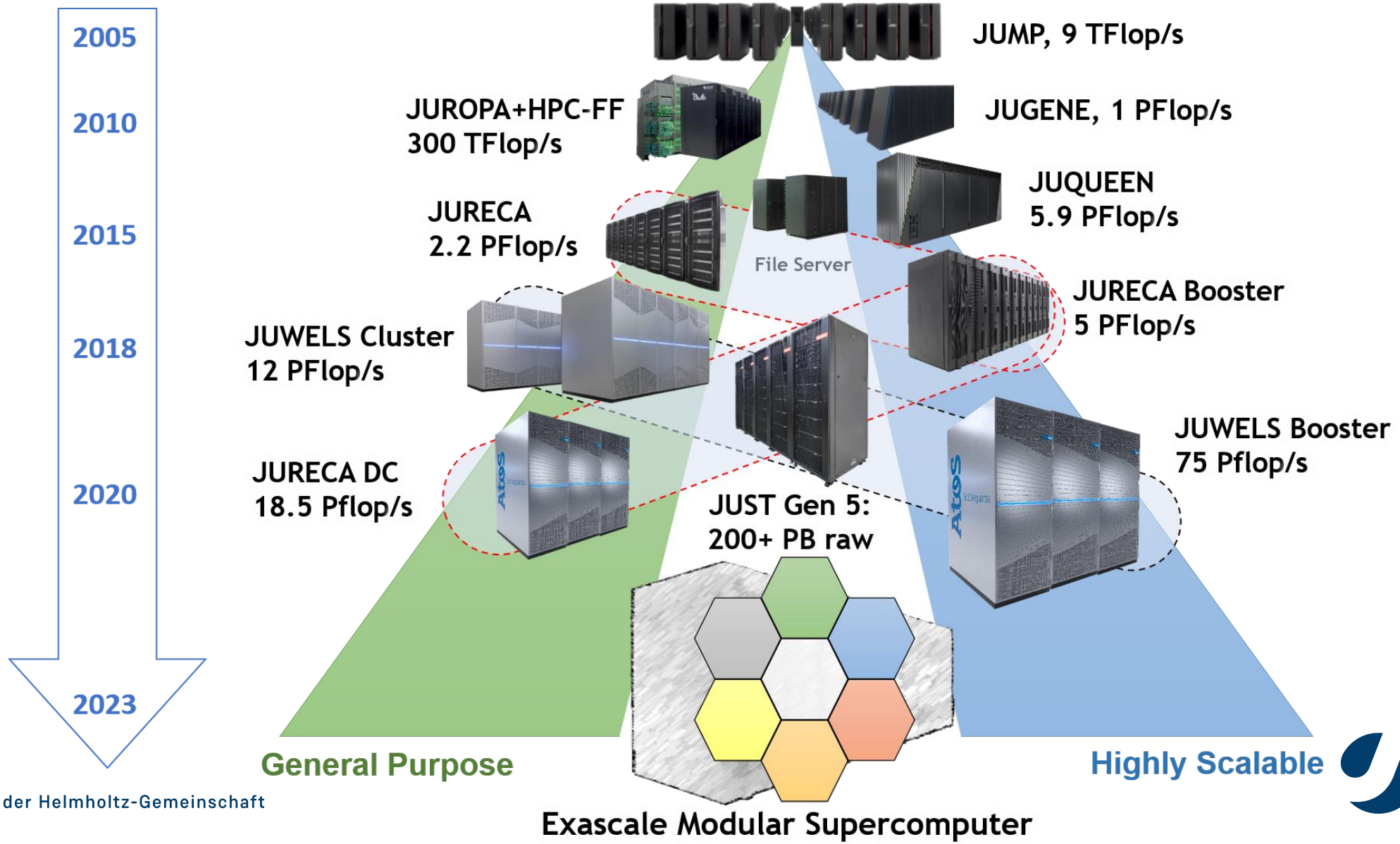


STAKEHOLDER‘S COMPUTE TIME SHARES

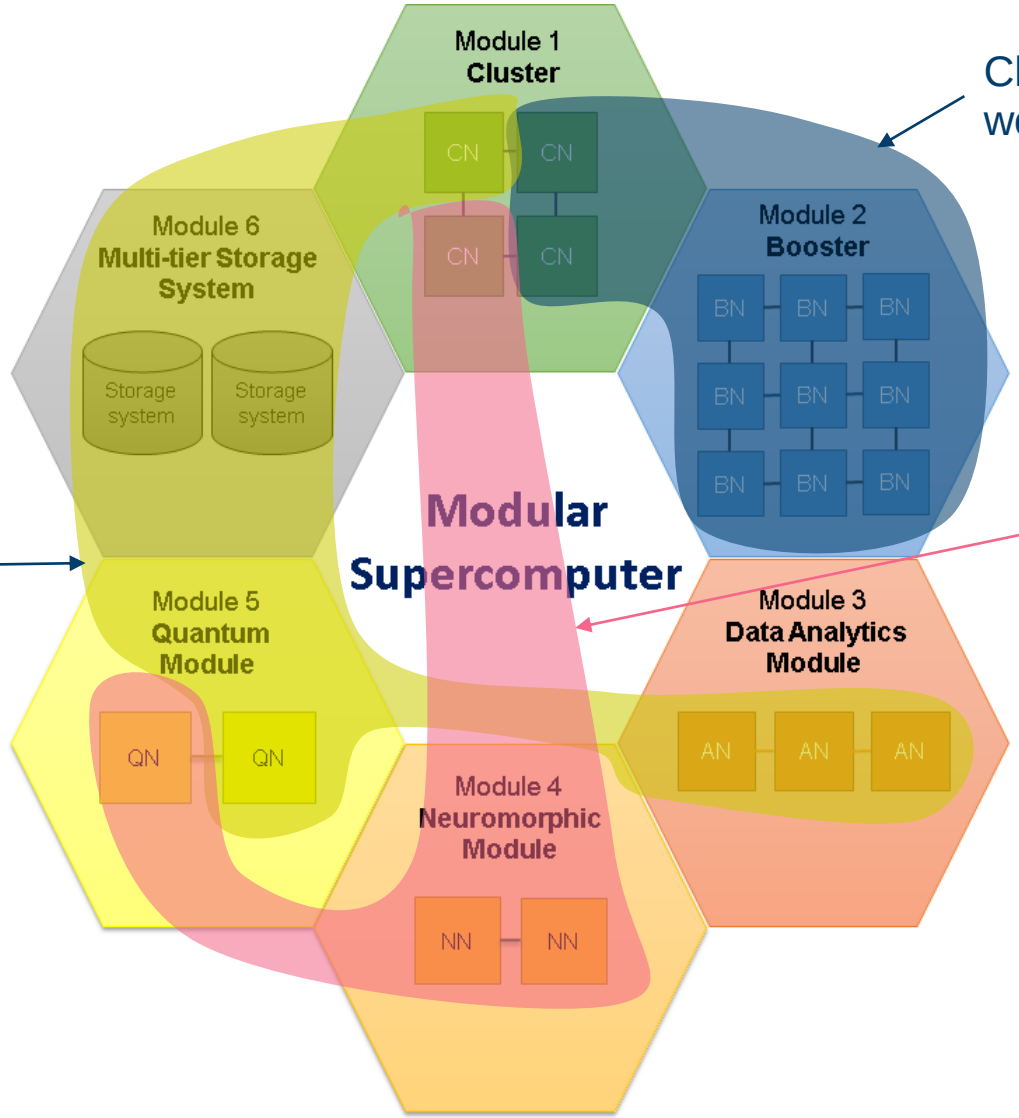


80% of the available time is being granted!

(DUAL) HARDWARE STRATEGY AT JSC



… AND EVOLUTION TO A MODULAR SUPERCOMPUTING ARCHITECTURE



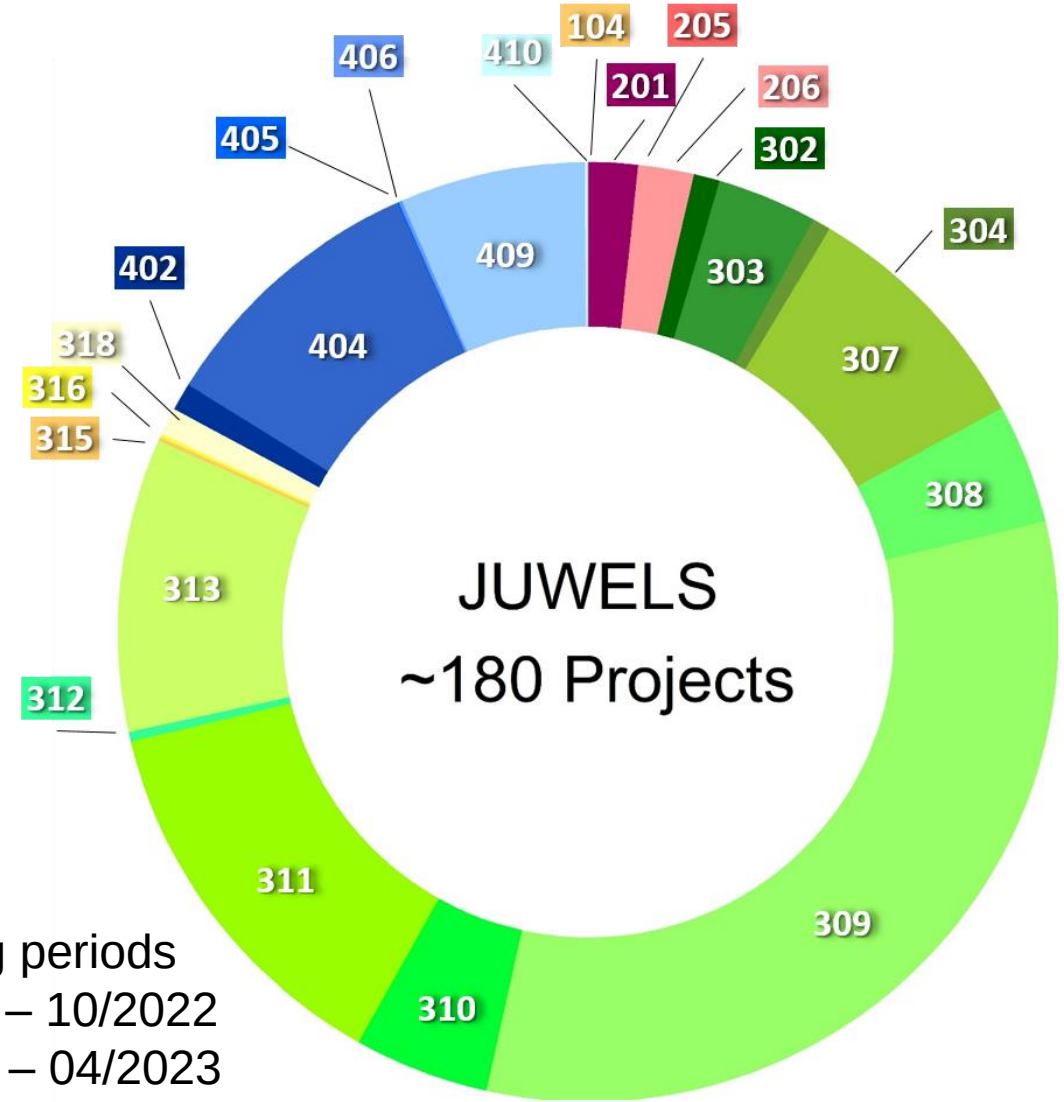
Climatology workflow

HBP Data Analytics workflow

Deep Learning workflow

*Patents granted and pending

RESEARCH FIELDS ON JUWELS (CLUSTER + BOOSTER)

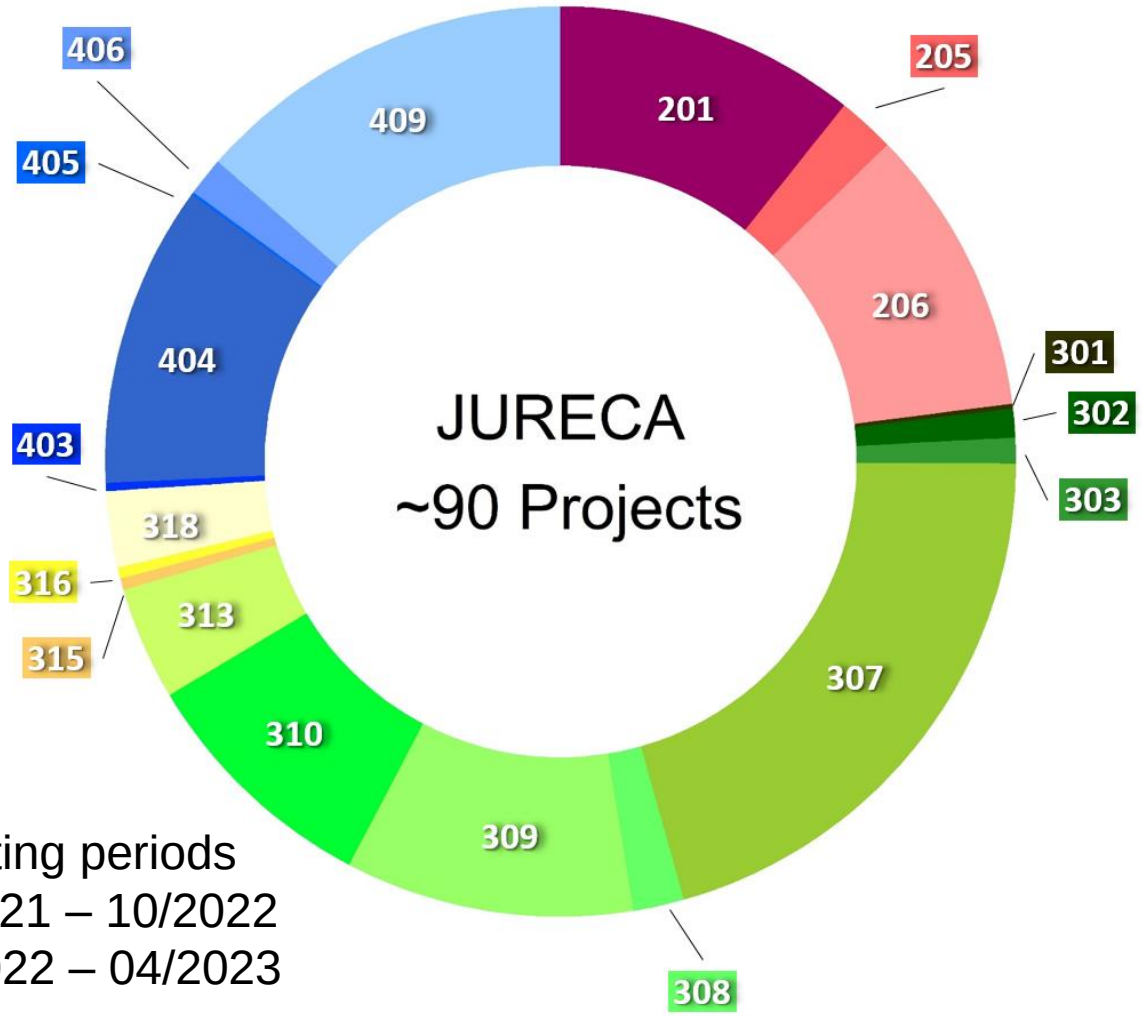


Granting periods
11/2021 – 10/2022
05/2022 – 04/2023

Reseach Fields

104	Linguistics
201	Basic Biological and Medical Research
205	Medicine
206	Neurosciences
302	Chemical Solid State and Surface Research
303	Physical and Theoretical Chemistry
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

RESEARCH FIELDS ON JURECA (CLUSTER + BOOSTER)



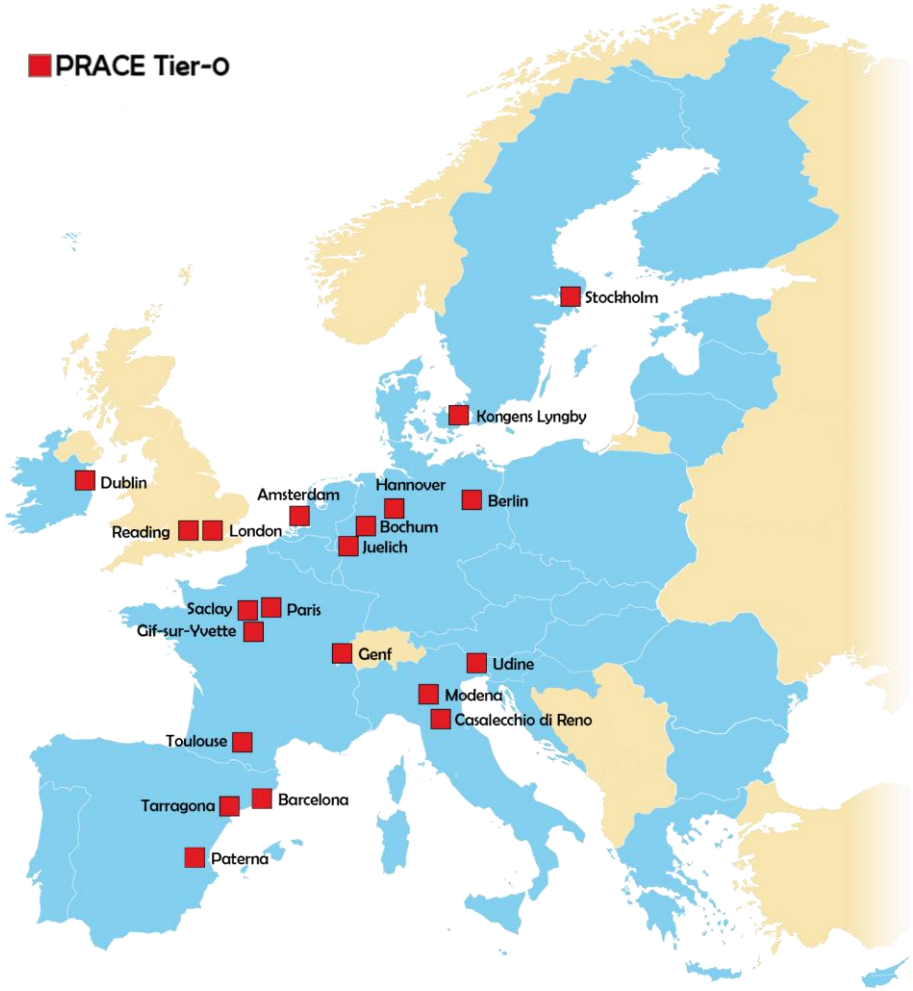
Reseach Fields

201	Basic Biological and Medical Research
205	Medicine
206	Neurosciences
301	Molecular Chemistry
302	Chemical Solid State and Surface Research
303	Physical and Theoretical 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
313	Atmospheric Science, Oceanography and Climate Research
315	Geophysics and Geodesy
316	Geochemistry, Mineralogy and Crystallography
318	Water Research
403	Process Engineering, Technical Chemistry
404	Heat Energy Technology, Thermal Machines, Fluid Mechanics
405	Materials Engineering
406	Materials Science
409	Computer Science

Granting periods
11/2021 – 10/2022
05/2022 – 04/2023

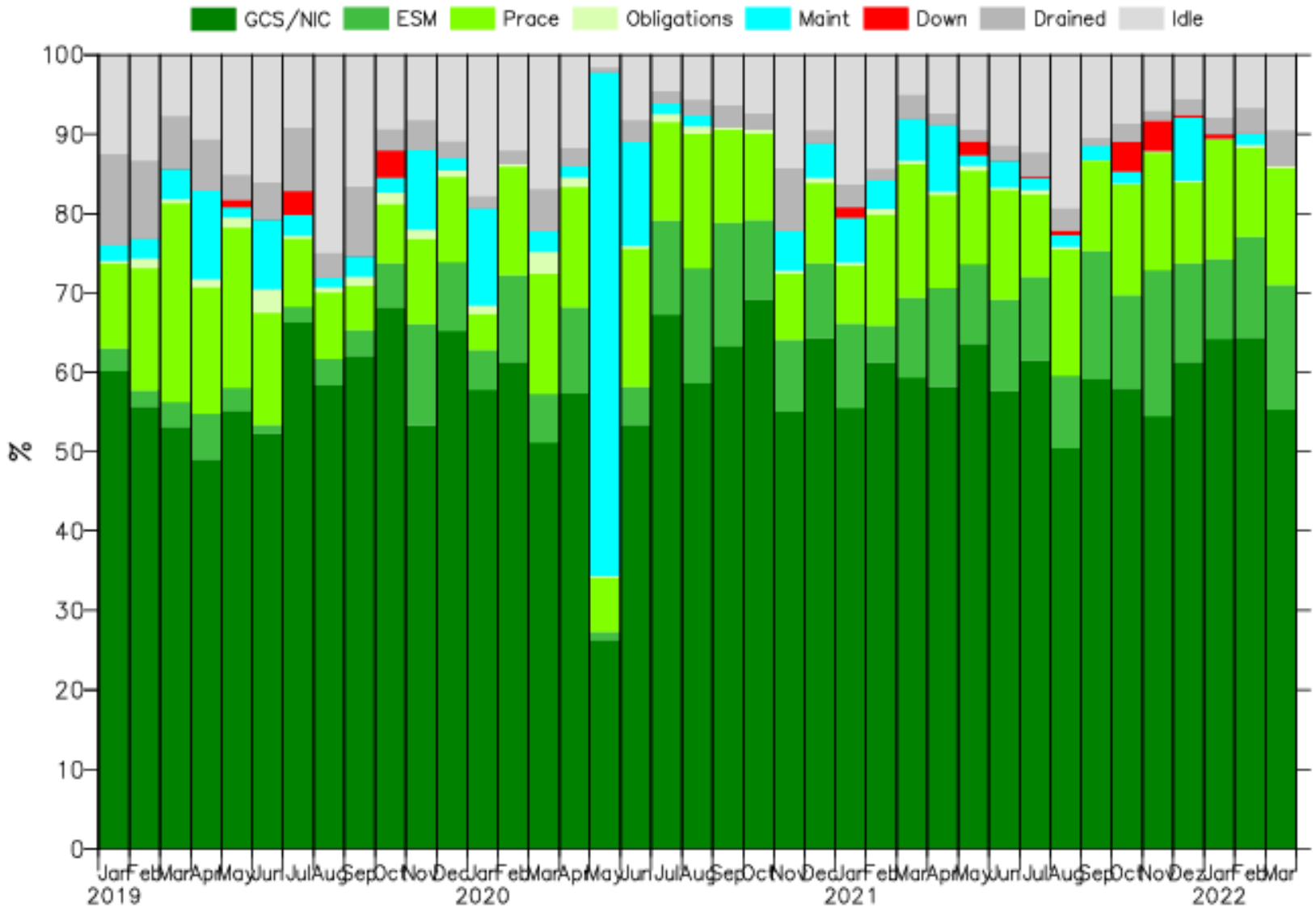
NATIONAL AND EUROPEAN USER GROUPS

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

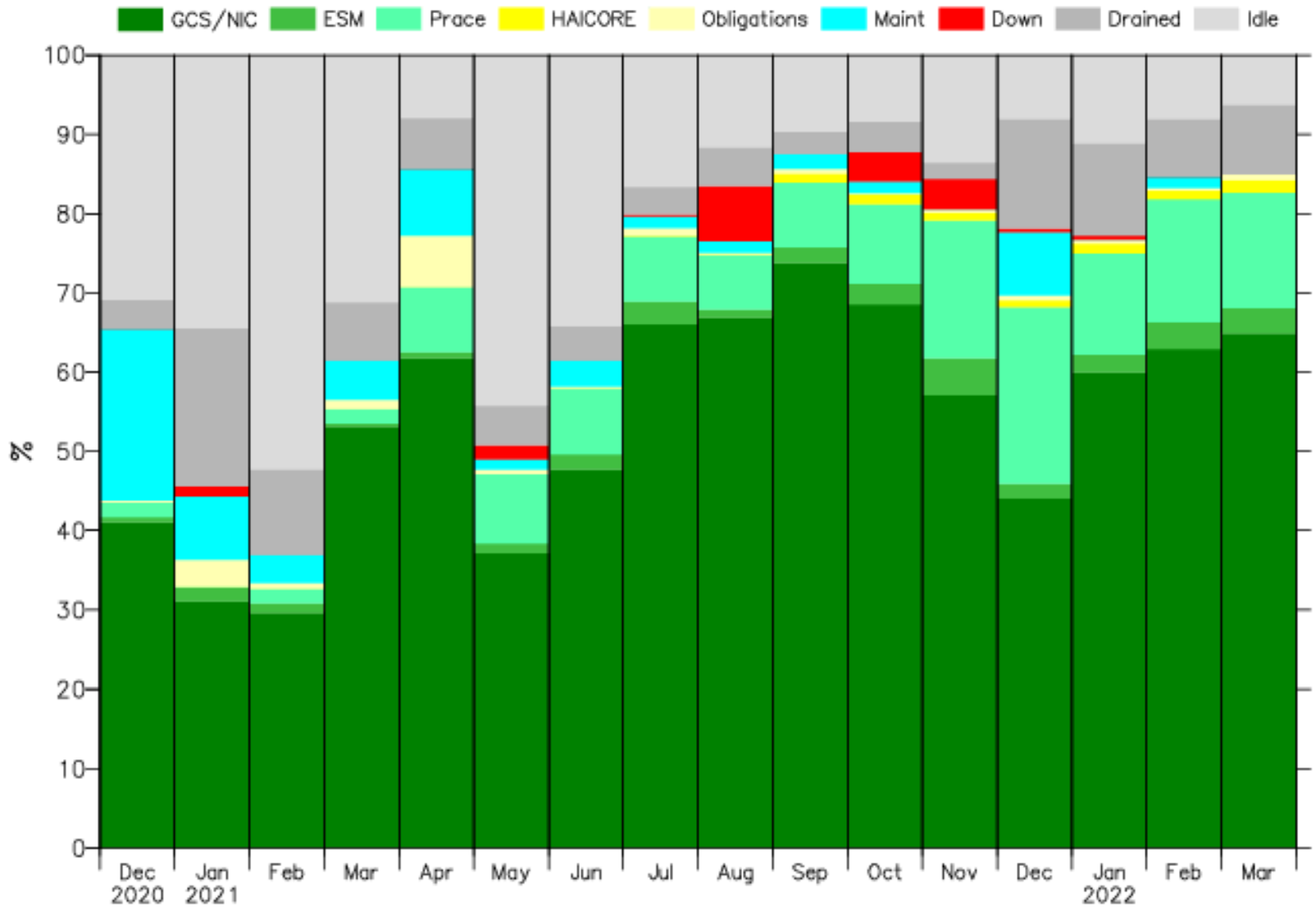


- Biology
- Medicine
- Chemistry
- Physics
- Mathematics
- Geosciences
- Mechanical and Industrial Engineering
- Thermal Engineering/Process Engineering
- Materials Science and Engineering
- Computer Science, System and Electrical Engineering
- Construction Engineering and Architecture

JUWELS CLUSTER USAGE



JUWELS BOOSTER USAGE



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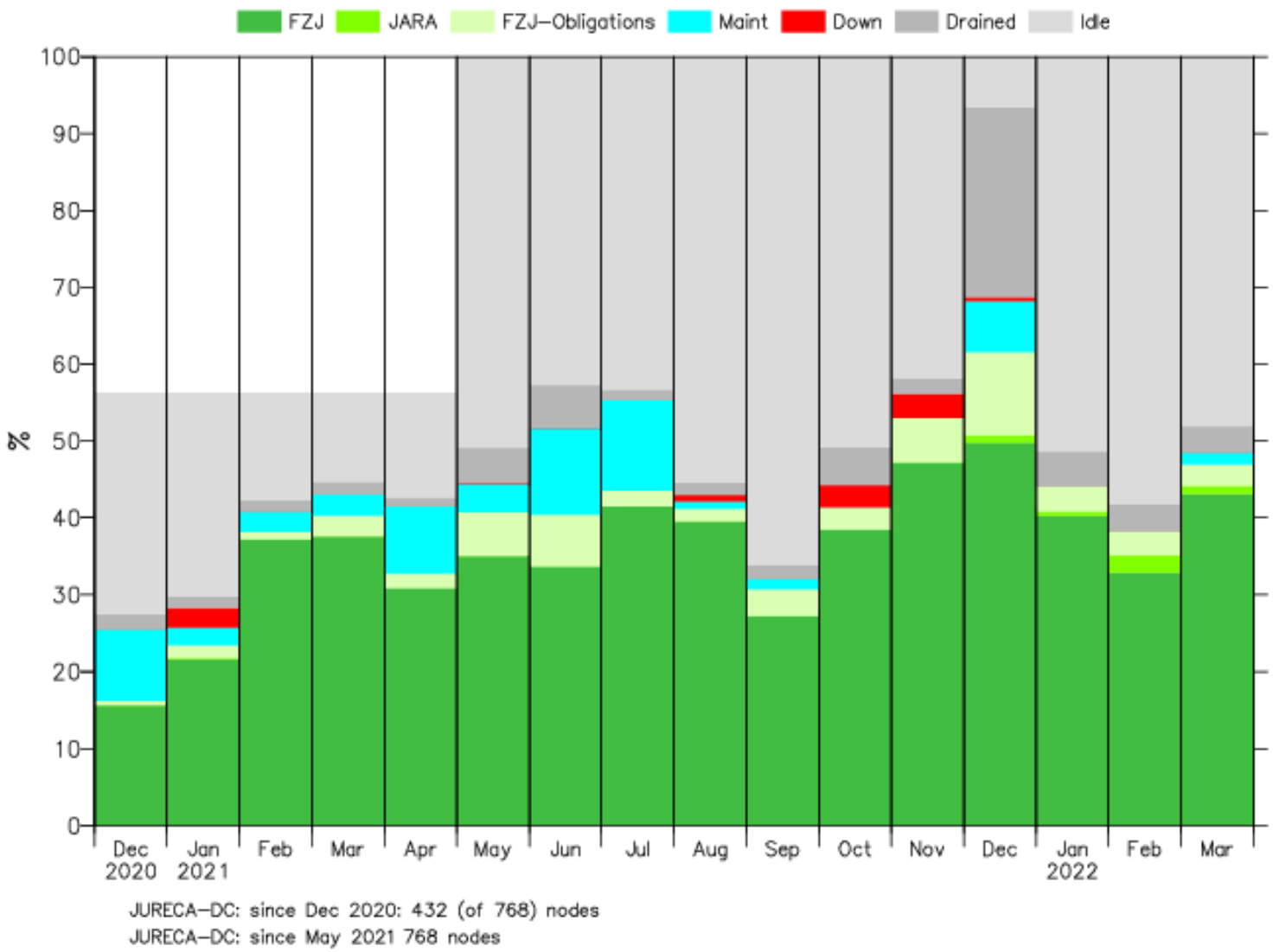
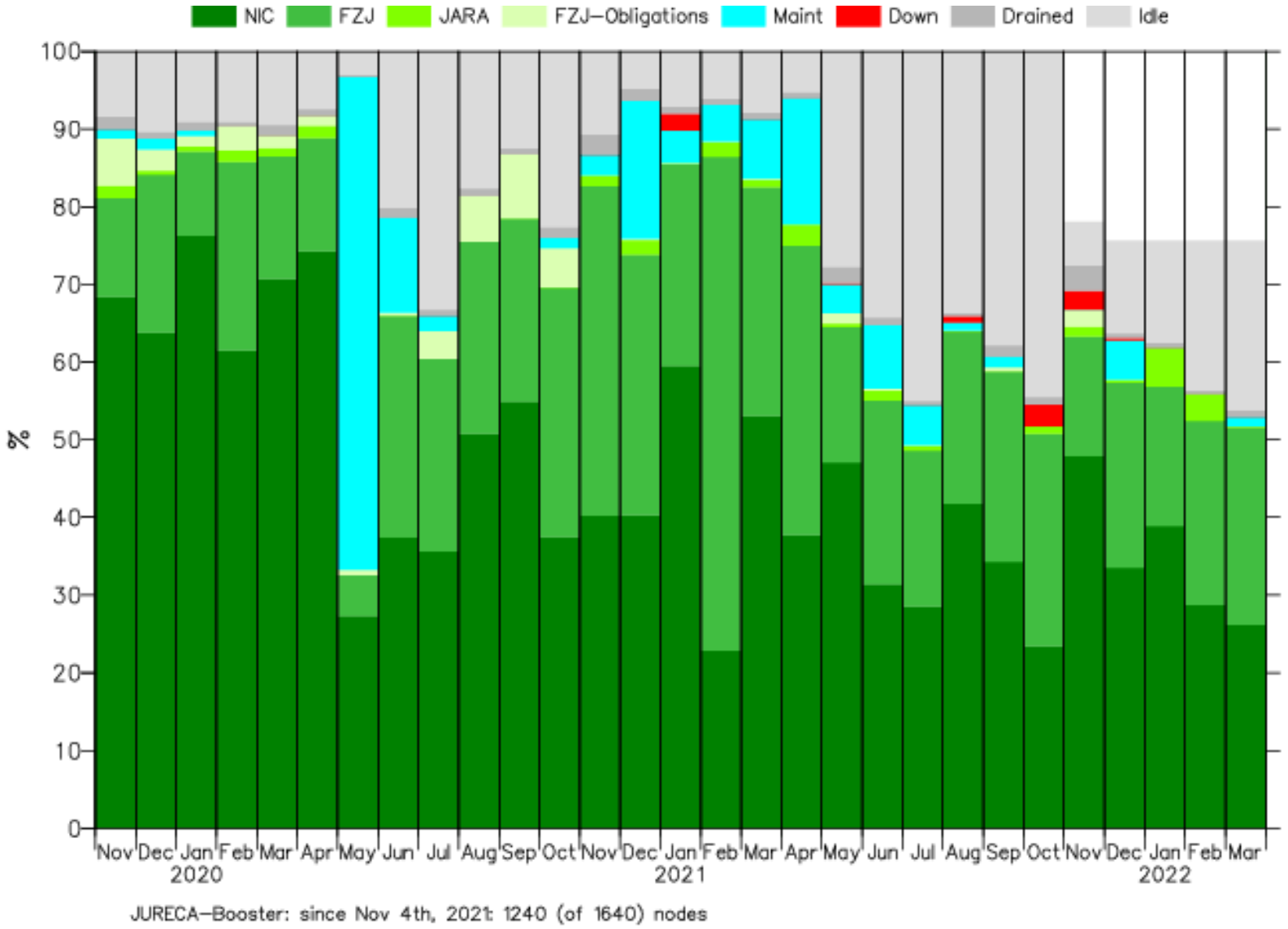
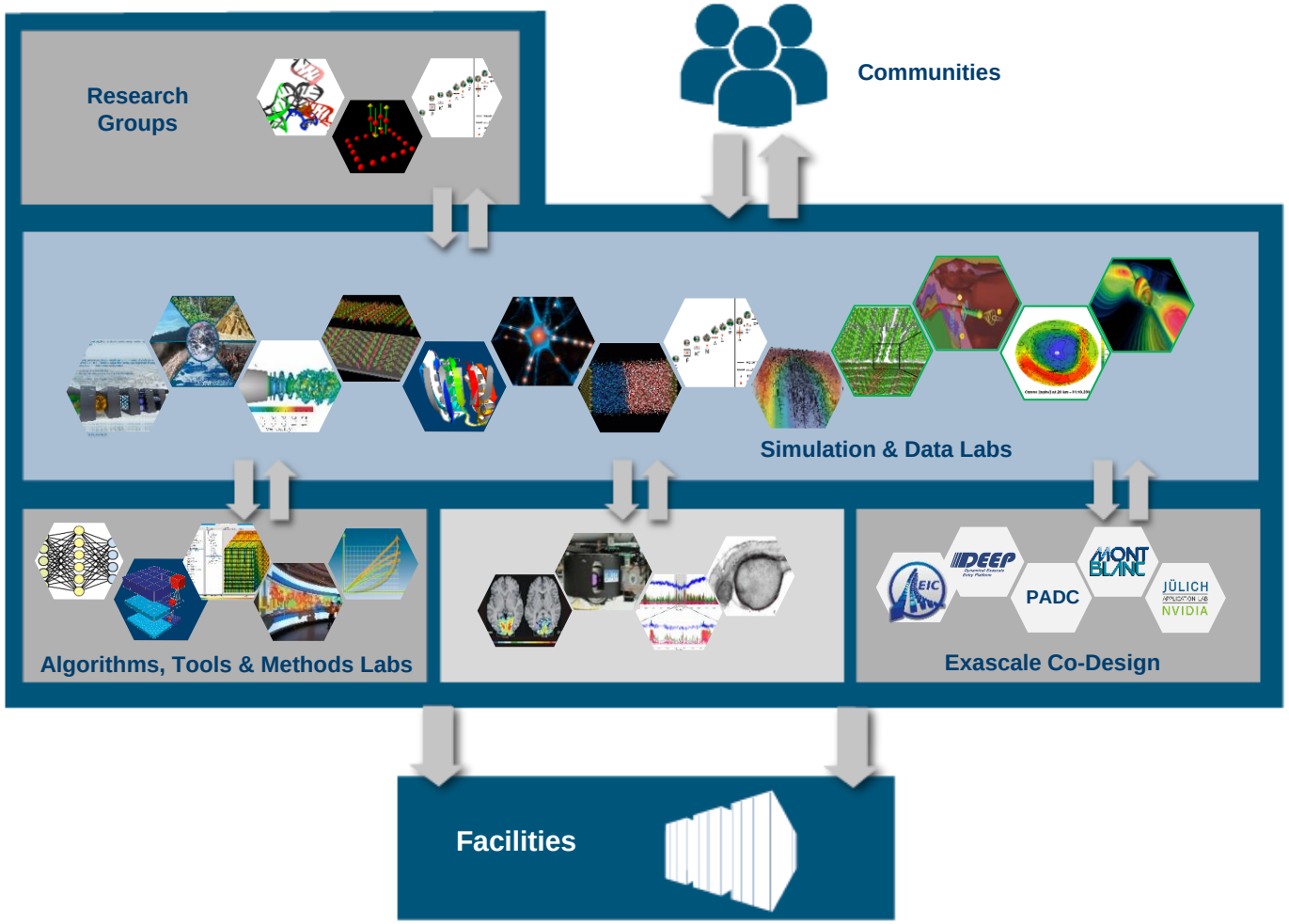
JURECA-DC USAGE



JURECA BOOSTER USAGE

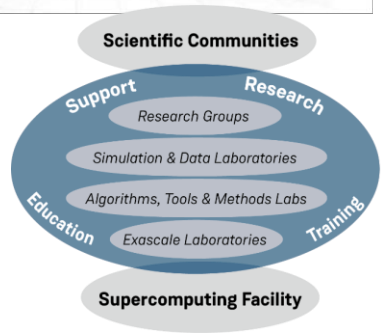


SUPPORT AND RESEARCH LANDSCAPE AT JSC



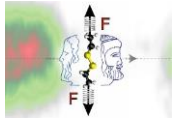
SUMMARY

- **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

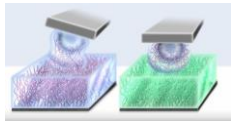


Sz. Borsanyi et al.,
Science **347** (2015) 6229

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



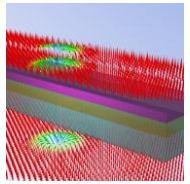
D. Marx et al.,
Nature Chemistry **5** (2013) 685



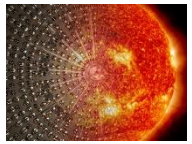
S. de Beer, M. Müser
Nature Communications **5** (2013)
doi 10.1038/ncomms4781

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

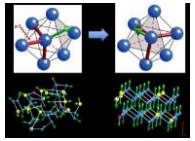
M. Lezaic et al.,
Nature Materials **9** (2010) 649



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