WELCOME TO THE

JÜLICH
SUPERCOMPUTING CENTRE

22.11.2018  I  NORBERT ATTIG, DANIEL ROHE
<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
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<tbody>
<tr>
<td>13:00 - 13:30</td>
<td>Welcome and Introduction to JSC – Norbert Attig (JSC)</td>
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<td>13:30 - 14:15</td>
<td>Work load management with Slurm – Chrysovalantis Paschoulas (JSC)</td>
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<td>14:15 - 14:45</td>
<td>JUST and IBM Spectrum Scale: Data management – Stephan Graf (JSC)</td>
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<td>14:45 - 15:15</td>
<td>Break</td>
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<td>15:15 - 16:00</td>
<td>JURECA Cluster and Booster – Philipp Thörnig (JSC)</td>
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<td>16:00 - 16:45</td>
<td>JUWELS Introduction – Michael Stephan (JSC)</td>
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<td>Bull Sequana Architecture – Thomas Knebel (Bull)</td>
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<td>16:45 – 17:30</td>
<td>ParTec Cluster Management – Frank Robel (ParTec)</td>
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<td>17:30</td>
<td>End of Day 1</td>
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<td>17:35</td>
<td>Bus SB20 from Seecasino to Rurtalbahn and Aachen/Jülich</td>
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<td>08:30 - 09:45</td>
<td>HPC Software - Compiler and Tools – Michael Knobloch (JSC)</td>
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<td>09:45 - 10:15</td>
<td>Break</td>
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<td>10:45 - 11:15</td>
<td>Remote Visualisation – Herwig Zilken (JSC)</td>
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<td>11:15 - 12:00</td>
<td>New Usage Model at JSC – Stefanie Janetzko (JSC)</td>
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<td>12:00 - 13:00</td>
<td>Lunch Break</td>
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<td>13:00 - 13:45</td>
<td>Using GPU accelerators on JURECA and JUWELS – Andreas Herten (JSC)</td>
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<td>13:45 - 14:30</td>
<td>Uniform Resource Access at JSC:UNICORE – Björn Hagemeier (JSC)</td>
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<td>LLview – Tobias Bauer (JSC)</td>
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<td>14:30 - 15:00</td>
<td>Break</td>
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<td>15:00 - 16:30</td>
<td>JURECA and JUWELS – Tuning and Tweaks – Heinrich Bockhorst (Intel)</td>
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<td>16:30</td>
<td>End of Day 2</td>
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<td>16:47</td>
<td>Bus 219 from Seecasino to Rurtalbahn, Bus 220 from Seecasino to Jülich</td>
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<tr>
<td>16:47</td>
<td>Bus SB 20 from Seecasino to Aachen</td>
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ORGANISATIONAL INFORMATION

- List of participants -> after coffee break
- Slides of all talks are available after the course at
  - [http://www.fz-juelich.de/jsc](http://www.fz-juelich.de/jsc), English
    - Expertise - Services - Documentation – Presentations
- WLAN access
  - Eduroam
  - Temporary access, forms will be handed out
- More workshops and conferences on JSC website: [www.fz-juelich.de/ias/jsc/events](http://www.fz-juelich.de/ias/jsc/events)
- Twitter: @fzj_jsc, @fzjjscuser
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, 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, Exascale Labs together with IBM, Intel, NVIDIA

- Education and training
ACCESS TO SUPERCOMPUTING RESOURCES AT JÜLICH

- **Access to JURECA via**
  - JARA-HPC Vergabegremium (VGG) and/or Kommission zur Vergabe von SC Ressourcen (VSR)
    (for FZJ and RWTH staff members only; JARA-HPC Partition)
  - John von Neumann Institute for Computing (NIC)
    - on the Cluster for Cluster-Booster proposals only
    - on the Booster (only temporarily)

- **Access to JUWELS via**
  - Gauss Centre for Supercomputing (GCS)
    (JUWELS CPU time proposals are evaluated by NIC); for FZJ and RWTH only for proposals >35 Mio. core-h
  - European Research Infrastructure PRACE
    - Project Access: Biannual CfPs since June 2010
    - Call for preparatory access open, no closing dates
  - ESM partition for Earth System scientists only (20% of JUWELS)
GAUSS CENTRE FOR SUPERCOMPUTING (GCS)

- GCS is the leading Tier-0 HPC centre in Europe
  - Alliance of the three German Tier-1 centres
  - Jülich Supercomputing Centre (JSC)
  - High Performance Computing Centre Stuttgart (HLRS)
  - Leibniz Rechenzentrum (LRZ), Garching

- Key facts
  - To date in sum more than 25 Petaflops (continuously expanding)
  - 400 people for Operation, HPC-research, Services, Training
  - Extensive know-how in key scientific fields
PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

The European HPC e-infrastructure (ESFRI)

PRACE 2
2017-2020

- 24 members, AISBL since 2010
- High Level Support Teams (HLST) at hosting member sites
- 7 supercomputers in 5 hosting countries, different architectures
- Research and industrial access (open R&D) for all disciplines based on excellence in science, free of charge
- More than 60 Pflop/s
- Up to 75 million node hours per year
DUAL HARDWARE STRATEGY AT JSC

IBM Power 6
JUMP, 9 TFlop/s

JUROPA
200 TFlop/s
HPC-FF
100 TFlop/s

IBM Power 4+
JUMP, 9 TFlop/s

IBM Blue Gene/L
JUBL, 45 TFlop/s

IBM Blue Gene/P
JUGENE, 1 PFlop/s

IBM Blue Gene/Q
JUQUEEN
5.9 PFlop/s

JURECA Cluster (2015)
2.2 PFlop/s

JURECA Booster (2017)
5 PFlop/s

JUST Gen 5:
100+ PB raw

JUWELS Cluster (2018)
12 PFlop/s

JUWELS Booster (2019/20)
50+ PFlop/s

General Purpose Cluster

Highly scalable
... AND EVOLUTION TO A MODULAR SUPERCOMPUTING ARCHITECTURE
Intel Skylake Cluster
- Dual-socket Skylake Platinum 8168 (24C, 2.7 GHz)
- 10 Sequana cells, ~2,500 nodes, ~120,000 cores
- 96 GB (in 88.7% of the cores) and 192 GB (9.4%); 4 Volta GPUs in 1.9% of nodes
- 12 Petaflop/s peak
- connected to a Global Parallel File System (GPFS)
- EDR InfiniBand, fat-tree interconnect
- Production start: July 2018

JUWELS Cluster: **#26 worldwide** (6,18 Petaflop/s Linpack)
JURECA Cluster (2015)

- 2 Intel Haswell 12-core processors, 2.5 GHz, SMT, 128 GB main memory
- 1,884 compute nodes or 45,216 cores, thereof
  - 75 nodes with 2 K80 NVIDIA graphics cards each and
  - 12 nodes with 512 GB main memory and
  - 2 K40 NVIDIA graphics cards each for visualisation
- 2.245 Petaflop/s peak (with K80 graphics cards)
  - 1.425 Petaflop/s Linpack from CPUs (out of 1,693 Petaflop/s peak)
- 281 TByte memory
- Mellanox Infiniband EDR
- Connected to the GPFS file system on JUST
JURECA – JÜLICH RESEARCH ON EXASCALE CLUSTER ARCHITECTURES

JURECA Booster (2017)

- Intel Xeon Knights Landing
- 1,640 compute nodes with 68 cores each
- 96 GiB memory per node
  - plus 16 GiB MCDRAM high-bandwidth memory per node
- Shared login infrastructure with the cluster module
- Intel Omni-Path Architecture high-speed network
  - with non-blocking fat tree topology
- 100+ GiB per second storage connection to JUST
- 5 Petaflop per second peak performance

JURECA Cluster & Booster: **#44 worldwide** (3.78 Petaflop/s Linpack)
STAKEHOLDER’S COMPUTE TIME SHARES

80% of the available time is being granted!

- FZJ obligations
- FZJ projects
- JARA-HPC (regional)
- NIC (Germany)
- GCS/NIC (Germany)
- PRACE (Europe)
- ESM partition
RESEARCH FIELD USAGE 11/2018-04/2019

JURECA
~130 Projects

JUWELS
~120 Projects

Granting periods
05/2018 – 04/2019
11/2018 – 10/2019

- Astrophysics
- Elementary Particle Physics
- Materials Science
- Soft Matter
- Other

- Biophysics
- Computer Science
- Earth & Environment
- Engineering

- Chemistry
- Condensed Matter
- Plasma Physics
- Fluid Dynamics
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
JURECA CLUSTER USAGE
JURECA BOOSTER USAGE
SUPPORT AND RESEARCH LANDSCAPE AT JSC
SUMMARY

- The Jülich Supercomputing Centre (JSC) provides
  - Tier-0/1 HPC resources
  - 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

S. de Beer, M. Müser, Nature Communications 5 (2013) 685
D. Marx et al., Nature Chemistry 5 (2013) 685
U. Meissner et al., Nature 528 (2015) 111
S. Blügel et al., Nature Communications 7 (2016) doi 10.1038/ncomms11779
D. Bravo et al., Nature 562 (2018) 505