JÜLICH
FORSCHUNGSZENTRUM

JURECA
An Overview

2017-11-23 | Philipp Thörnig | HPS group @ JSC

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 decomissioned 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`**
  - In a separate **`mem512`** partition due to lower node 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**
  - ≥512 GiB memory (2 nodes with 1 TiB), 2× 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× NVIDIA K80 (4 visible GPUs per host)
  - `-p gpus --gres=gpu:[1-4]`

JURECA node quantities

Node type	#	Characteristics
Standard/Slim	1605	24 cores, 128 GiB
Fat (type 1)	128	24 cores, 256 GiB
Fat (type 2)	64	24 cores, 512 GiB
Accelerated	75	24 cores, 128 GiB, 2× K80
Login	12	24 cores, 256 GiB
Visualization (type 1)	10	24 cores, 512 GiB, 2× K40
Visualization (type 2)	2	24 cores, 1 TiB, 2× K40

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 availables 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 **Jü**lich **St**orage Cluster (JUST)
  - **Exception:** Node local **`/tmp`** filesystem (**ext4**), $\mathcal{O}$(10 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 (`$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

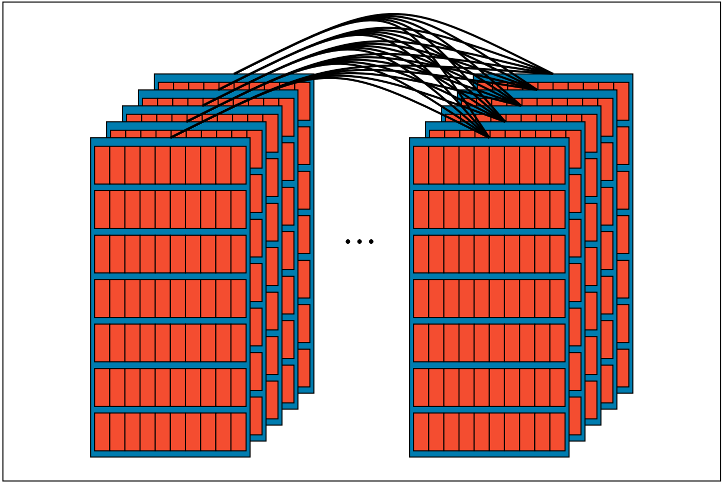
```
$ q_dataquota [-l]
```

- Copy important files to **`$HOME`** or **`$ARCH`**

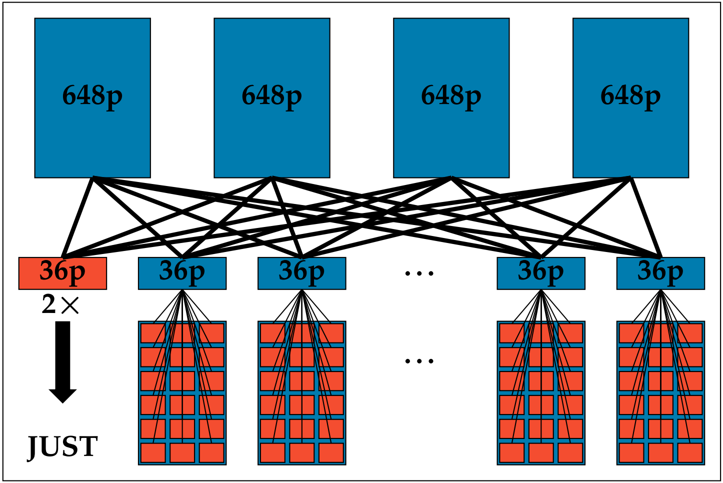
JURECA: Filesystems (`$ARCH`)

- **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

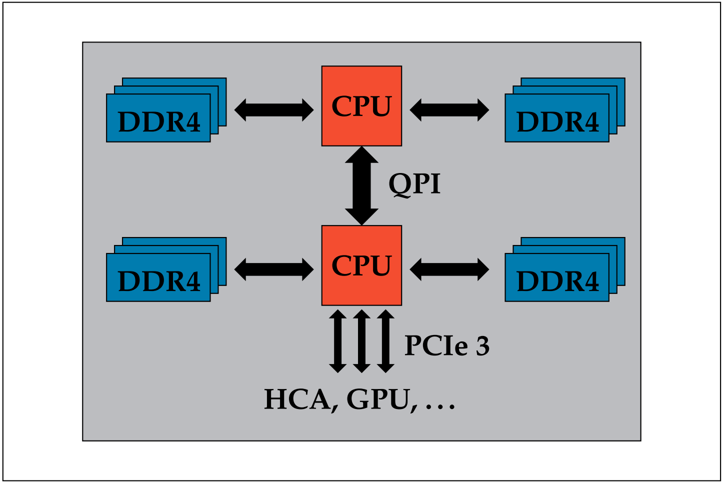
JURECA: Sketch



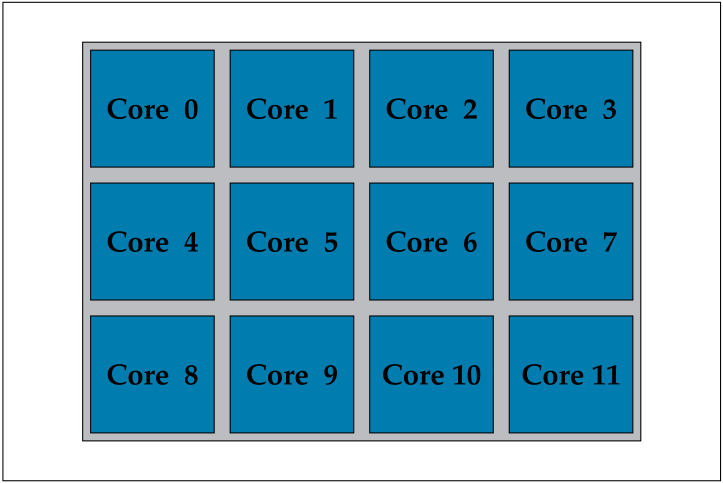
JURECA: Fat-tree InfiniBand topology



JURECA: NUMA architecture

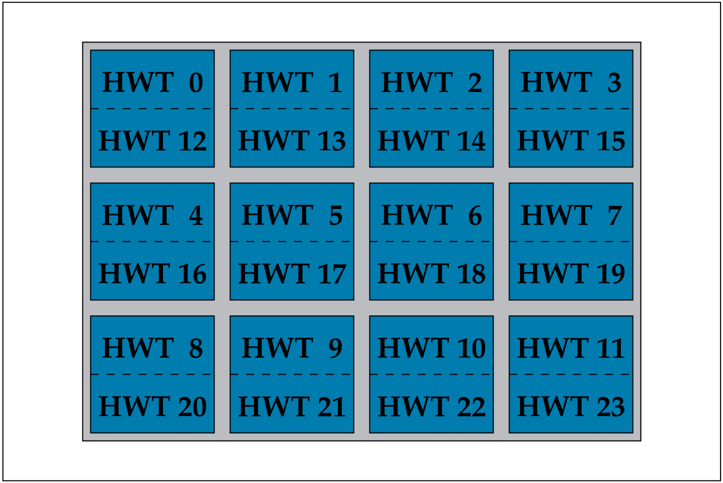


JURECA: Multicore



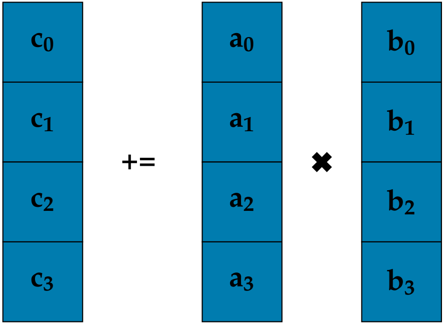
Core 0	Core 1	Core 2	Core 3
Core 4	Core 5	Core 6	Core 7
Core 8	Core 9	Core 10	Core 11

JURECA: Hyper-Threading Technology



HWT 0 HWT 12	HWT 1 HWT 13	HWT 2 HWT 14	HWT 3 HWT 15
HWT 4 HWT 16	HWT 5 HWT 17	HWT 6 HWT 18	HWT 7 HWT 19
HWT 8 HWT 20	HWT 9 HWT 21	HWT 10 HWT 22	HWT 11 HWT 23

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**
- User support at FZJ
  - **sc@fz-juelich.de**
  - Phone: 02461 61-2828