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Dynamical Exascale Entry Platform

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Definition Of Environmental Requirements
Approved

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Executive Summary

Target of this deliverable is to define the environmental requirements for deploying the DEEP System focusing energy efficiency. Energy efficiency will be an important aspect within the project and for the prototype system itself. Considerations and concepts regarding energy efficiency, that will be applied here, are based on the outcome of WP7 “Energy Efficiency” using recommendations given in D7.1 "Datacentre infrastructure requirements" (submitted in month 6).

Multiple aspects have to be considered when installing an energy efficient HPC system. The configuration and properties of the prototype system have been taken into account to plan the infrastructure changes at installation site that will be described in this document. Key objectives for environmental requirements are:

- The cooling system
- Building infrastructure (including power supply and floor space)
- Networking and interconnects

Several results have been achieved with this deliverable. The decision on the cooling concept of the DEEP System, which consists of a Cluster part and a Booster part both based on Eurotech’s Aurora platform, has been made [4]. The configuration of the Cluster part has been defined including additional hardware components for system management and integration. Infrastructure changes according to the requirements have been identified and planned, e.g. the integration of the prototype into the existing network infrastructure.

1 Introduction

Within WP6 the technologies developed in WP3 to WP5 will be integrated into the DEEP System with respect to energy efficiency aspects investigated in WP7. Hence the installation details and most of the environmental requirements are defined by the specifications and developments in WP3, WP4 and WP7.

The compute part of the DEEP system consists out of one cabinet holding an Intel Xeon based CPU cluster (128 nodes) and one cabinet for the Intel Xeon Phi based Booster (512 KNCs). An additional rack will be placed between the two cabinets containing hardware for power supply and network interconnects. For more details on the compute hardware, please refer to the respective WP3 documentation. Additional servers for login and management of the system and an external storage system for maintaining application data will be required. Figure 1 on page 7 gives an overview on the DEEP System including additional hardware and cooling system. The overall power consumption of the system can be estimated with 300 kW.

A successful integration of the prototype hardware into the infrastructure at the installation site as well as the deployment of the system are critical for investigation and approval of the DEEP Architecture for building energy efficient HPC systems.

This includes the following topics:

- **Floor space:** An appropriate machine room for running the DEEP System has to be provided.
- **Power supply:** The power requirements of the DEEP system make special solutions for cabling and cutouts necessary.
- **Liquid cooling:** Cooling loops, pumps, and filters have to be installed for deployment of water cooled systems.
- **System management and user access:** For running the DEEP System, additional hardware for user login, system management and administration has to be installed.

Among others, the DEEP system will be used for further experiments in hot water cooling and energy efficient computing extending the experiences and results that have been obtained with existing hot water cooling experimentation platforms at BADW-LRZ and UniReg. Changing the inlet temperature for the inner cooling loops in the range from 20°C (standard cold water cooling) to about 40°C (allows for 100% free cooling) the most energy efficient configuration will be of high interest. This includes stability of the running system and power consumption of the hardware and of the cooling system itself (e.g. fans in dry cooler and pumps in the water loops). Increase of the outlet temperatures for possible reuse of the waste energy like done in the CooLMUC experiment platform at BADW-LRZ is also to be inspected. In doing so, the behavior of the hardware components regarding stability and performance dependent on the operating temperature have to be observed. For doing measurements and experiments with the system, sensors and monitoring capabilities have to be installed within the cooling loops and along with the DEEP prototype hardware. WP6 has to provide a flexible installation to maximize the range of investigations.

This document describes the process of defining environmental requirements with respect to the configuration of the DEEP System and including the collaboration with other work packages (especially WP3 “System Hardware” and WP7 “Energy Efficiency”). Section 2 reiterates the energy efficiency aspects that have been discussed in D7.1 before. The decision for using hot water cooling is explained and an overview on the cooling concept for the DEEP System is given. Special requirements that hot water cooling might imply will also be mentioned. A detailed description of different scopes of environmental requirements is provided in section 3. Infrastructures details and decisions that have already been taken will be presented together with considerations for certain aspects of environmental requirements. Further installation details and specifications of infrastructure components will be presented later in D6.2 “Environment Preparation Completed”.

Along with the European Commission the intended audience of this document is the project partners from other work packages, especially those involved in the system integration and installation process, as well as people interested in deploying energy efficient HPC systems.

2 Energy Efficiency Aspects

As D7.1 already has shown, energy efficiency is an important aspect of high-performance computing systems. This will even get more challenging when developing systems in the Exascale range. Along with the peak performance of a system the number of FLOPs per Watt will become increasingly important. The DEEP System will demonstrate that the power efficiency of HPC systems can be improved by an order of magnitude using energy efficient hardware and an innovative efficient cooling concept. Investigation on energy efficiency aspects is done in WP7. Its results, especially regarding liquid cooled systems, will guide the work in WP6.

In traditional data centers, the compute hardware is cooled with air. Computer room air conditioning (CRAC) units suck in warm air from the ceiling. After cooling the air with an external cooling medium (water in most cases), the cold air is blown under the false floor. In such a scenario, the system integrator's task for cooling is restricted to ensuring proper air flows through the hardware. Air cooled systems are easy to design, quick to set up, and can be manufactured at low costs.

However, increased compute and power densities, especially in HPC, require the use of a cooling medium with better thermal properties than air. D7.1 refers to two prototype implementations featuring water based cooling solutions for the entire cooling chain down to individual CPUs, memory and network components on the mainboard. On these systems, it was shown that in direct liquid cooled systems, even inlet water temperatures of over 40ºC are still sufficient to keep the CPUs under the same thermal conditions as similar air-cooled systems operating at 23ºC inlet temperature. In almost every region on earth, water can be re-cooled to 40ºC using free cooling only avoiding intermediate chilling, which leads to significant energy savings.

Along with high temperature direct liquid cooling it also becomes more attractive to reuse waste energy. Higher temperature levels and the high thermal capacity of water make it feasible to even use the energy remotely outside the data center (e.g. office heating)

When not reusing waste heat, the inlet temperature of a direct liquid cooled system with free cooling can be brought near the outside temperature leading to lower junction temperatures of the silicon components. This results in less leakage losses and may improve component lifetime.

2.1 Cooling Concept for the DEEP System

Hot water cooling with inlet temperatures up to 50°C is applicable for the DEEP hardware using Eurotech's Aurora platform. With JSC being the installation site, a climate with maximum outside temperatures below 40°C can be expected even on hot summer days. Hence free cooling will provide under normal operation conditions the whole cooling capacity needed.

However, to improve availability and safety a backup cooling solution relying on the central cold water supply of JUELICH is implemented in parallel. Coupling the cooling systems with heat exchangers allows separating the individual circuits for reasons of water quality and provides optimal control of the inlet temperature for the Aurora water cooling. A stageless regulation of the inlet temperature will be possible with this configuration.

Since the Cluster part and the Booster part of the DEEP System have different power consumption and cooling requirements, two inner cooling circuits are necessary to allow for independent control of the cooling for each of the two parts. Hence the DEEP liquid cooling concept consists of all together four different water loops coupled through heat exchangers.

While almost all of the hardware components integrated into the DEEP System are water cooled, there will still be some parts that have to be cooled by air in a traditional way. This includes the power converters and the additional hardware that has to be installed for running and administering the system (e.g. storage and management servers). Table 1 gives an overview on the estimated waste heat of the components and how it will be captured:

Component	Waste heat	Type of cooling
DEEP Cluster	100 kW	Direct liquid cooled
DEEP Booster	200 kW	Direct liquid cooled
AC/DC converters	16 kW	Air cooled
Storage	2 kW	Air cooled
Management-Servers	6 kW	Air cooled
Network Components	6 kW	Air cooled

Table 1: Cooling requirements

A room air conditioner with a capacity of at least 30 kW has to be added to the machine room where the prototype system will be placed to cover the waste heat of the air cooled components. Besides it has to be assured, that the relative humidity within the machine room will not be in the range of 20% to 60%. Figure 1 gives a simplified overview on the overall concept of the DEEP cooling system.

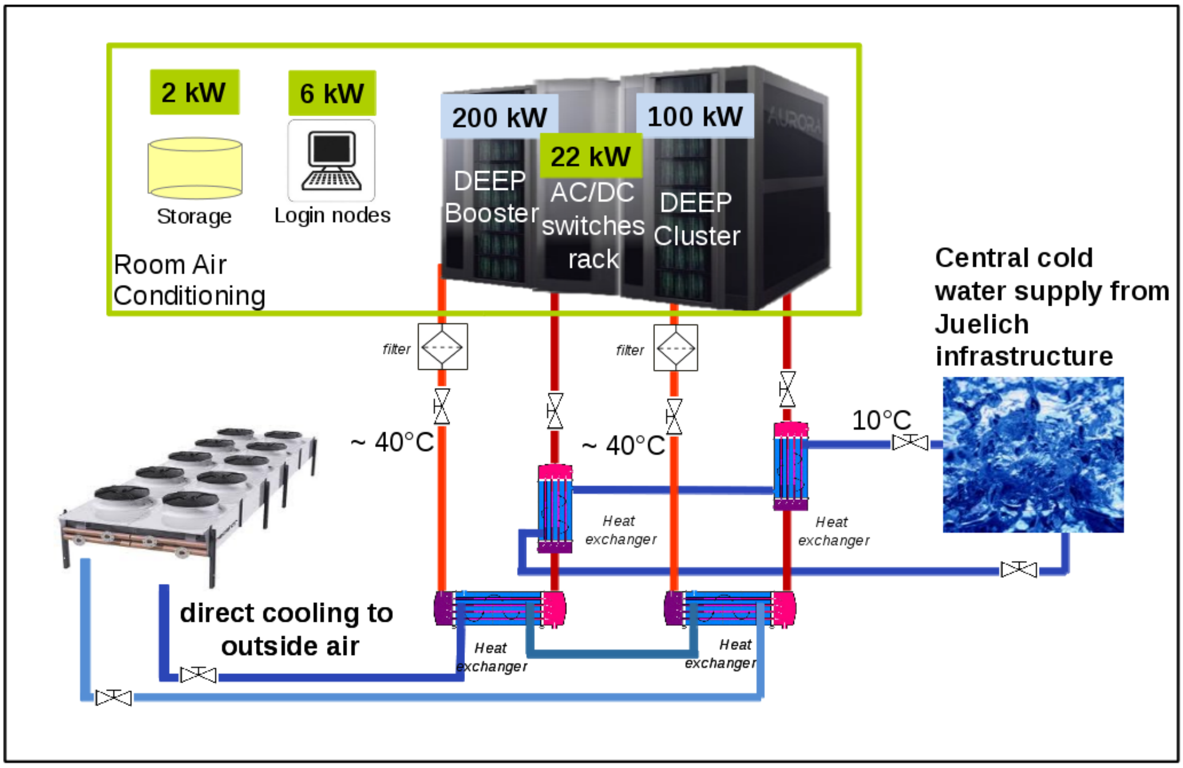


Figure 1: Cooling Concept for the DEEP System

The Aurora platform brings certain requirements and constraints for the liquid cooling system, e.g. the flow rate and pressure inside the racks and the type of connection that has to be used for tubing. Table 2 lists the specifications that have to be followed.

Description	Specification
Connection type for water pipes	M 45 / 2 mm
Pressure for inner cooling loops	2 bar
Flow rate for Cluster cooling loop	370 to 560 lpm (20°C to 40°C inlet)
Flow rate for Booster cooling loop	740 to 1120 lpm (20°C to 40°C inlet)
Filter for inner cooling loops	25 um
Flow reduction to be balanced by pumps	35% – 40%
Delta T (T_out – T_in)	3.5°C (max. 5°C)
Relative humidity in room	20% - 60 %
Minimum inlet temperature for inner loops (assuming 60 % humidity)	Max. 5 °C under room temperature
Input temperature for dry cooler	Up to 45°C

Table 2: Specifications for inner cooling circuits

With the concept of having a free cooling loop backed up by the cold water loop both circuits have to be capable to cover all the waste heat produced by the direct liquid cooled components, this means 300 kW. Hence the heat exchangers and dry coolers have to provide corresponding capacities.

Although D7.1 recommends hybrid coolers the combination of direct cooling backed by a cold water based backup seems more appropriate. In addition of not giving a substantial benefit spray-on water to be used in evaporative cooling often needs to be preprocessed as the minerals contained in the water can cause corrosion and scale on the coolers. Such treatment causes additional costs and/or energy inefficiencies.

For the free cooling circuit an anti-freeze protection like glycol has to be used, since parts of this water loop reside outside the building and temperatures could fall below zero. For the inner circuits directly connected to the Aurora racks water quality will be an important issue as well and has to be observed critically, especially when moving from cold to hot water cooling. Special requirements have to be fulfilled, to avoid problems such as corrosion and growth of microorganisms. The combination of different materials for the cooling loops has to be considered carefully.

Water quality details for the cooling system and other environmental requirements are described in section 3.

3 Infrastructure Requirements at Installation Site

This section provides a detailed description of the infrastructure requirements and changes at installation site for deploying the DEEP System. Along with the preparation of an appropriate machine room this includes the integration into the existing infrastructure regarding power supply, cooling and networking. Environmental requirements are defined by the configuration of the prototype hardware and the properties of the components developed in WP3. Installation guidelines providing in-depth specifications for the Aurora platform have been provided by Eurotech and are taken into account for planning necessary infrastructure changes.

3.1 Floor Space

As mentioned before, the compute part consists of two Aurora racks, the DEEP Cluster and the DEEP Booster, with an additional power supply rack in between. Figure 2 shows the dimensions and the floor space needed for system installation.

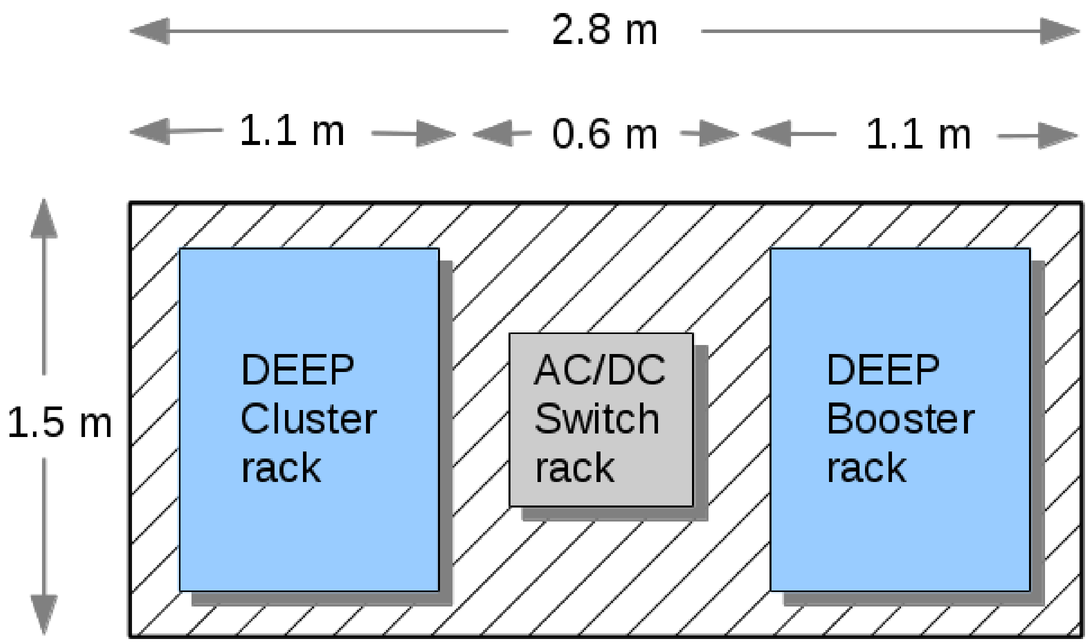
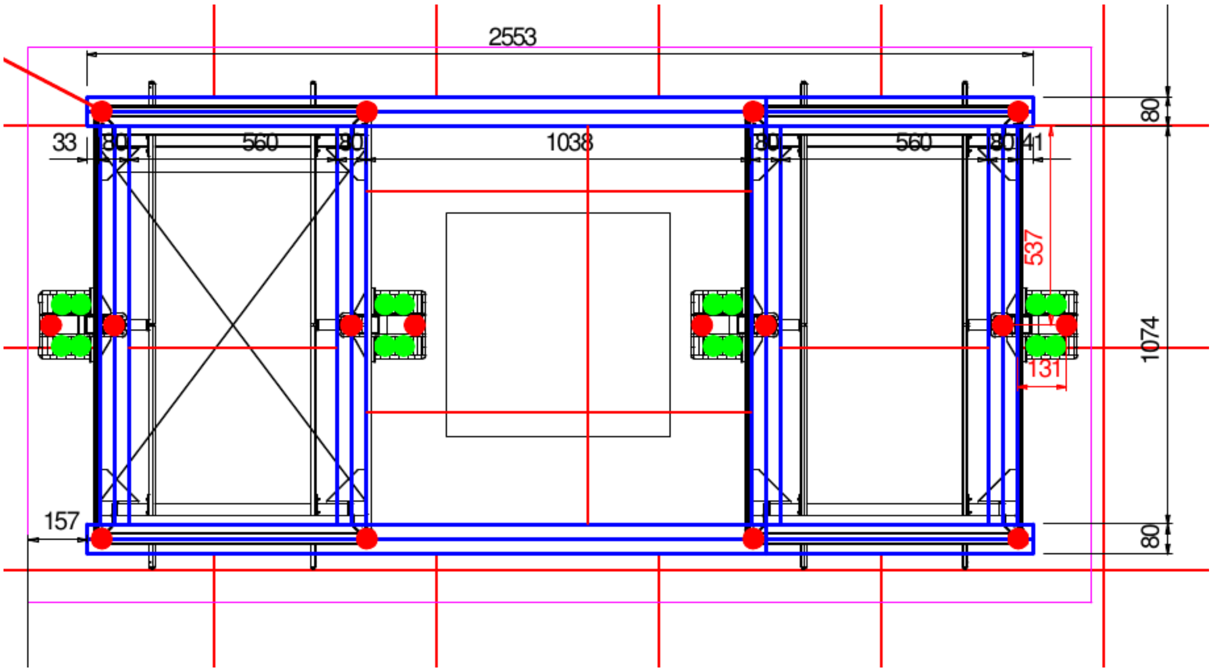


Figure 2: Floor Space Requirements for the DEEP System

Since the Aurora cabinets have larger height than standard racks, respective modifications to the building like to the access doors may become necessary. A floating floor has to be provided for cabling and placing the water pipes for the cooling loops. Additional floor space should be considered for operation and easy access to the racks, e.g. for system installation and future maintenance. To avoid impact on other compute systems at installation site and to have the opportunity of doing experimentation with the temperatures inside the cooling circuits a constructional separated and insulated machine room is advisable. As introduced before, the machine room has to provide an air conditioner to cover the waste heat of the air cooled system components, which will amount to about of 30 kW.

Due to the heavy weight of the Aurora racks (about two tons per rack) a supporting frame has to be installed with the floating floor. It has to meet the composition of the racks accurately covering the base plates. Besides it must not hinder the positioning of the inlet and outlet water pipes of the racks. Figure 3 shows the composition of the Aurora racks highlighting the foot positions that have to be carried by the frame.

Cutouts in the floating floor will be necessary for conducting the water pipes of the Aurora cooling loops into the floating floor. The cutouts should allow for easy access to the connections and help avoiding strong bends of the pipes, which could have a negative impact on the flow rates within the cooling loops and might promote material fatigue. On the other hand the cutouts should be as small as possible to avoid circulation of heat by air and not to interfere with the direct liquid cooling.



- Support frame
- Tiles of floating floor
- Pipes
- Feet of racks
- Outside cover
- Racks

Figure 3: Aurora Rack Composition and Supporting Frame

3.2 Power Supply

The DEEP prototype system has special requirements regarding power supply that are listed in Table 3 below. As of now, the values are estimations.

Description	**Specification / Value**
Power consumption DEEP Cluster	100 kW
Power consumption DEEP Booster	200 kW
Power consumption additional hardware	30kW
Connection type of AC/DC converters	3 phase, 230 V, 50 Hz
Cabling needed for Cluster and Booster	26 x 2 cables
Number of cut-outs needed for Cluster and Booster	52 (32 A)
Cabling needed for additional hardware	About 20 cables

Table 3: Requirements for Power Supply

To provide sufficient electrical power, an electrical sub-distribution has to be implemented in the machine room. Since this is a prototype system with no requirement for high availability, an uninterruptible power supply will not be necessary.

Power consumption of the system will be an important aspect for doing investigations on energy efficiency. To allow for accurate measurements and evaluation of energy efficiency, power sensors have to be added to the whole power supply chain outside the racks including the cooling system (e.g. dry cooler and pumps) and additional hardware components. They should be integrated into the DEEP management plane covering the DEEP internal sensors.

3.3 Liquid Cooling and Water Quality

Applying the cooling concept introduced with Figure 1, four cooling loops and corresponding heat exchangers have to be installed. Tubing has to be done in aluminum, stainless steel or plastic to ensures a compatible material mix and avoid corrosion of the aluminum in the cold plates inside the racks. High quality stainless steel with properties similar to aluminum is used for pipes and heat exchangers at the installation site.

For the two inner loops connected to the Cluster and the Booster racks, special water quality is needed which can be derived from the ASHRAE (American Society of Heating, Refrigerating and Air Conditioning Engineers) guidelines [2]. The following table shows the aspects and characteristics of importance for the water quality:

Description	**Specification**
pH value	7 – 9
Sulfides	< 1 ppm
Sulfate	< 10 ppm
Chloride	< 5 ppm
Bacteria	< 100 CFU / ml
Total hardness (as $CaCO_3$)	< 20 ppm
Conductivity	0.2 to 20 micromho / cm^2
Total suspended solids	< 3 ppm
Residue after evaporation	< 50 ppm
Turbidity	< 20 NTU (nephelometric)
Biocide	needed
Corrosion inhibitor	needed

Table 4: Water Quality Specifications

Providing high water quality is essential for hot water cooling to avoid several problems. For instance:

- Corrosion of aluminum parts leading to leakages
- Growth of microorganisms, which impedes water flow and reduces thermal conductivity
- Occurrence of flaking metal particles, that can jam the filters or the cooling channels

Hence it is very important to keep the values specified in the guide lines and to frequently control the water quality. There is no clear recipe available on the water mixture to fill the cooling loops with, because water quality within hot water cooling loops is a very complex subject. There are lots of influences and dependencies to be considered and therefore the water quality forms a very interesting research aspect for the DEEP project that will be addressed in WP7.

For example, chemical additives have a direct impact on the pH value. Growth of bacteria and algae strongly depends on the water temperature, what makes it even more complicated when changing the inlet temperatures of the system as planned within the DEEP project. Besides, for the use of chemicals like biocide and corrosion inhibitors special constraints have to be observed:

- Corrosion inhibitors have to be compatible with the materials used for the cooling loops
- Adding biocide might create resistant bacteria
- Health and safety aspects have to be taken into account

The advice of the project partners (Eurotech, BADW-LRZ and UniReg), who have already some experience with water quality in hot water cooling systems, has been taken into account. Furthermore suppliers of additives may be consulted.

High quality purified water fulfilling the restrictions mentioned above is available at the installation site. However, purified water can become very aggressive when it gets in contact with oxygen. Since water loops can usually not be guaranteed to be entirely gas tight this might become a problem, when no corrosion inhibitor is added to protect the aluminum.

A good approach to handle all this obstacles will be as follows:

1. **Clean the loops**

   Before filling the loops they have to be cleaned to flush out particles and dirt that might be present from installation. Applying a chemical cleaner will help to achieve better results and can also improve the properties and resistance of the aluminum cold plates. Furthermore it has to be ensured that no leakages exist.

2. **Use a reasonable start configuration**

   When filling the loops for the first time all the requirements described before have to be hold. Purified water available at installation site can be used, but de-airing of the system as to be processed very carefully then. A small amount of biocide and corrosion inhibitor compatible with the used materials might be added.

3. **Frequent analysis of water quality**

   In the first period the water quality has to be observed very frequently including

   - pH value
   - Conductivity
   - Carbonates (hardness)
   - Metal particles
   - Level of chemistry
   - Level of microorganisms

   Ingredients can then be added on demand. For example the amount of biocide should be increased if the growth of microorganisms is too high, which can be determined through water quality analysis at installation site. When the water quality seems to be getting stable the frequency of water quality analysis can be reduced, but measurements should be done at least twice a year. As the temperature of the coolant has an influence on the quality additional tests might be necessary.

Along with measurements of power consumption sensors for the cooling loops have to be installed to observe the water flow rates and the water temperature for each of the four input and output channels of each rack. Just as the electric sensors they should be integrated in the general management plane. Devices for automatic water quality analysis (like pH value) might be considered as well.

3.4 Network and Additional Hardware

The DEEP System will be used by several partners within the project. Hence access to external users outside JUELICH has to be provided. A high capacity networking infrastructure is available at installation site, both for internal and external connections, where the DEEP System has to be integrated.

For monitoring and administering the system as well as user logins, an Ethernet based admin network has to be installed. This will also enable access to the DEEP management plane. A 1 Gb/s Ethernet provides enough bandwidth to cover the network traffic caused by administrative tasks and monitoring. Components that have to be integrated into the Ethernet admin network will be the compute parts and additional hardware of the management plane. This includes management servers, a storage system and available sensors. WP6 has to take care, that necessary hardware components like Ethernet switches will be available and the cabling between the network components will possible which might affect several rooms within the installation site. Figure 4 gives an overview on the administration network.

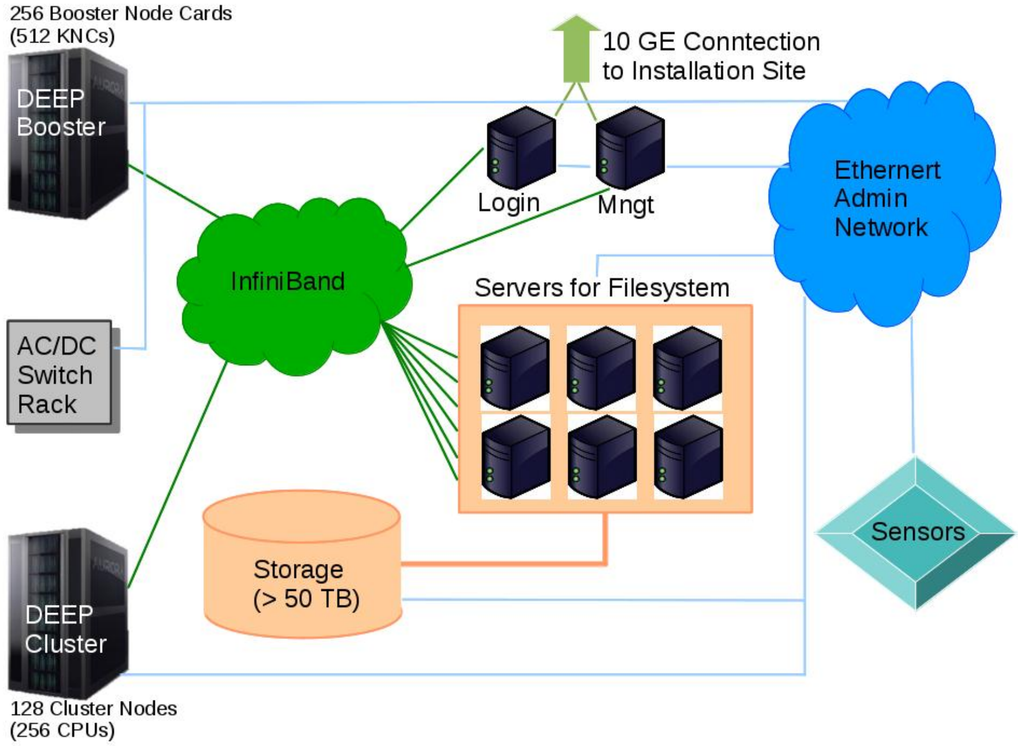


Figure 4: Administration Network

In addition to the Ethernet admin network, a fast InfiniBand interconnect has to be set up between the Cluster and the DEEP Booster. It has to include fast access to the storage system. The concept for the interconnect between the Cluster and the Booster has already been described in D3.1. It has to be ensured, that the InfiniBand connections provide sufficient capacity to avoid bottlenecks in Cluster - Booster communications. Therefore a two-layer InfiniBand connection scheme, developed within WP4, is being installed depicted in Figure 5. The Cluster nodes are connected with eight root cards, each of them providing InfiniBand interconnect for 16 node cards.

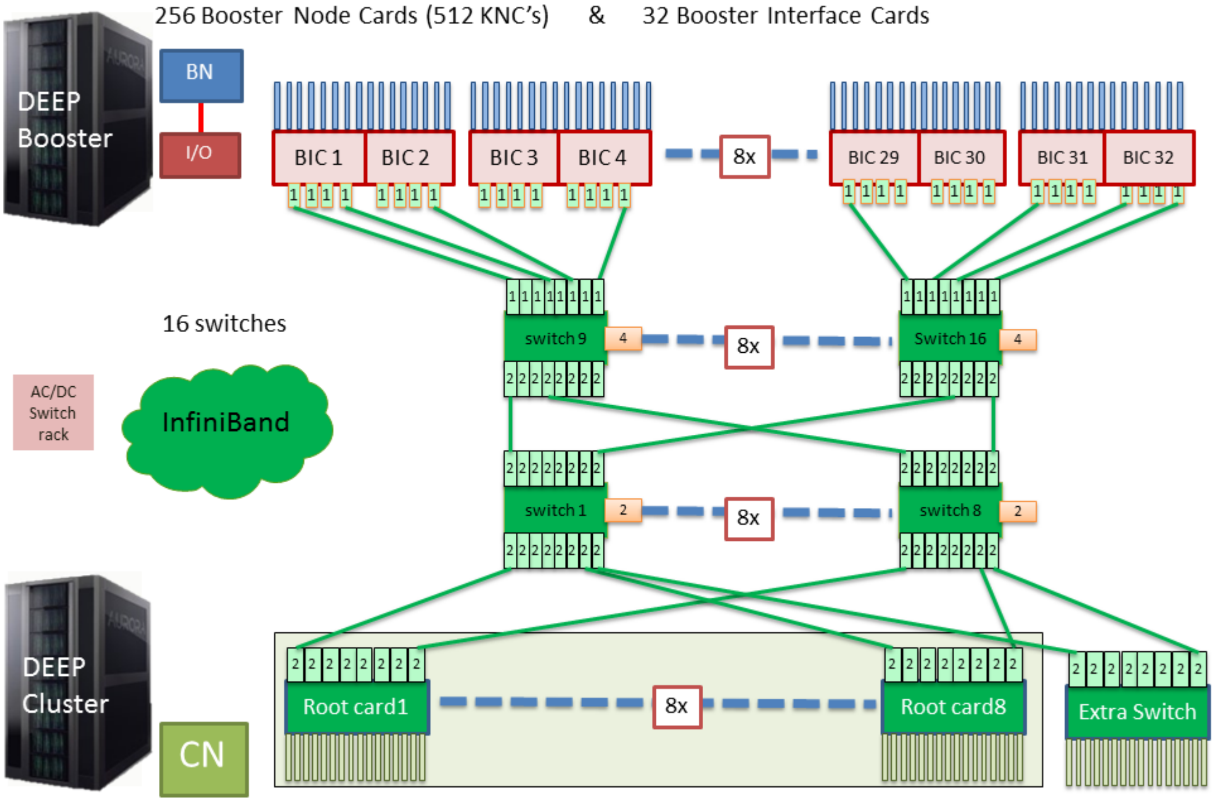


Figure 5: DEEP InfiniBand Network

Several hardware components like InfiniBand switches and cables have to be procured for the implementation. Due to the high temperatures that might occur in the Cluster and the Booster racks, the network components have to be placed into the middle supply rack, to avoid failures and a negative impact on the MTBF.

Additional hardware is necessary for deployment and operation of the system. A storage system including access through a parallel file system has to be installed to provide sufficient disk space (at least 50 TB) for application data. Besides, some login and management nodes will be needed to allow for external user login and administration. Several software components will have to be installed to run the system.

This includes:

- Operating System (OS) on the Cluster compute nodes with low update frequency to reduce maintenance costs, compatible with DEEP Software Stack
- Parallel filesystem (servers and clients)
- Cluster Management Software (ParaStationMPI)
- Software for user and data management on login node (e.g. LDAP)
- Batch system for resource management on management node (e.g. Torque)

To have fast and easy access to the compute hardware and the components for cooling and power supply, installation of panels and consoles has to be considered. Additional hardware has to be provided to monitor and evaluate the various sensors included in the installation and to be used as a frontend for the global management plane.

References and Applicable Documents

[1] http://www.deep-project.eu
[2] Ashrae TC 9.9: „2011 Thermal Guidelines for Liquid Cooled Data Processing Environments", Whitepaper, 2011
[3] http://www.guentner.de
[4] http://www.eurotech.com/en/hpc/

List of Acronyms and Abbreviations

A

AC/DC: Alternating Current / Direct Current
ASHRAE: American Society of Heating, Refrigerating and Air-Conditioning Engineers
Aurora: The name of Eurotech's cluster systems

B

BADW-LRZ: Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften.Computing Centre, Garching, Germany
BN: Booster Node (functional entity)
Booster System: Hardware subsystem of DEEP comprising of BNC, BIC and Intra-Booster network
BoP: Board of Partners for the DEEP project

C

CN: Cluster Node (functional entity)
CooLMUC: Prototype at BADW-LRZ with direct warm water cooling
CPU: Central Processing Unit
CRAC: Computer room air conditioning

D

DC: Direct Current (electricity)
DEEP: Dynamical Exascale Entry Platform: EU-FP7 Exascale Project led by Forschungszentrum Juelich
DEEP Architecture: Functional architecture of DEEP (e.g. concept of an integrated Cluster Booster Architecture)
DEEP Booster: Booster part of the DEEP System
DEEP System: The production machine based on the DEEP Architecture developed and installed by the DEEP project

E

EC: European Commission
Energy Efficiency evaluator: Platform used for the investigations of the energy-aware functionality of DEEP, used only in the DEEP project
EU*:* European Union
Eurotech: Eurotech S.p.A., Amaro, Italy
Exaflop: 10^{18} floating point operations per second
Exascale: Computer systems or applications, which are able to run with a performance above 10^{18} floating point operations per second

F

FLOP: Floating point Operation

G

H

HPC: High Performance Computing

I

IB: InfiniBand
Intel: Intel GmbH Braunschweig, Germany
IT: Information Technology

J

JSC: Juelich Supercomputing Center
JUELICH: Forschungszentrum Jülich GmbH, Jülich, Germany

K

KNC: Knights Corner: Code name of a processor based on the MIC architecture

L

LDAP: Lightweight Directory Access Protocol

M

MTBF: Mean Time Between Failures

N

O

OS: Operating System

P

ParaStation Consortium: Involved in research and development of solutions for high performance computing, especially for cluster computing
ParaStationMPI: Software for cluster management and control developed by ParTec
ParTec: ParTec Cluster Competence Center GmbH, Munich, Germany
PC: Normally Personal Computer, but in the context of the proposal also Project Coordinator
PMT: Project Management Team of the DEEP project

Q

R

S

SW: Software

T

U

UniReg: University of Regensburg, Germany
UPS: Uninterruptible Power Supply

V

W

WP: Work Package

X

Y

Z