JÜLICH
FORSCHUNGSZENTRUM

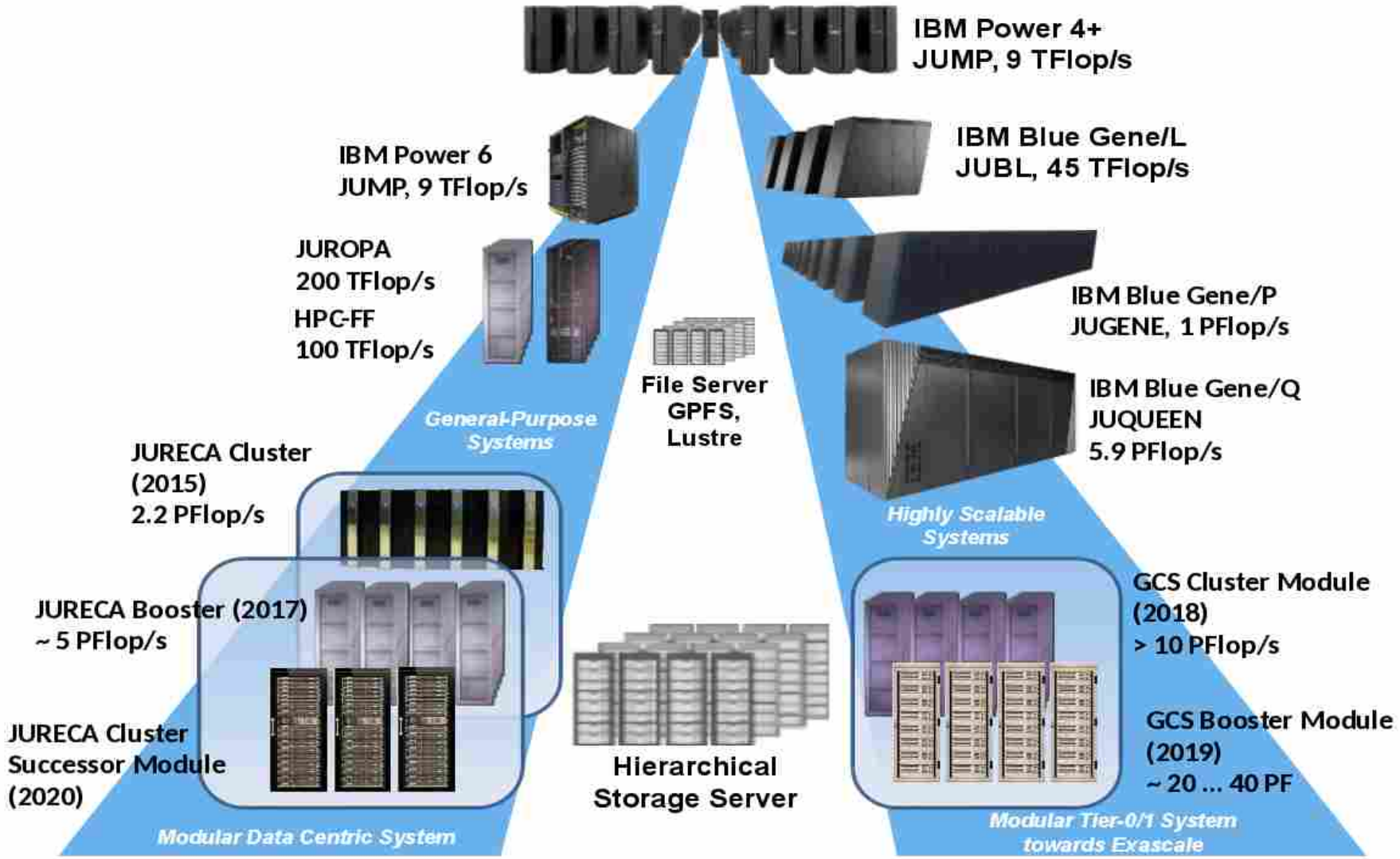
Vectorisation and Portable Programming using OpenCL

Andreas Beckmann, Ilya Zhukov, Willi Homberg, JSC
Wolfram Schenck, FH Bielefeld

Course no. 95/2017 in the trainings programme of Forschungszentrum Jülich

Jülich Supercomputing Centre (JSC)

Supercomputer Systems: Dual Track Approach



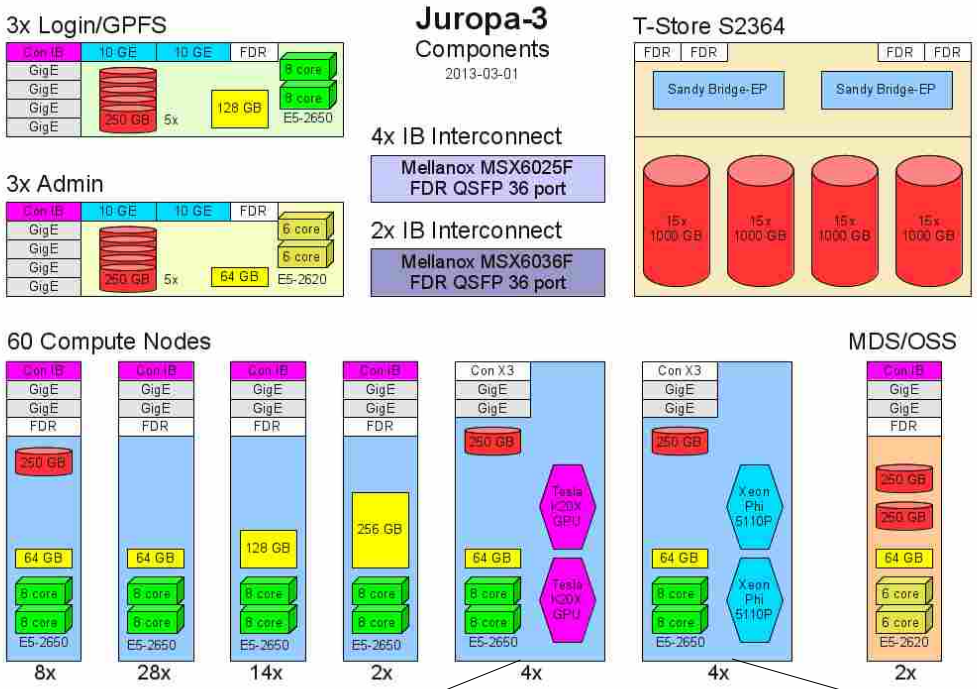
JURECA – Juelich Research on Exascale Cluster Architectures

General purpose cluster

- 2.24 Pflop/s
- #50 Top500
- 1872 compute nodes
  - Two Intel Xeon E5-2680 v3 Haswell CPUs per node
  - 2 x 12 cores, 2.5 GHz
- **75 compute nodes equipped with two NVIDIA K80 GPUs**
  - **2 x 4992 CUDA cores (4 visible devices per node)**
  - **2 x 24 GiB GDDR5 memory**
- 12 visualization nodes
  - Two Intel Xeon E5-2680 v3 Haswell CPUs per node
  - Two NVIDIA K40 GPUs per node

    2 x 12 GiB GDDR5 memory

JUROPA-3 Accelerated Nodes (NVIDIA Tesla K20x, Intel Xeon Phi 5110P)



4x K20x accelerated compute nodes

- 2 Intel Xeon E5-2650 (Sandy Bridge-EP)
- eight-core processors
  - 2.0 GHz
  - SMT (Simultaneous Multithreading)
- 64 GB memory (DDR3, 1600 MHz)
- IB FDR HCA
- **2 NVIDIA Tesla K20X GPU**
  - 2688 CUDA cores
  - 6 GB memory

4x Xeon Phi accelerated compute nodes

- 2 Intel Xeon E5-2650 (Sandy Bridge-EP)
- eight-core processors
  - 2.0 GHz
  - SMT (Simultaneous Multithreading)
- 64 GB memory (DDR3, 1600 MHz)
- IB FDR HCA
- **2 Intel Xeon Phi 5110P**
  - 60 cores

JÜLICH
FORSCHUNGSZENTRUM

Agenda Day 1

09:00	Welcome
09:15	Introduction to parallel computing
10:00	Login to test systems and query OpenCL capable devices
10:30	Coffee break
10:45	OpenCL programming concepts (I)
11:45	Lunch at Casino
12:45	OpenCL programming concepts (II)
13:45	Exploit OpenCL vectorisation features
14:45	Coffee break
15:00	Example: parallel reduction

Agenda Day 2

9:00	Portable performance
10:30	Coffee break
10:45	Matrix multiplication (I)
11:45	Lunch at Casino
12:45	Matrix multiplication (II)
13:45	Heterogeneous multi-device programming
14:45	Coffee break
15:00	Appendix

- OpenCL: History & Future
- OpenCL compared with CUDA

Acknowledgements

- Many previous presentations on OpenCL have been read in preparation for this course. You are encouraged to look at these:
  - OpenCL – An Introduction for HPC Programmers, ISC2011, Tim Mattson, Intel, Udeepta Bordoloi, AMD
  - Introduction to OpenCL, Training course June 2012, George Leaver, University of Manchester
  - OpenCL: An Introduction, Simon McIntosh-Smith, University of Bristol
    - http://handsonopencl.github.io
  - NVIDIA OpenCL SDK
  - AMD Accelerated Parallel Processing SDK
  - Intel SDK for OpenCL Applications

Course test platforms

- OpenCL – Open Computing Language
  - Open, royalty-free standard
  - For cross-platform, parallel programming of modern processors
  - An Apple initiative
  - Specified by the Khronos group
- Code hardware agnostic and portable (contrary to CUDA)
- Intended for accessing heterogeneous computational resources
  - **CPUs (Intel processors, Intel Xeon Phi coprocessors (KNC), ...)**
  - **GPUs (NVIDIA Fermi, Kepler, …)**
  - not available during course:
    - AMD APUs/CPUs/GPUs, ARM SoCs, FPGAs, DSPs, ...

JURECA – Juelich Research on Exascale Cluster Architectures

General purpose cluster

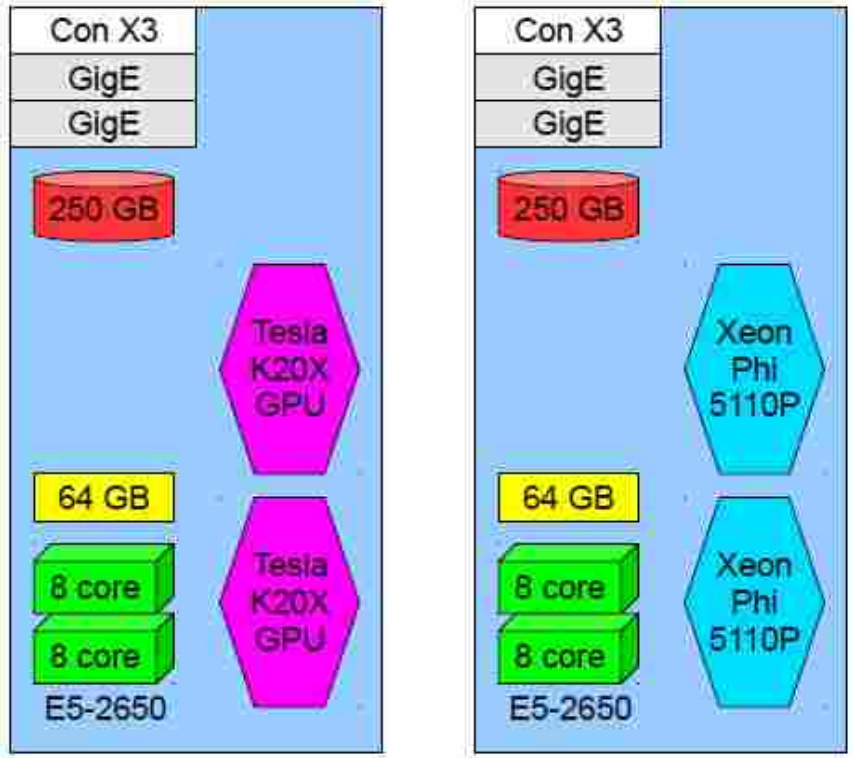
- 2.24 Pflop/s
- #50 Top500
- 1872 compute nodes
  - Two Intel Xeon E5-2680 v3 Haswell CPUs per node
  - 2 x 12 cores, 2.5 GHz
- **75 compute nodes equipped with two NVIDIA K80 GPUs**
  - **2 x 4992 CUDA cores (4 visible devices per node)**
  - **2 x 24 GiB GDDR5 memory**
- 12 visualization nodes
  - Two Intel Xeon E5-2680 v3 Haswell CPUs per node
  - Two NVIDIA K40 GPUs per node

    2 x 12 GiB GDDR5 memory

JUROPA-3 – JUROPA Update Prototype System

Heterogeneous prototype system:60 compute nodes

- 52 nodes
  - 2 Intel Xeon E5-2650 (Sandy Bridge)
  - 8-core processor, 2-2,8 GHz
  - 64 – 256 GB memory
- 4 nodes
  - 2x Sandy Bridge, 64 GB memory
  - 2x NVIDIA K20x GPUs (Kepler)
  - 3,94/1,31TFLOPS SP/DP
- 4 nodes
  - 2x Sandy Bridge, 64 GB memory
  - 2x Intel Xeon Phi 5110P
  - 2,02/1,01TFLOPS SP/DP



OpenCL Course Cheat Sheet

Workstations

Logging in

Username: `train0??`, where ?? is the number assigned to you.
Password: see whiteboard
Here, you find course materials under:
`~train060/OpenCL_Course`
Please copy the required files to the remote systems.

Editing

On JURECA and JUROPA3 you will find the same GPFS-based HOME filesystem! kate provides remote editing, thus you could use:
`sftp://juropa3/homea/hpclab/train0??`
to access your files on JURECA and JUROPA3 and edit them locally.

Command line

Start a terminal window: <ALT>+<F2> opens a window to enter commands, then type konsole:
`cd <dir>` - switches the working directory
`ls` - lists files in current directory
`ll` - same as ls but gives more detail
`rm <file>` - deletes (removes) a file. Cannot be undone!
`less <file>` - shows the context of a file.

JURECA

Logging in:

Type `ssh-add` and passphrase/word then
`ssh jureca.zam.kfa-juelich.de`

Choosing an SDK

OpenCL comes with the NVIDIA platform:
`module load CUDA`

Accessing a compute node

JURECA uses the slurm batch system.
Allocate compute resources:

```
salloc --nodes=1 --gres=gpu:4
       --partition=gpus
       --reservation=opencl
```

Start interactive shell on allocated node:

```
srun --cpu_bind=none --nodes=1
     --pty /bin/bash -i
```

Device query

For all test systems you find a script under
`~train060/OpenCL_Course/Device_Query`
to query all available OpenCL capable GPU devices

```
module load CUDA
make
export CUDA_VISIBLE_DEVICES=0,1,
```

JUROPA3

Logging in:

Type `ssh-add` and passphrase/word then
`ssh juropa3.zam.kfa-juelich.de`

Accessing a compute node

We have a reservation of 4 NVIDIA K20X-based GPU nodes and 4 Intel Xeon Phi accelerated MIC nodes.
JUROPA3 uses the slurm batch system:

```
salloc -N1 -n16 -p q_gpus --reservation=opencl_gpus
```

or

```
salloc -N1 -n16 -p q_mics --reservation=opencl_mics
```

then
srun --pty /bin/bash -i

Device query

For all test systems you find a script under
`~train060/OpenCL_Course/Device_Query`
to query all available OpenCL capable devices on an MIC node

```
module load Intel
make
LIB=/usr/local/intel/OpenCL/intel/
                    opencl-1.2-3.2.1.16712/lib64
export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$LIB
```

Exercise OpenCL_Platforms/device-query

- Login to all test systems (cf. Cheat Sheet on previous slide)
  - JURECA node
  - JUROPA-3 GPU node
  - JUROPA-3 MIC node
- and query platform information to find all OpenCL capable devices
  - copy local directory Device_Query to the remote host
  - inspect correspondig run script and run it
    - ./run_device_query_*.sh

OpenCL Architecture: Platform Model

- A host is connected to one or more (possibly heterogeneous) OpenCL devices
  - A device is divided into compute units (CUs)
    - CUs are subdivided into processing elements (PEs)