Jülich Supercomputing Centre

Introduction

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Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
Outline

- JSC in a Nutshell
- Production systems
  - System use
  - How to get access
  - Training
- Architecture evolution
  - Dual approach
  - Cluster-Booster
  - Modular Supercomputing
- JSC vision
JSC in a Nutshell

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

Education and training

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
Domain-specific User support

SimLabs
PRODUCTION SYSTEMS
JURECA Cluster – Hardware

- Dual-socket Intel Haswell (E5-2680 v3)
  - 12× cores/socket
  - 2.5 GHz
  - ≥ 128 GB main memory

- 1,884 compute nodes (45,216 cores)
  - 75 nodes: 2× K80 NVIDIA GPUs
  - 12 nodes: 2 × K40 NVIDIA GPUs
  - 512 GB main memory

- Peak performance: **2.2 Petaflop/s** (1.7 w/o GPUs)

- Mellanox InfiniBand EDR

- Connected to the GPFS file system on JUST
  - ~15 PByte online disk and
  - 100 PByte offline tape capacity

**June 2017: #26 in Europe
#80 worldwide
#168 in Green500**
JUQUEEN - Hardware

- IBM Blue Gene/Q
- PowerPC® A2
  - 16× cores per node
  - 1.6 GHz
  - 16 Gbyte main memory
- 28,672 nodes
  - 458,752 cores
  - 28 racks
- Peak performance: 5,9 PFlop/s
- Connected to a GPFS:
- 5D network

June 2017:
#7 in Europe
#21 worldwide
#94 in Green500
JUST: Storage server

- **8 PB**
  - $WORK
  - $DATA
- **$HOME**
  - 3 x 600 TB
- **$ARCH**
  - 2 x 600 TB

220 GB/sec

- JUQUEEN
- JURECA
- JUROPA3
- JUDAC
  - Jülich Data Access
- TSM Server
JURECA Cluster – Software

- **Operating system**: Linux CentOS 7.X
- **Scheduler**: SLURM
- **Filesystem**: GPFS ($HOME, $WORK, $ARCH)
- **Compilers** (C/C++, Fortran, CUDA): Intel, GNU, PGI, CUDA
- **Debuggers**: TotalView, DDT, MUST
- **Programming**: Intel MPI, ParaStation MPI, OpenMP, CUDA
- **Performance analysis tools**: Score-P, Scalasca, Vampir, TAU, NVIDIA Visual Profiler, Darshan…
- **Libraries** (modules): MKL, SIONlib, HDF5, netcdf, PETSc …
- **Domain specific packages**: NAMD, QuantumExpresso, …

Support: [sc@fz-juelich.de](mailto:sc@fz-juelich.de)
On-line documentation: [http://www.fz-juelich.de/ias/jsc/jureca](http://www.fz-juelich.de/ias/jsc/jureca)
JUQUEEN – Software

- **Operating system**: Linux
- **Scheduler**: SLURM
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- **Libraries (modules)**: MKL, SIONlib, HDF5, netcdf, PETSc …

Support: sc@fz-juelich.de

On-line documentation: [http://www.fz-juelich.de/ias/jsc/juqueen](http://www.fz-juelich.de/ias/jsc/juqueen)
SYSTEMS USE
System Usage

JURECA Cluster

Launch of JURECA, phase 1: 260 nodes: Jul 13, 2015
Launch of JURECA, phase 2: 1,884 nodes: Nov 2, 2015
Research fields – Current projects

General-Purpose Cluster

- JURECA
  - ca. 170 Projects

- Research fields:
  - 1. Earth & Environment
  - 2. Biophysics
  - 3. Particle Physics
  - 4. Soft Matter
  - 5. Condensed Matter
  - 6. Plasma Physics
  - 7. Chemistry
  - 8. Fluid Dynamics

Massively Parallel system

- JUQUEEN
  - ca. 95 Projects

- Research fields:
  - 9. Materials Science
  - 10. Computer Science
  - 11. Astrophysics

Granting periods:
- JURECA: 11/2016 – 10/2017
- JUQUEEN: 05/2017 – 04/2018
How to get access – peer review process

To JURECA via:
- JARA-HPC: for FZJ + RWTH staff members only
  - Vergabegremium (VGG) and/or
    Kommission zur Vergabe von SC Ressourcen (VSR)
- John von Neumann Institute for Computing (NIC)

To JUQUEEN via:
- JARA-HPC (for FZJ + RWTH staff only): VGG and/or VSR
- Gauss Centre for Supercomputing (GCS)
  - Proposals evaluated by NIC
- PRACE: European Research Infrastructure
  - Project Access: Biannual CfPs since June 2010
  - Call for preparatory access open, no closing dates
How to use the systems

- Introductory courses every 6 months
- Detailed documentation (slides) on JSC website:

Further training events

- Very varied training events: jsc-events-join@fz-juelich.de

Events at JSC

If you would like to receive regular information on our events per e-mail, please send an e-mail to jsc-events-join@fz-juelich.de.

<table>
<thead>
<tr>
<th>Date</th>
<th>Title</th>
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<tbody>
<tr>
<td>25 Sep 2017 - 29 Sep 2017</td>
<td>International HPSH TerrSys Fall School 2017</td>
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<tr>
<td>09 Oct 2017 - 11 Oct 2017</td>
<td>Training course &quot;Einführung in Python&quot;</td>
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<tr>
<td>09 Oct 2017 - 10 Oct 2017</td>
<td>Training course &quot;Porting code from Matlab to Python&quot;</td>
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<tr>
<td>16 Oct 2017 - 17 Oct 2017</td>
<td>Training course &quot;Introduction to GPU programming using OpenACC&quot;</td>
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<td>19 Oct 2017 - 20 Oct 2017</td>
<td>GMM CSE Workshop 2017</td>
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<td>06 Nov 2017 - 15 Nov 2017</td>
<td>Training course &quot;Programmierung in C&quot;</td>
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<tr>
<td>15 Nov 2017</td>
<td>Training course &quot;JusD - JUNet/Internet Security Day&quot;</td>
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<tr>
<td>20 Nov 2017</td>
<td>Training course &quot;Software Development in Science&quot;</td>
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<tr>
<td>21 Nov 2017 - 22 Nov 2017</td>
<td>Training course &quot;Vectorisation and portable programming using OpenCL&quot;</td>
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<tr>
<td>23 Nov 2017 - 24 Nov 2017</td>
<td>Training course &quot;Introduction to the programming and usage of the supercomputer resources at Jülich&quot;</td>
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<tr>
<td>27 Nov 2017 - 28 Nov 2017</td>
<td>Training course &quot;Advanced Parallel Programming with MPI and OpenMP&quot;</td>
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<tr>
<td>29 Nov 2017</td>
<td>Training course &quot;Das Programmierwerkzeug make&quot;</td>
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http://www.fz-juelich.de/ias/jsc/EN/News/Events
High-Q-Club: >30 generic codes at scale!

- dynQCD
- Gysela
- JusPIC
- MP2C
- $\mu\varphi$

- PEPC
- PMG+PFASST
- TeraNEO
- WalBerla

Gyrokinetic code
Laser-Plasma
CFD with Particles
Water in Porous Media
Particle Tree Code
ODE-Solver
MG for Geophysics
Lattice Boltzmann
etc.

Non-trivial kernels only!
From *dual* to *Modular Supercomputing*

**ARCHITECTURE EVOLUTION**
Dual Architecture

- JUROPA: Intel Nehalem, 300 TFlop/s
- JURECA Cluster: Intel Haswell, ~2.2 PFlop/s
- JUGENE: IBM Blue Gene/P, 1 PFlop/s
- JUQUEEN: IBM Blue Gene/Q, 5.9 PFlop/s

General purpose clusters vs. massively parallel architecture
The DEEP projects
DEEP, DEEP-ER and DEEP-EST

EU-Exascale projects
27 partners
Total budget: 44 M€
EU-funding: 30 M€
Nov 2011 – Jun 2020

Both combine:
-Hardware
-Software
-Applications
in a strong co-design
Homogeneous cluster
Heterogeneous cluster

Network
Cluster-Booster architecture
DEEP Prototype

- Installed at JSC
- 1,5 racks
- 500 TFlop/s peak perf.
- 3.5 GFlop/s/W
- Water cooled
Software environment

- **Scheduler**: Torque/Maui → future moving to SLURM
- **Filesystem**: BeeGFS
- **Compilers**: Intel, gcc, PGI
- **Debuggers**: Intel Inspector (threading, memory), TotalView (source code, memory debugger)
- **Programming**: ParaStation MPI (mpich), OpenMP, OmpSs
- **Performance analysis tools**: Extrae/Paraver, Scalasca, Intel Advisor, Intel, VTune
- **Libraries**: SIONlib, SCR, E10, HDF5, netcdf, PETSc …
DEEP projects applications (15):

- Brain simulation (EPFL + NMBU)
- Space weather simulation (KU Leuven)
- Climate simulation (Cyprus Institute)
- Computational fluid engineering (CERFACS)
- High temperature superconductivity (CINECA)
- Seismic imaging (CGG + BSC)
- Human exposure to electromagnetic fields (INRIA)
- Geoscience (LRZ)
- Radio astronomy (Astron)
- Lattice QCD (University of Regensburg)
- Molecular dynamics (NCSA)
- Data analytics in Earth Science (UoI)
- High Energy Physics (CERN)
Cluster-Booster architecture advantages

- **Full user flexibility** – many different use modes
  - Dynamic ratio of processors/coprocessors
  - Use Booster as pool of accelerators (globally shared)
  - Discrete use of the Booster
  - Discrete use + I/O offload
  - Specialized symmetric mode

- **More efficient use of system resources**
  - Only resources really needed are blocked by applications
  - Dynamic allocation further increases system utilization

- **Better I/O performance and resiliency**
Dual Architecture

- JUROPA: Intel Nehalem, 300 TFlop/s
- JURECA Cluster: Intel Haswell, ~2.2 PFlop/s
- JUGENE: IBM Blue Gene/P, 1 PFlop/s
- JUQUEEN: IBM Blue Gene/Q, 5.9 PFlop/s
- JURECA Booster: DELL/Intel Xeon Phi, 5 PFlop/s

2005: JUROPA
2009: JUGENE
2012: JUQUEEN
2017: JURECA Booster

* Fictive picture
Dual Architecture

- **JUROPA**
  - Intel Nehalem
  - 300 TFlop/s

- **JURECA Cluster**
  - Intel Haswell
  - ~2.2 PFlop/s

- **JUQUEEN**
  - IBM Blue Gene/Q
  - 5.9 PFlop/s

- **JUGENE**
  - IBM Blue Gene/P
  - 1 PFlop/s

- **JURECA Booster**
  - DELL/Intel Xeon Phi
  - 5 PFlop/s

*Fictive picture

General purpose cluster

Massively parallel architecture
Dual Architecture

General purpose cluster

Massively parallel architecture

2005
2009
2012
2017

JUROPA
Intel Nehalem
300 TFlop/s

JUQUEEN
IBM Blue Gene/Q
5.9 PFlop/s

JUGENE
IBM Blue Gene/P
1 PFlop/s

JURECA Cluster
Intel Haswell
~ 2.2 PFlop/s

JURECA Booster
DELL/Intel Xeon Phi
5 PFlop/s

* Fictive picture
MODULAR SUPERCOMPUTING
Cluster – Booster architecture
Modular Supercomputing

Generalization of the Cluster-Booster concept
Module 0
Exascale Storage
- Storage system
- Storage system

Module 1
HPC Cluster
- CN
- CN

Module 2
Extreme Scale Booster
- BN
- BN
- BN

Module 3
Data Analytics Module
- DN
- DN
- DN

Module 4
Graphics Module
- GN
- GN

Module 5
Neuromorphic
- NN
- NN

Module n:
- N
- N
Modular Supercomputing

Module 0: Exascale Storage
- Storage system
- Storage system

Module 1: HPC Cluster
- CN
- CN
- CN

Module 2: Extreme Scale Booster
- BN
- BN
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- BN
- BN
- BN
- BN
- BN

Module 3: Data Analytics Module
- DN
- DN
- DN

Module 4: Graphics Module
- GN
- GN

Module 5: Neuromorphic
- NN
- NN

Module n:
- N
- N
JSC Vision

Neuromorphic

Quantum Computer

Cluster

Booster

Data Analytics Module