Welcome to the Jülich Supercomputing Centre

St. Janetzko and N. Attig
Jülich Supercomputing Centre (JSC), Forschungszentrum Jülich
Schedule: Monday, May 21

13:00 - 13:30  Welcome and Introduction of JSC
                Norbert Attig, Stefanie Janetzko, JSC
13:30 - 15:00  JUROPA/HPC-FF - An Overview
                U.Detert, U.Ehrhart, B.Tweddell, F.Heckes, JSC
15:00 - 15:20  Break
15:20 - 16:35  JUROPA/HPC-FF - Tuning for the platform
                Heinrich Bockhorst, Intel
16:35 - 16:45  Break
16:45 - 17:30  JUROPA/HPC-FF - Tuning for the platform II
                Ralph Krotz, Peter Niessen, ParTec

17:39  Bus from Seecasino to Rurtalbahn, Jülich
Schedule: Tuesday, May 22 (morning)

08:30 - 08:35  Welcome of new participants
               Stefanie Janetzko, JSC

08:35 - 09:45  HPC Software - Compiler and Tools
               Markus Geimer, Bernd Mohr, JSC

09:45 - 10:00  Break

10:00 - 10:30  HPC Software - Math Libs & Application Software
                Inge Gutheil, JSC

10:30 - 11:00  Postprocessing/Visualization-Cluster JUVIS
                Herwig Zilken, JSC

11:00 - 11:30  UNICORE - Uniform Resource Access at JSC
                Michael Rambadt, JSC

11:30 - 12:30  Lunch break
Schedule: Tuesday, May 22 (afternoon)

12:30 - 14:00  An overview on BlueGene/P and BlueGene/Q
    Michael Stephan, JSC
14:00 - 14:15  Break
14:15 - 15:15  Tuning for the platform – BlueGene/P
    Christoph Pospiech, IBM
15:15 - 15:30  Break
15:30 - 16:30  Introduction to the platform – BlueGene/Q
    Christoph Pospiech, IBM
16:30       End of Day 2

16:36           Bus from Seecasino to Rurtalbahn
16:47           Bus from Seecasino to Aachen/Jülich
Organizational Information

- List of participants
- Course foils after the course available via
  - http://www.fz-juelich.de/ias/jsc/events/sc
- WLAN access
  - MAC-address needed (→ List)
Introduction of the Jülich Supercomputing Centre

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

Supercomputing is being supported by the

Jülich Supercomputing Centre (JSC)

The main tasks of JSC are:

- **Operation of the supercomputers** for local, regional, national and European scientists
- **User support** in programming and optimisation of applications, support of research groups from different research domains by means of simulation laboratories
- **R&D** work on new computer architectures, algorithms, performance analysis and tools, GRID computing, etc.
- **Education** and training of users, education of students (bachelor and master courses, PhD programmes)
Access to Supercomputing Resources at Jülich

- “Traditional access” via
  - John von Neumann Institute for Computing (NIC); JUROPA
  - Gauss Centre for Supercomputing (GCS); JUGENE (currently granting the JUGENE CPU time via NIC)
  - Kommission zur Vergabe von SC Ressourcen (VSR) (for FZJ staff members only; JUROPA)
  - NEW: JARA-HPC Vergabegremium (VGG) (for FZJ and RWTH staff members only; JARA-HPC Partition)

- Further access to JUGENE via European RI PRACE, …
  - Biannual CfPs since June 2010
  - Call for preparatory access open, no closing dates

- Access to HPC-FF via
  - HPC-FF Board (Secretary: Roman Zagorsky); www.efda-hlst.eu
Gauss Centre for Supercomputing (GCS)

- Alliance of the three German national supercomputing centres
  - Jülich Supercomputing Centre (JSC)
  - Leibniz-Rechenzentrum (LRZ) der Bayerischen Akademie der Wissenschaften
  - Höchstleistungsrechenzentrum Stuttgart (HLRS)

- Support of computational science through
  - Multi-Petaflop/s supercomputers
  - Multi-Petabyte storage
  - Multi-Gigabit networking infrastructure
  - Large-Scale projects → Gauss projects → Call for Proposals

- German representative in PRACE
PRACE
Partnership for Advanced Computing in Europe

- Consists of 24 European partner states, each represented by one institution
- Prepares the creation of a persistent, sustainable pan-European HPC service
- Prepares the establishment of three to five Tier-0 supercomputing centres at different European sites
- Defines and establishes a legal and organisational structure involving HPC centres, national funding agencies, and scientific user communities
- Develops funding and usage models and establishes a peer review process
- Provides training for European scientists and creates a permanent education programme
Supercomputer Systems: Dual Concept

- **2004**: IBM Power 4+ JUMP, 9 TFlop/s
- **2006-8**: IBM Power 6 JUMP, 9 TFlop/s
- **2009**: JUROPA 200 TFlop/s, IBM Blue Gene/L JUBL, 45 TFlop/s
- **2012**: JUROPA++ Cluster, 1-2 PFlop/s + Booster, IBM Blue Gene/P JUGENE, 1 PFlop/s
- **2014**: General-Purpose, Highly-Scalable, IBM Blue Gene/Q JUQUEEN 5.7 PFlop/s

**File Server**
- GPFS, Lustre

**IBM Blue Gene/Q JUQUEEN**
- 5.7 PFlop/s
JUGENE: Jülich’s Scalable Petaflop System

IBM Blue Gene/P JUGENE

- 32-bit PowerPC 450, 850 MHz, 4-way SMP
- 72 racks, 294,912 procs
- 1,00 Petaflop/s peak
- 0,82 Petaflop/s Linpack
- 144 TByte main memory
- connected to a Global Parallel File System (GPFS) with 5 PByte online disk and up to 25 PByte offline tape capacity
- Torus network
- Production start: July 1, 2009

First Petaflop system in Europe, no 13 in Top500 (Nov 2011)
IBM Blue Gene/Q JUQUEEN

- IBM PowerPC® A2 1.6 GHz, 16 cores per node
- 8 racks, 131,072 cores
- 5,7 Petaflop/s peak
- ?? Petaflop/s Linpack
- 128 TByte main memory
- connected to a Global Parallel File System (GPFS) with 6 PByte online disk and up to 25 PByte offline tape capacity
- 5D network
- Production start: May 16, 2012

Extension to 20 (28) racks in autumn 2012 (winter 2013)
JUROPA: Jülich’s General-Purpose Supercomputer

JUROPA, an Intel-based cluster

- 2 Intel Nehalem quad-core processors, 2.93 GHz, SMT
- 2,208 compute nodes, 17,664 cores
- 207 Teraflop/s peak
- 184 Teraflop/s Linpack
- 52 TByte memory
- Mellanox Infiniband QDR with non-blocking Fat Tree topology
- 500 TByte disk storage on Lustre file system, connected to GPFS

JUROPA designed in co-development with HPC companies

JUROPA serves as prototype for HPC-FF, U. of Cambridge, CHPC (Cape Town), PRACE
HPC-FF
High-Performance Computer for Fusion

- Intel-based Linux cluster identical in construction with JUROPA
- 1,080 compute nodes
- 101 Teraflop/s peak
  87 Teraflop/s Linpack
- funded by EU, EFDA and FZJ
- dedicated to European fusion community

HPC-FF and JUROPA can be used as a single system

308 Teraflop/s peak
275 Teraflop/s Linpack, no. 36 in Top500 (Nov 2011)
Use by Compute Time Shares

80% of the available time is being granted!

- JUGENE
- JUQUEEN
- JUROPA

- FZJ obligations
- FZJ projects
- JARA-HPC
- GCS/NIC (Germany)
- PRACE (Europe)
Research Fields of Current National Projects

Leadership-Class System

JUGENE
~ 60 Projects

General-Purpose Supercomputer

JUROPA
~ 200 Projects

High oversubscription factor

Granting periods
05/2012 – 04/2013

Research Fields:

- Astrophysics
- Biophysics
- Chemistry
- Earth & Environment
- Plasma Physics
- Soft Matter
- Fluid Dynamics
- Elementary Particle Physics
- Computer Science
- Condensed Matter
- Material Science

Research Fields of Current National Projects:

- JUROPA
  ~ 200 Projects
- JUGENE
  ~ 60 Projects
Research Fields of Current European Projects

**JUGENE**
PRACE: 21 Projects

- Astrophysics
- Chemistry and Materials
- Earth Sciences and Environment
- Engineering and Energy
- Fundamental Physics
- Mathematics and Computer Science
- Medicine and Life Sciences

High oversubscription factor!

Granting periods
11/2011 – 10/2012 3rd Regular Call
05/2012 – 04/2013 4th Regular Call
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
JUGENE Usage

![JUGENE Usage Chart]

[Graph showing JUGENE usage across different categories and months from 2010 to 2012.]
JUROPA Usage
HPC-FF Usage

![HPC-FF Usage Chart]

- FZJ
- HPC-FF
- Queue "nc_hpcff"
- Maint
- Down
- degraded
- System
- Idle

21. May 2012
Supercomputing Resources in Jülich: Welcome and Introduction of JSC
Traditional Support Structure

User Support
- Technical Support
- Technical Support
- Methods and Optimisation
- Advisor

Training
- Courses
- Tutorials and Seminars
- High-level Workshops
Domain-Specific User Support and Research

Simulation Laboratories

<table>
<thead>
<tr>
<th>Plasma Physics</th>
<th>Biology</th>
<th>Molecular Systems</th>
<th>Climate Science</th>
<th>Solid &amp; Fluid Engineering</th>
<th>Nuclear and Particle Physics</th>
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Parallel Performance | Application Optimisation | Methods & Algorithms

Cross-Sectional Teams

Quantum Information | Comp. Materials Physics

Research Groups
Summary

- The Jülich Supercomputing Centre provides
  - world-class supercomputers
  - 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