Welcome to the Jülich Supercomputing Centre

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Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
### Schedule: Thursday, November 23

<table>
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<th>Time</th>
<th>Event</th>
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| 13:00 – 13:30 | Welcome and Introduction of JSC  
               Norbert Attig (JSC)                                                            |
| 14:50 – 15:20 | Break                                                                |
| 15:20 – 16:00 | JURECA – Tuning for the platform – part I  
               F. Robel (ParTec)                                                            |
| 16:00 – 16:30 | Using GPU accelerators on JURECA  
               W. Homberg (JSC)                                                             |
| 16:30 – 17:30 | JURECA – Tuning for the platform – part II  
               Heinrich Bockhorst (Intel)                                                  |
| 17:35       | Bus SB20 from Seecasino to Rurtalbahn and  
               Aachen/Jülich                                                              |
Schedule: Friday, November 24 (morning)

08:45 – 10:00  HPC Software – Compiler and Tools
                M. Knobloch (JSC)

10:00 – 10:15  Break

10:15 – 10:45  HPC Software – Math Libs & Application Software
                I. Gutheil (JSC)

10:45 – 11:15  Remote Visualization – H. Zilken (JSC)

11:15 – 12:00  Uniform Resource Access at JSC
                UNICORE – B. Hagemeier (JSC)
                LLView – C. Karbach (JSC)

12:00 – 13:00  Lunch break
Schedule: Tuesday, May 23 (afternoon)

13:00 – 13:30  JURECA Booster – Intro, D. Krause (JSC)
13:30 – 14:45  JURECA Booster – Tuning and Tweaks
                Heinrich Bockhorst (Intel)
14:45 – 15:15  Break
15:15 – 16:30  Taming Wild Threads – Tips and Pitfalls in Hybrid
                Programming, Christoph Pospiech, Lenovo/IBM
16:30          End of Day 2

16:35          Bus 219 from Seecasino to Rurtalbahn
16:47          Bus SB 20 from Seecasino to Aachen/Jülich
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, @fzj_jscuser
Jülich Supercomputing Centre

Introduction

N. Attig
Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
Jülich Supercomputing Centre

Supercomputer operation for:

- Centre – FZJ
- Region – RWTH Aachen University
- Germany – Gauss Centre for Supercomputing
  John von Neumann Institute for Computing
- 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)

- Access to JUQUEEN via
  - JARA-HPC Vergabegremium (VGG) and/or Kommission zur Vergabe von SC Ressourcen (VSR) (for FZJ and RWTH staff members only; JARA-HPC Partition)
  - Gauss Centre for Supercomputing (GCS) (JUQUEEN CPU time proposals are evaluated by NIC)
  - European Research Infrastructure PRACE
    - Project Access: Biannual CfPs since June 2010
    - Call for preparatory access open, no closing dates
Gauss Centre for Supercomputing (GCS)

A German Success Story:

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 20 Petaflops (continuously expanding)
- 400 people for Operation, HPC-research, Services, Training
- Extensive know-how in key scientific fields
PRACE - Partnership for Advanced Computing in Europe
The European HPC e-infrastructure (ESFRI)

- 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 FZJ ...

- IBM Power 4+ JUMP
  - 9 TFlops/s

- IBM Power 6 JUMP
  - 9 TFlops/s

- IBM Blue Gene/L JUBL
  - 45 TFlops/s

- IBM Blue Gene/P JUGENE
  - 1 PFlops/s

- IBM Blue Gene/Q JUQUEEN
  - 5.9 PFlops/s

- JURECA
  - 2.2 PFlop/s

- JURECA Booster
  - 5 PFlop/s

- JUROP A
  - 200 TFlops/s

- HPC-FF
  - 100 TFlops/s

- File Server
  - GPFS Lustre

- Hierarchical Storage Server

- General-Purpose Cluster

- Highly Scalable System
... and Evolution to Modular Supercomputer Architecture

- **GPU Module**
- **Cluster Module**
- **Many-core Booster**
- **Data Analytics Module**
- **Memory Module**
  - Neuro-morphic Device
  - Quantum Device

Storage Module:
- Disk
- Disk
- Disk
- Disk
JUQUEEN: Jülich’s Scalable Petaflop System

IBM Blue Gene/Q JUQUEEN

- IBM PowerPC® A2 1.6 GHz, 16 cores per node
- 28 racks, 458,752 cores
- 5,9 Petaflop/s peak
  5,0 Petaflop/s Linpack
- 448 TByte main memory
- connected to a Global Parallel File System (GPFS) with O(10) PByte online disk and O(50) PByte offline tape capacity
- 5D network
- Production start: Nov 5, 2012
JURECA: Jülich Research on Exascale Cluster Architectures

JURECA Cluster

- 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 (II)

JURECA Booster

- 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: #29 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)
Research Field Usage 05/2017-04/2018

Leadership-Class System

- **JUQUEEN**
  - ca. 80 Projects
  - **Astrophysics**
  - **Biophysics**
  - **Chemistry**
  - **Earth & Environment**

General-Purpose Supercomputer

- **JURECA**
  - ca. 160 Projects
  - **Plasma Physics**
  - **Soft Matter**
  - **Fluid Dynamics**
  - **Elementary Particle Physics**
  - **Computer Science**
  - **Condensed Matter**
  - **Materials Science**

Granting periods

- 11/2017 – 10/2018
- 05/2017 – 04/2018
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
JUQUEEN Usage
JURECA Usage

Launch of JURECA, phase 1, 260 nodes: Jul 13, 2015
phase 2, 1,884 nodes: Nov 02, 2015
Support and Research Landscape at JSC

- Research Groups
- Communities
- Simulation Labs
- Cross-Sectional Teams
- Data Life Cycle Labs
- Exascale co-Design
- Facilities
Summary

- The Jülich Supercomputing Centre provides
  - Tier-0/1 HPC resources
  - high-end primary and domain-specific user support
  - …

...to German and European research groups working in the computational sciences and in engineering

- JSC expects to see
  - breakthrough science
  - parallel applications, using a substantial number of processors simultaneously
End of Presentation