JURECA
An Overview

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JURECA

- Jülich Research on Exascale Cluster Architectures
- Project partners: T-Platforms, ParTec
- FZJ next-generation general purpose production system
  - NIC, VSR and commercial projects
  - Replaces the decommissioned JUROPA system
- Intended for mixed capacity and capability workloads
  - Designed with big-data science needs in mind
- Cluster architecture
  - Commodity hardware
  - Largely based on a open-source software stack
JURECA hardware overview

- Dual-socket Intel Xeon **E5-2680 v3** Haswell nodes
  - 24 cores @ 2.5 GHz
- NVIDIA K40 and K80 GPUs
- 128/256/512 GiB memory per node (DDR4 @ 2133 MHz)
- 1884 compute nodes ⇒ 45,216 cores
  - **1800 TFps** + 430 TFps peak performance
- InfiniBand **EDR** (100 Gbps per link and direction)
  - Full fat tree topology
- 100 GiBps I/O bandwidth to central GPFS storage cluster
JURECA software overview

- **Operating system:** CentOS 7.X
- **Batch system** based on **Slurm/Parastation**
  - Workload management and UI ⇒ Slurm
  - Resource management ⇒ Parastation (psid + psslurm)
- **Programming environment:**
  - GNU Compilers, Intel Professional Fortran, C/C++ Compilers, OpenMP (Intel, GNU)
  - CUDA
  - Parastation MPI (based on **MPICH3**), Intel MPI, MVAPICH2-GDR
  - Optimized mathematical libraries (Intel Math Kernel Library, etc.) and applications (/usr/local)
JURECA node types

- **Login nodes**
  - 256 GiB memory
  - Intended for interactive work: development, compilation, interactive pre- and post-processing
  - CPU time limits (2 hours)

- **Standard/slim nodes**
  - 128 GiB memory
  - Default for batch jobs (**batch** partition)
  - Smallest allocation is one node, charge based on wall-clock time
  - No direct login ⇒ Interactive sessions with `salloc` and `srun --forward-x --pty`
JURECA node types (2)

- Fat (type 1): 256 GiB memory
  - `--gres=mem256`
  - Included in `batch`

- Fat (type 2): 512 GiB memory
  - `-p mem512 --gres=mem512`
  - Currently in a separate `mem512` partition (lower performance)

- Fat (type 3): 1 TiB memory
  - `-p mem1024 --gres=mem1024`
  - Intended for memory-intense, lowly scalable pre- and post-processing tasks
JURECA node types (3)

- **Visualization nodes**
  - $\geq 512$ GiB memory (2 nodes with 1 TiB), $2\times$ NVIDIA K40
  - `-p vis --gres=gpu:[1-2]`
  - `--gres=mem1024` for large memory nodes
  - Client-server visualization requires **ssh** tunneling

- **GPU nodes**
  - 128 GiB memory, $2\times$ NVIDIA K80 (4 visible GPUs per host)
  - `-p gpus --gres=gpu:[1-4]`
# JURECA node quantities

<table>
<thead>
<tr>
<th>Node type</th>
<th>#</th>
<th>Characteristics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard/Slim</td>
<td>1605</td>
<td>24 cores, 128 GiB</td>
</tr>
<tr>
<td>Fat (type 1)</td>
<td>128</td>
<td>24 cores, 256 GiB</td>
</tr>
<tr>
<td>Fat (type 2)</td>
<td>64</td>
<td>24 cores, 512 GiB</td>
</tr>
<tr>
<td>Accelerated</td>
<td>75</td>
<td>24 cores, 128 GiB, 2× K80</td>
</tr>
<tr>
<td>Login</td>
<td>12</td>
<td>24 cores, 256 GiB</td>
</tr>
<tr>
<td>Visualization (type 1)</td>
<td>10</td>
<td>24 cores, 512 GiB, 2× K40</td>
</tr>
<tr>
<td>Visualization (type 2)</td>
<td>2</td>
<td>24 cores, 1 TiB, 2× K40</td>
</tr>
</tbody>
</table>
JURECA: Accessing the system

$ ssh <user>@jureca.fz-juelich.de
$ ssh <user>@jureca[01-12].fz-juelich.de

- Access with SSH keys
  - Recommendation: 2048 bit RSA
    (ssh-keygen -t rsa -b 2048)
  - Protection of private key with non-trivial pass phrase is mandatory!
- CPU time limits apply
  - Soft limit: 2 hours
JURECA: Accessing software (hierarchical modules)

1. List available toolchains
   $ module avail

2. Load the desired compiler and MPI
   $ module load <Compiler> <MPI>

3. List available packages based on current list of modules
   $ module avail

4. Load additional applications/libraries
   $ module load <module name>

Search for an application/library
   $ module spider <name>
JURECA: Filesystems

- All user filesystems mounted from the central GPFS fileserver Jülich Storage Cluster (JUST)
  - Exception: Node local /tmp filesystem (ext4), $O(10\, \text{GiB})$

- $\$HOME$
- $\$WORK$
- $\$ARCH$
JURECA: Filesystems ($HOME$)

- **Purposes**
  - Storage of regularly used files and applications
  - Storage of smaller files used for current computation
- **Daily backup**
- **Quota:** Max. 10 TiB disk space and max. 3 mio. inodes per group

```
$ q_dataquota [-l]
```

- Careful with `chmod -R`!
  - **Safer alternative:** Access control lists (ACL)
JURECA: Filesystems ($\text{WORK}$)

- **Purpose**
  - Storage of large files used or generated by the current computation
- Scratch filesystem with highest performance
- No backup
- Files will be deleted 90 days after last usage!
  - atime is not updated for performance reasons
- **Quota:** Max. 30 TiB disk space and max. 4 mio. inodes per group

```
$ \text{q\_dataquota \{-l\}}
```

- Copy important files to $\text{HOME}$ or $\text{ARCH}$
JURECA: Filesystems ($ARCH$)

- **Purpose**
  - Storage of large, not recently used, files
- Not available on compute nodes!
- Daily backup
- Files migrated to tapes
- **Quota:** No space quota and max. 2 mio. inodes per group
- **Usage recommendations**
  - `tar/zip` many small files
  - Do not touch/move files
JURECA: Sketch
JURECA: Fat-tree InfiniBand topology
JURECA: NUMA architecture
JURECA: Multicore

Core 0
Core 1
Core 2
Core 3
Core 4
Core 5
Core 6
Core 7
Core 8
Core 9
Core 10
Core 11
JURECA: Hyper-Threading Technology
JURECA: AVX 2.0 ISA extension

- AVX 2.0 ISA extension ⇒ Two 256-bit wide multiply-adds per cycle!
Further information

- **motd**: Message of the day
  - Information about preventive and emergency maintenances
  - Information about system configuration changes

- On-line documentation
  - [http://www.fz-juelich.de/ias/jsc/jureca](http://www.fz-juelich.de/ias/jsc/jureca)

- User support at FZJ
  - [sc@fz-juelich.de](mailto:sc@fz-juelich.de)
  - Phone: 02461 61-2828