DEEP

Dynamical Exascale Entry Platform

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D7.3
Preparation of energy and cooling experimentation infrastructure

Approved

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Date: 16.01.2015
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<td>EC Project Officer:</td>
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Approved by: BoP/PMT

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Executive Summary

Energy efficiency is one of the most important topics in the DEEP project, as it will be pivotal for building Exascale systems. While different strategies and approaches have been proposed to improve the energy efficiency of HPC systems, most of these systems lack the infrastructure to test different approaches and assess their impact and effectiveness. The DEEP project will therefore commission a second prototype system specifically for such experiments: the Energy Efficiency Evaluator. It will employ a sophisticated liquid cooling infrastructure with extensive monitoring capabilities and flexible control loops. High-precision sensors will allow for very accurate measurements of all important parameters, such as temperatures, water pressure, and flow rates, and hence facilitate a wide range of energy efficiency experiments.

This document gives a detailed description of the cooling infrastructure and its monitoring and controlling capabilities. Its design takes into account the IT system requirements as specified by WP3 (System Hardware) with regard to monitoring and cooling capabilities, as well as the requirements from WP7 (Energy Efficiency) for energy efficiency experiments, such as water inlet temperatures, variable pump speeds, high-precision measurements of temperatures and heat flows, and monitoring of water quality.
1 Introduction

In addition to the DEEP System at the Juelich Supercomputing Centre, a second, small-scale system is to be installed at the facilities of Leibniz Supercomputing Centre (BADW-LRZ). We refer to this smaller system as the “Energy Efficiency Evaluator” (EEE) since its purpose is to:

- Conduct experiments with the liquid cooling system at higher temperatures
- Improve firmware for system power-measurement and the DEEP software stack for Reliability, Availability, and Serviceability (RAS)
- Conduct experiments to explore the power saving techniques of the DEEP System

Since operational stability cannot be ensured during these activities and frequent reboots are to be expected, using a separate Energy Efficiency Evaluator for these experiments minimises the impact on the application porting and optimisation efforts of WP8 (Pilot Applications).

As outlined in D7.1 [1], attention has to be paid to the material mix of the cooling loop and the water quality in liquid cooled supercomputers. Hence, it is necessary to build a separate cooling infrastructure to decouple the existing cooling water loops of the BADW-LRZ data centre from the cooling water within the DEEP hardware using a heat exchanger.

This document describes the high-level goals and the resulting design of this cooling infrastructure. It therefore starts with a description of the existing facilities at BADW-LRZ, the requirements from WP3 for safe machine operations, and the goals and requirements of WP7 for conducting energy efficiency related experiments. It then explains the setup in detail including the piping structure and electronics for monitoring and control.

2 Existing Infrastructures and Conditions at BADW-LRZ

BADW-LRZ’s data centre is located in Garching, roughly 20 minutes north of the city of Munich in southern Germany. The computer building spreads over five floors and contains 3,160m² of IT equipment space. Additional 6,393m² of space are occupied by the surrounding building infrastructures. The centre is designed for a maximum power draw of 10MW that are supplied via two redundant 20kV underground power supply lines.

The room in which the Energy Efficiency Evaluator will be set up is located on the second floor of the building and provides an area for IT equipment of 21x21m². The room has a total height of 4.98m out of which 4.09m are above the false floor. Ceiling mounted lights and power rails restrict the maximum height for IT equipment to 2.69m.

Power supply in the room is provided using overhead power rails that provide standard IEC 60309 CEE 32A 3L+N+PE power outlets. Power quality (e.g. protection against brown-outs) is ensured using fly-wheel uninterruptible power supply units (UPS). Yet, there is no backup generator for IT equipment in this room, meaning that outages in the electric grid of more than a few seconds will lead to a loss of power to the room’s IT equipment and cooling infrastructure. Not providing backup power for prototype system is one of BADW-LRZ’s means of improving overall data centre energy efficiency since the electrical overhead for standby UPS systems would not be justified.

The room has already been prepared for liquid cooling during its construction in 2010 and provides both, cold and warm-water cooling loops. The cold water supply originates from the central cold-water facilities located on the ground level of the building and is currently operated with a set point of 14°C. The warm-water cooling loop is a chiller-free water circuit that connects the room’s infrastructure to the cooling towers on the roof. The warm-water
loop currently operates at a set point of 40°C. As of today, the room hosts the CooLMUC PRACE prototype system as well as a small direct liquid cooled GPGU test system. Both systems remove their heat via the warm-water cooling loop solely. In addition to the water-cooling infrastructure, the room is equipped with standard computer room air conditioning (CRAC) units, with water-to-air heat exchangers which blow cold air into the false floor. The current set point for the air outlet temperature of the CRACs is 22°C.

All cooling loops have separate control units that locally manage pump speeds, valve settings, etc. The control units are connected via a dedicated Ethernet infrastructure to the central cooling manager using the BACnet protocol [2]. All high-level cooling parameters in the individual control units are configured and monitored via this network by the central building infrastructure-management solution based on Johnson Control’s MetaSys 5 software.

Figure 1 Screenshot of the central infrastructure management tool based on Johnson Control MetaSys

BADW-LRZ’s data centre is located in southern Germany and hence in a mild climate zone. It rarely observes summer temperatures above 35°C. Our own records from 2013 show that even during the warmest days of the year at the end of July, wet-bulb temperatures never exceeded 25°C (Figure 2). Therefore, even including some safety-margins, it has been possible in the past to provide chiller-less cooling using the warm-water cooling loops for the SuperMUC supercomputer all year-round for inlet temperature set points of 35°C and above.
3 System Design Specifications and Requirements

The DEEP Energy Efficiency Evaluator will consist of 4 Cluster Nodes, 1 Booster Interface Node, and 8 Booster Node Cards (16 Booster Nodes). The goal of the infrastructure preparation is to ensure that the requirements of the EEE hardware as well as the requirements for the planned experiments on energy efficiency are met. The IT system requirements originate from WP3, the requirements for the energy efficiency experiments originate from the discussions in WP7.

3.1 IT System Requirements

WP3 has defined the following infrastructure requirements for the EEE’s IT-hardware:

**Power**
- Max. power consumption: 10kW
- Power supply via 4x 230V single phase cables

**Cooling Water (physical properties)**
- Flow-rate for Cluster Nodes and Root Card: 580 lph
- Flow-rate for Booster Nodes and Booster Interface Nodes: 1800 lph
- Working pressure: 2 bar
- Target ΔT inlet/outlet: 3.5 - 6°C
- Coolant temperature always > dew point

**Cooling Water (quality)**
- Corrosion inhibitor: Clariant Proctectogen C Acqua 2% v/v
Biocide: Clariant Nipacide BIT20 0.2%
Input filtering: 25µm preferred, 50µm allowed
No Teflon gasket after filter
Materials in the loop: Aluminium preferred, stainless steel allowed
All other parameters according to ASHRAE "Liquid Cooling Guidelines for Datacom Equipment Centers"

Monitoring
- Coolant input temperature to the rack
- Coolant output temperature at the rack
- Coolant flow rate
- Differential pressure over the filter
- Absolute system pressure

3.2 Requirements for Energy Efficiency Experiments

For the planned experiments on energy efficiency and warm-water cooling in WP7, the following requirements have been identified:

High Inlet Temperature Range
It should be possible to operate the EEE at varying coolant temperatures. As has been reported in D7.1 and D7.2, results from our current water-cooled experimentation platforms showed dependencies between semiconductor operating temperatures and power consumption due to leakage currents. However, we also know that the extent to which higher chip temperatures result in higher power draw varies between different semiconductor manufacturing processes. We would like the EEE infrastructure to allow for measuring this effect on DEEP hardware and therefore operate the system at varying temperatures ranging from ~16°C to up to 50°C. Obviously, special care will have to be taken of particularly low and high temperatures due to the risks of condensation and overheating.

Variable Pump Speeds
One of the key aspects for improved energy efficiency in HPC is to recapture waste-heat for energy reuse. Due to the Carnot principle, the efficiency of such efforts is restricted by the difference between the waste heat’s temperature and the temperature of the re-cooling medium such as outside air, or river water. To improve the reuse efficiency, high outlet temperatures of the HPC system’s waste heat are desirable. Apart from driving the system at higher inlet temperatures, higher outlet temperatures can also be achieved by reducing the water flow in order to increase the temperature delta over the EEE’s hardware. Therefore, the system should be equipped with a pump allowing for variable pump speeds.

Measuring Heat Flows
In D7.1 and D7.2, we have discussed the superiority of water over air as a cooling medium. In most cases, HPC systems are cooled using a mix of water and air cooling, since some components (e.g. power supplies) typically remain air cooled. Even when all components are being water-cooled, convection typically causes some heat to be picked up by the ambient air surrounding the machine. Thus, the overall cooling efficiency of a liquid cooled HPC system depends on the fraction of heat that is being removed by the water. Due to the principle of energy conservation, we can measure the amount of heat energy removed from the system using water and compare that to the amount of electrical energy that was spent to power the system to derive this fraction.

Temperature Monitoring Accuracy
Measuring heat flows into or out from a system (as described above) is performed by taking into account the inlet and outlet water temperatures of the system and the flow rate. The thermal output (e.g. through a heat-exchanger) is then defined as:

\[
\dot{Q} = \dot{V} \cdot \rho \cdot c_W \cdot (t_{\text{out}} - t_{\text{in}})
\]

where

- \( \dot{Q} \): Heat output in kW
- \( \dot{V} \): Flow rate in l/s
- \( \rho \): Water density in kg/m³
- \( c_W \): Specific heat capacity of water in kJ/(kgK)
- \( t_{\text{in}} \): Inlet temperature in °C
- \( t_{\text{out}} \): Outlet temperature in °C

When taking into account a temperature delta of 3.5-6°K as specified by WP3, it becomes clear that accurate temperature measurements are necessary. The widely used PT100 / PT1000 temperature probes require accurate digitalisation and extensive calibration, an effort, which we like to avoid by using digital temperature probes.

**Water Quality Measurements**

Retaining water quality can become an issue in liquid cooled computer systems, particularly when aluminium is part of the material mix. Therefore, the EEE cooling infrastructure should facilitate taking water samples for analysis and refill the system afterwards. Since it is believed that the pH and conductivity of the cooling water can provide hints for ongoing corrosion, we also would like to continuously monitor these two parameters using electronic probes.

## 4 Final Infrastructure Setup

Based on the requirements described in the previous sections, a piping scheme has been developed that interfaces between the DEEP System and the existing cooling loops. It is capable of satisfying all needs in a flexible, yet economic manner. Since the infrastructure is an in-kind contribution by BADW-LRZ, reusability for future installations has also been considered.

### 4.1 Pipe System Setup

The final system plan is shown in Figure 3. It is based on a simple temperature controlled 3-way mixing loop comprising a pump, a heat exchanger and a 3-way mixing valve. We refer to this part of the system as the primary circuit since it also contains the DEEP hardware to be cooled. In the primary circuit, the 3-way valve controls the inlet temperature to the DEEP System: short-circuiting water from outlet to inlet increases the temperature, diverting water to the heat exchanger on the other hand will result in heat being removed from the primary circuit and thus from the DEEP System.

With respect to the DEEP hardware, the pipe system splits into two legs - one for the Cluster and one for the Booster. Each leg then splits again into two, providing four pairs of system connectors in total. For the Energy Efficiency Evaluator, we will only use two pairs, the other pairs are reserved for future use when cooling higher heat loads.

On the other side of the heat exchanger, water from the existing building side cooling loops is responsible to remove the heat from the room. We refer to this as the secondary circuit. Manual ball valves in the secondary circuit are used to select among the room’s cold or warm-
water cooling loops. This enables a large temperature range for the cooling experiments when driven by the cold water loop and allows for energy-efficient standard operations using the warm-water loop.

To retain pressure and to compensate for temperature-induced expansion, the primary circuit contains a pressure compensation vessel. A mechanical pressure gauge is used to monitor water pressure when filling the system. A separate safety valve protects against overpressure.

All vertical pipes in the system are equipped with manual breather valves. Manual de-airing is preferred over automatic de-airing due to the risk of water leaking out of automatic breather valves when contained in pressurised loops under continuous operation.

The design is capable of serving cooling loads of up to 50kW. The pump speed is electronically controllable and thus, the entire setup can be adapted to lower cooling needs.

In terms of flexibility, all connectors to the building’s cooling loops as well as to the DEEP hardware are realised using flexible EPDM rubber hoses. Thus, the entire setup can easily be moved within the data centre. This setup also facilitates connecting to future systems. Apart from the EPDM rubber, all other components in the primary circuit are made of stainless steel to avoid incompatibilities in the material mix.

Multiple measures are in place to monitor and improve water quality in the system. A special dosage sluice is used to take water samples and inject additives such as biocides and corrosion inhibitors into the water. Flowing from the 3-way valve towards the DEEP System, water first passes a 50µm filter before some of the water is diverted to flow through a special fitting hosting a pH and conductivity probe.

For temperature measurements, the pipes are equipped with sensor fitting sleeves that reach into the center of the pipes. Temperature sensors are placed within these sleeves using thermal grease. Temperatures being monitored are the two in- and outlet temperatures to the heat exchanger as well as the in- and outlet legs to the Cluster and Booster part.

Heat flow measurements are accomplished by inserting flow meters into the Cluster and Booster legs respectively. A third flow meter monitors the secondary circuit. In conjunction with the temperature sensors, heat removed from Cluster and Booster can be measured separately as well as the total heat flow towards the room’s cooling loops.

To detect obstruction events and to monitor pump performance, differential pressure measurements over the filter, the compute system, and the pump are desirable. Instead of using differential pressure sensors, the system contains three simple pressure sensors that measure water pressure against the atmospheric pressure of the room. The sensors are located between the pump and the filter, between the filter and the DEEP System, and between the system and the pump. When calibrated, these sensors provide the same insight towards filter obstruction as a special differential pressure sensor.
Figure 3 Piping diagram of the Energy Efficiency Evaluator infrastructure
4.2 Monitoring and Control

Most commercially available monitoring and control systems for cooling infrastructures are designed for industrial, production-level applications. Those systems typically focus on providing constant cooling year-round with hard limits and provide only limited flexibility with regard to varying workloads and changing operational parameters. Most of them employ proprietary protocols which prohibit mixing components from different vendors. Often, the initial setup has to be done by a specialist with vendor-specific software tools that are not publicly available. Any modification of the control algorithm can only be done by the specialist and needs to be paid for.

For these reasons, we decided not to use an industrial monitoring and control system but develop our own solution based on a low-cost Raspberry Pi model B minicomputer. As it employs a Broadcom BCM2835 ARM SoC which provides a wide range of general purpose input and output (GPIO) pins that can be used for connecting actuators and sensors, it is particularly well suited for this task [3].

4.2.1 Hardware

As described in section 4.1, there will be a large amount of sensors and actuators in the Energy Efficiency Evaluator that need to be connected to the Raspberry Pi: a total of 17 sensors and 2 actuators. A detailed list of these can be found in Table 1.

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<td>Analogue: 0-10V</td>
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<tr>
<td>1</td>
<td>Actuator</td>
<td>Electrical 3-way valve</td>
<td>Analogue: 0-10V</td>
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<td>8</td>
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<td>Water flow</td>
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<tr>
<td>1</td>
<td>Sensor</td>
<td>PH</td>
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<tr>
<td>1</td>
<td>Sensor</td>
<td>Electrical conductivity</td>
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<tr>
<td>1</td>
<td>Sensor</td>
<td>Feedback from 3-way valve</td>
<td>Analogue: 2-10V</td>
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Table 1: Actuators and sensors

In the industrial automation industry, actuators and sensors typically use analogue signalling systems that either employ voltages between 0 and 10V or currents between 4 and 20mA. As the Raspberry Pi provides no analogue input and output channels, additional circuitry is required to deal with these signalling systems. For analogue input, analogue/digital converters (ADC) can be used to translate voltage levels into digital values. ADCs are available from multiple vendors with a wide range of different characteristics such as sampling frequency, sampling precision, number of channels, digital interface, and packaging. Reading the signals of voltage driven sensors via the digital interface is then straightforward with an ADC. As the acceptable voltage range of most ADCs is typically below 5V, an additional voltage divider may be required to adjust the 0-10V voltage levels of the sensors accordingly. Current driven sensors can also be read with such an ADC by measuring the potential difference across a shunt resistor between the two connectors of the sensor.
In an early prototype setup (see Figure 4) we used a Microchip MCP3208 analogue/digital converter, an ADC with 8 channels, 12-bit resolution, and a maximum sampling rate of 100,000 samples/s. It provides a Serial Peripheral Interface (SPI) digital interface that connects to one of the two SPI ports of the Raspberry Pi. However, as the planning of the cooling infrastructure has now been finalised, it became clear, that the 8 channels of this ADC were not sufficient to read the measurements from the 9 analogue sensors. We are therefore planning to switch to the Texas Instruments TLC1543 with 11 channels and which also connects via SPI [4]. Compared to the MCP3208, it only provides 10-bit resolution and a maximum sampling rate of 38,000 samples/s, which however is still expected to meet our requirements.

For the two voltage controlled actuators, digital/analogue converters (DACs) will be required to generate the required analogue output signals with voltages between 0 and 10V. In the prototype setup we used the hardware PWM (Pulse-Width Modulation) output of the Raspberry Pi and a low-pass filter for that purpose. However, as there is only one PWM port available, but two actuators (the pump and the electrical 3-way valve), two DACs will be required for the final Energy Efficiency Evaluator. Instead of implementing an additional PWM port on one of the GPIO pins in software, we decided to use a dedicated DAC chip instead. Similarly to the ADCs, there is a large variety of different DACs available. We chose the Microchip MCP4812, a dual-channel 10-bit DAC with SPI interface that will connect to the second SPI port of the Raspberry Pi [5]. As the maximum output voltage of the MCP4812 is limited to 2.048V, an additional non-inverting operational amplifier circuit will have to be added between the DAC output and the actuator input to increase the voltage levels to the required 0-10V range.
As temperature sensors we chose the TSIC-306 digital sensors from Innovative Sensor Technology with a typical accuracy of +/- 0.3°C, 0.1°C resolution, and a sampling rate of 10Hz [6]. The use of digital temperature sensors instead of the widely used analogue sensors like PT1000 allows for more precise temperature measurements as it avoids the need for error-prone sensor calibrations. The TSIC sensor series employs the ZACwire protocol [7], a custom 1-wire digital interface that can easily be implemented in software on the Raspberry Pi's GPIO pins.

4.2.2 Software

The Raspberry Pi runs on Rasbian Linux, a customised Debian-based Linux distribution for ARM. It provides kernel drivers to access the SPI interface as well as the Raspberry's GPIO ports.

For reading the TSIC-306 temperature sensors via the GPIO pins, we developed a Linux kernel module for the ZACwire protocol. The kernel module consistently enumerates all connected sensors and provides read access to them via the Linux Industrial I/O (iio) subsystem.

The Industrial I/O subsystem of the Linux kernel provides an easy to use interface to sensors and actuators via the sysfs filesystem interface. Depending on the actual hardware and the implementation of the driver, it allows for reading and writing raw values as well as derived values like °C, mV, or mA. As it is a filesystem interface, any environment that provides read/write access to files can be used to read sensors and to set actuators. This is particularly useful in a prototyping environment like the Energy Efficiency Evaluator as it allows for reading sensors and setting actuators from a command line shell.

Currently, no kernel driver exists for the MCP4812 DAC and the TLC1543 ADC. However, as both chips utilise the SPI digital interface, a corresponding driver should be straightforward to implement based on their datasheets. Additionally, there are drivers available for other DACs and ADCs with similar protocols from the same vendors that can be used for reference. For the MCP4812, there exists a user-space driver in the wiringPi framework that could be easily used as additional reference for the implementation of a kernel space driver. Similarly to the TSIC-306 driver, the kernel drivers for the DAC and the ADC will also be developed for the iio subsystem.

5 Conclusion

The final design of the infrastructure for the DEEP Energy Efficiency Evaluator fulfills the requirements of WP3 and WP7. It has been designed with flexibility and cost in mind. With its monitoring capabilities, the infrastructure will enable many experiments related to energy efficient HPC systems operation. It will also help in gaining further experience with direct (warm-)water cooled HPC systems.

It is expected that most of the results originating from the experiments conducted on the Energy Efficiency Evaluator will be applicable to the full DEEP System in Jülich. Also, the additional insight in the field of cooling water quality will hopefully be helpful to all operators of liquid cooled supercomputers.
References and Applicable Documents


# List of Acronyms and Abbreviations

## A

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<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>ADC</td>
<td>Analog Digital Converter</td>
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<tr>
<td>ASHRAE</td>
<td>American Society of Heating, Refrigerating and Air-Conditioning Engineers</td>
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<tr>
<th>Acronym</th>
<th>Description</th>
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<tr>
<td>BADW-LRZ</td>
<td>Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Computing Centre, Garching, Germany</td>
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<td>BACNet</td>
<td>Building Automation and Control Network; a protocol used in building automation and monitoring. In DEEP, BACNet is used to manage the cooling and power infrastructure surrounding the DEEP System.</td>
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<tr>
<td>BMC</td>
<td>Baseboard Management Controller</td>
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## C

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<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>CooLMUC</td>
<td>Prototype at BADW-LRZ with direct warm water cooling</td>
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<tr>
<td>CRAC</td>
<td>Computer room air conditioning</td>
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## D

<table>
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<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
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<td>DAC</td>
<td>Digital Analog Converter</td>
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<td>DEEP</td>
<td>Dynamical Exascale Entry Platform: EU-FP7 Exascale Project led by Forschungszentrum Juelich</td>
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<td>DEEP System</td>
<td>The production machine based on the DEEP Architecture developed and installed by the DEEP project</td>
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<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy Efficiency evaluator (EEE)</td>
<td>Platform used for the investigations of the energy-aware functionality of DEEP, used only in the DEEP project</td>
</tr>
<tr>
<td>EPDM</td>
<td>Ethylene propylene diene monomer, a synthetic rubber with a wide range of applications</td>
</tr>
</tbody>
</table>

## G

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>GPIO</td>
<td>General Purpose Input/Output</td>
</tr>
</tbody>
</table>

## J

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>JUELICH</td>
<td>Forschungszentrum Jülich GmbH, Jülich, Germany</td>
</tr>
</tbody>
</table>

## L

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LINUX</td>
<td>A Unix-like computer operating system assembled under the model of free and open source software development and distribution</td>
</tr>
<tr>
<td>Lph</td>
<td>Litres per hour</td>
</tr>
</tbody>
</table>

## P

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PWM</td>
<td>Pulse-Width Modulation</td>
</tr>
</tbody>
</table>
D7.3 Preparation of energy and cooling experimentation infrastructure

**R**

**RAS:** Reliability, Availability and Serviceability

**S**

**SPI:** Serial Peripheral Interface  
**SoC:** System-on-Chip  
**SuperMUC:** Tier-0 supercomputer at BADW-LRZ  
**SysFs:** Virtual file system provided by the Linux kernel to export information from devices and drivers to the user.

**U**

**UPS:** Uninterruptible Power Supply