



Leibniz Supercomputing Centre  
of the Bavarian Academy of Sciences and Humanities



**GCS@LRZ update: HPC, Data Center Infrastructure and  
Machine Learning**

HPC User Forum, February 28, 2017 Stuttgart

**Arndt Bode** Chairman of the Board, Leibniz-Rechenzentrum of the Bavarian Academy of  
Sciences and Humanities and Technische Universität München



# Leibniz Supercomputing Centre (LRZ)



- IT Equipment Floor Space: **3160.5 m<sup>2</sup>**  
(34 019 ft<sup>2</sup> 6 rooms on 3 floors)
- Infrastructure Floor Space: **6393.5 m<sup>2</sup>**  
(68 819 ft<sup>2</sup>)



**Generic IT services to all Munich universities**

- Internet Access, Munich Scientific Network
- IT Service & Support
- ...



**IT services to all Bavarian universities**

- Software License Management
- Backup & Archive Services
- ...



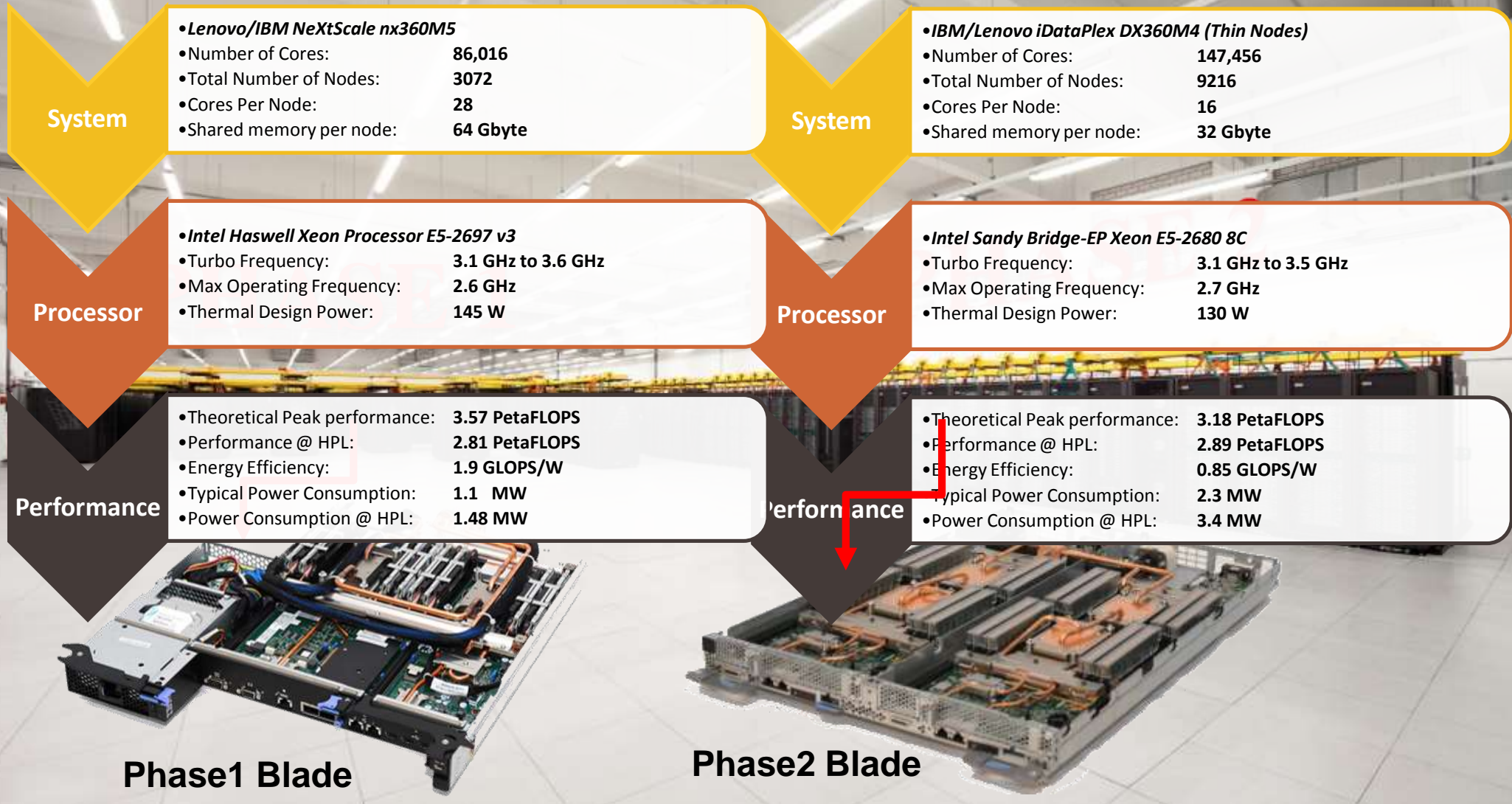
**HPC resources to scientist in Europe**

- European Tier 0 level of HPC
- PRACE Member
- ...





# SuperMUC – The First High Temperature Direct Liquid Cooled Petascale Supercomputer



# HPC: New Procurements

- SuperMUC-NG:
  - negotiations started in 2017, contract end 2017
  - Funding: project SiVeGCS
- Overview over current systems:

Architecture				Total Numbers		Max Job Limits				How to get access	
System Name	CPU	Cores per Node	RAM per Node [GB]	Nodes	Cores	Nodes	Cores	Wall Time	Max. aggreg. RAM	Queue	Login Node
SuperMUC Phase 1 Fat Nodes	Intel Xeon E7-4870 ("Westmere")	40	256	205	8200	52	2080	192h	13 TB	fat, fattest, fatter	wm.supermuc.lrz.de
SuperMUC Phase 1 Thin Nodes	Intel Xeon E5-2680 ("Sandy Bridge")	16	32	9216	147456	4096	65538	48h	131 TB	test, general, large	sb.supermuc.lrz.de
SuperMUC Phase 2 Haswell Nodes	Intel Xeon E5-2697 v3 ("Haswell")	28	64	3072	86016	512	14336	48h	33 TB	test, micro, general	hw.supermuc.lrz.de
SuperMUC Phase 2 Big Nodes	Intel Xeon E5-2697 v3 ("Haswell")	28	256	8	224	8	224	6h	2 TB	big	hw.supermuc.lrz.de
SuperMIC Many-Core Nodes	Intel Xeon E5-2650 v2 ("Ivy Bridge") + Intel Xeon Phi KNC	16	32	32	3840 (Phi)	16	3840	48h	512 GB	phi	sb.supermuc.lrz.de, supermic.smuc.lrz.de
SuperMUC Phase 1 Remote Visualization	Intel Xeon E5-2650 v2 ("Ivy Bridge") + NVidia GPU K20x	16	128	8	128 + GPU	1	16	48h	128 GB	rva	sb.supermuc.lrz.de, submit job
SuperMUC Phase 2 Remote Visualization	Intel Xeon E5-2697 v3 ("Haswell") + NVidia GPU K40	28	256	3	84 + GPU	1	28	48h	256 GB	vis	hw.supermuc.lrz.de, submit job

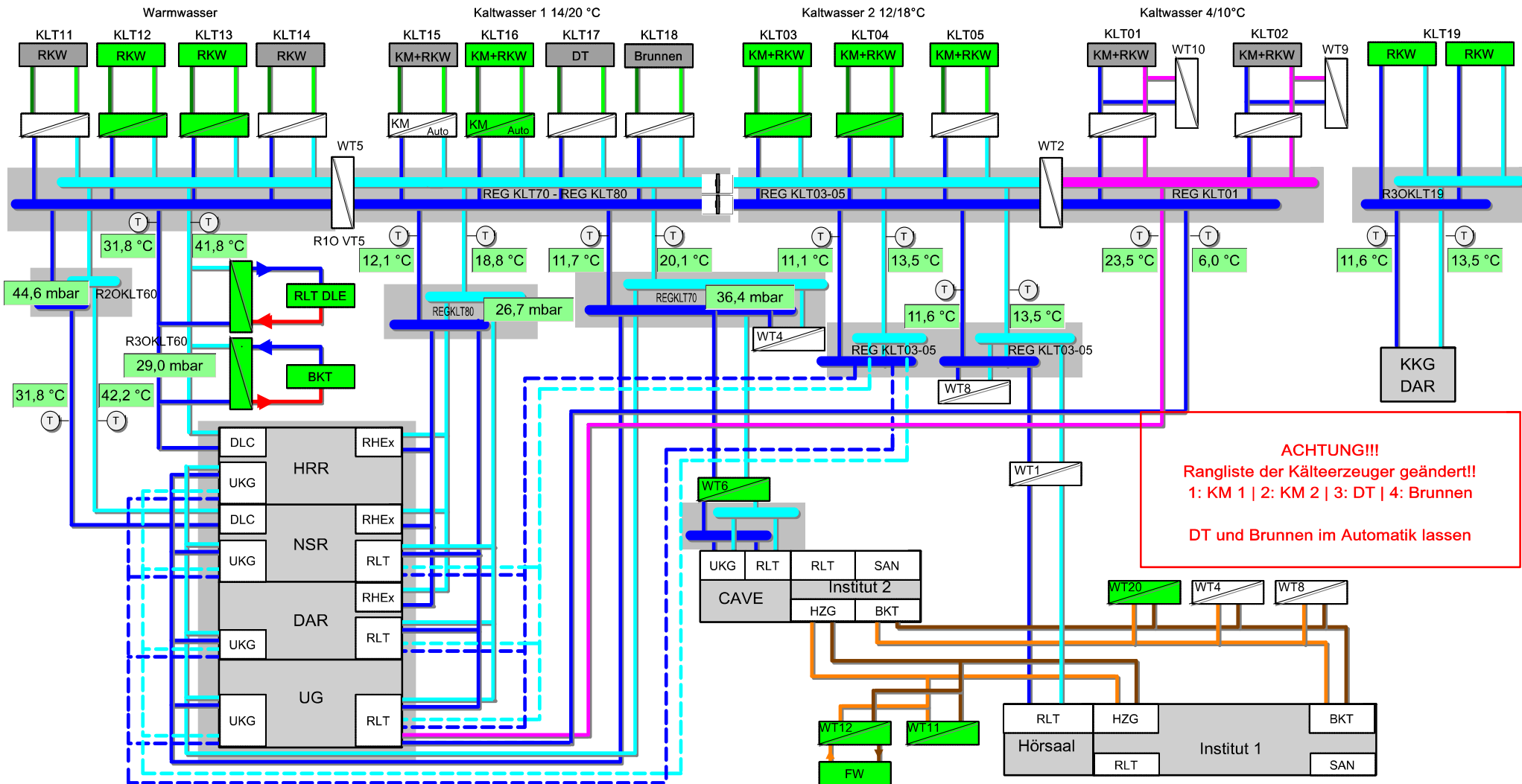


# Overview HPC Systems @LRZ (continued)

Architecture				Total Numbers		Max Job Limits				How to get access	
System Name	CPU	Cores per Node	RAM per Node [GB]	Nodes	Cores	Nodes	Cores	Wall Time	Max. aggreg. RAM	Queue	Login Node
Linux-Cluster CoolMUC2	Intel Xeon E5-2690 v3 ("Haswell")	28	64	384	10752	60	1680	48h	3.8 TB	mpp2	lxlogin5.lrz.de, lxlogin6.lrz.de
Linux-Cluster CoolMUC2	Intel Xeon E5-2690 v3 ("Haswell")	28	64	1	28	1	28	96h	64 GB	serial	lxlogin5.lrz.de, lxlogin6.lrz.de
Linux-Cluster Hugemem	Intel Xeon E5-2660 v2 ("Sandy Bridge")	20	240	11	220	1	20	168h	240 GB	hugemem	lxlogin1.lrz.de
Linux-Cluster Hugemem	Intel Xeon E5-2660 v2 ("Sandy Bridge")	20	480	1	20	1	20	168h	480 GB	hugemem	lxlogin1.lrz.de
Linux-Cluster Teramem	Intel Xeon E7-8890 v4	96	6144	1	96	1	96	48h	6.1 TB	inter	any cluster login node
Linux Cluster Many Core	Intel Xeon Phi (Knights Landing)	64	96	1	64	1	64	24h	RAM:96GB +HBM:32GB		contact servicedesk
Machine Learning System	Nvidia Pascal P100	8 GPU	128	1	n.a.	1	n.a.	12h	128GB GPU 512GB CPU		contact servicedesk
LRZ Compute Cloud	Intel Xeon E5540 X5650 E5-2660v2	1-20	1-240	95	852		64		720	N.A.	<a href="http://www.cloud.mwn.de">www.cloud.mwn.de</a> Self-Service VMs with custom operating system
LRZ Virtual Machines	Intel Xeon E5-2660 v2 ("Sandy Bridge")	1-8	1-32	90	1800					Managed Hosting	<a href="http://www.lrz.de/services/serverbetrieb/">http://www.lrz.de/services/serverbetrieb/</a>

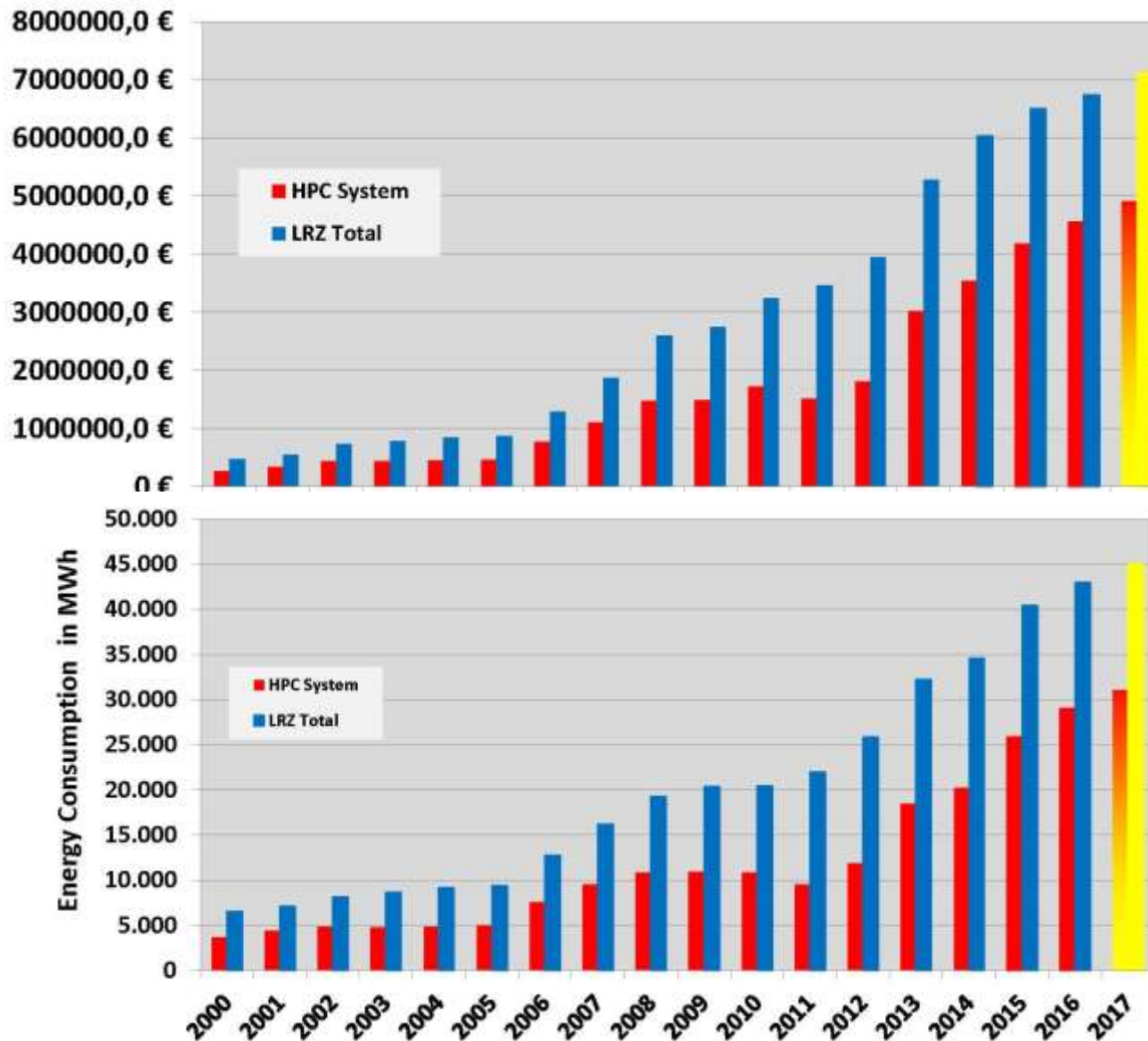


# Schematic overview of LRZ's cooling infrastructure





# Costs @LRZ ...

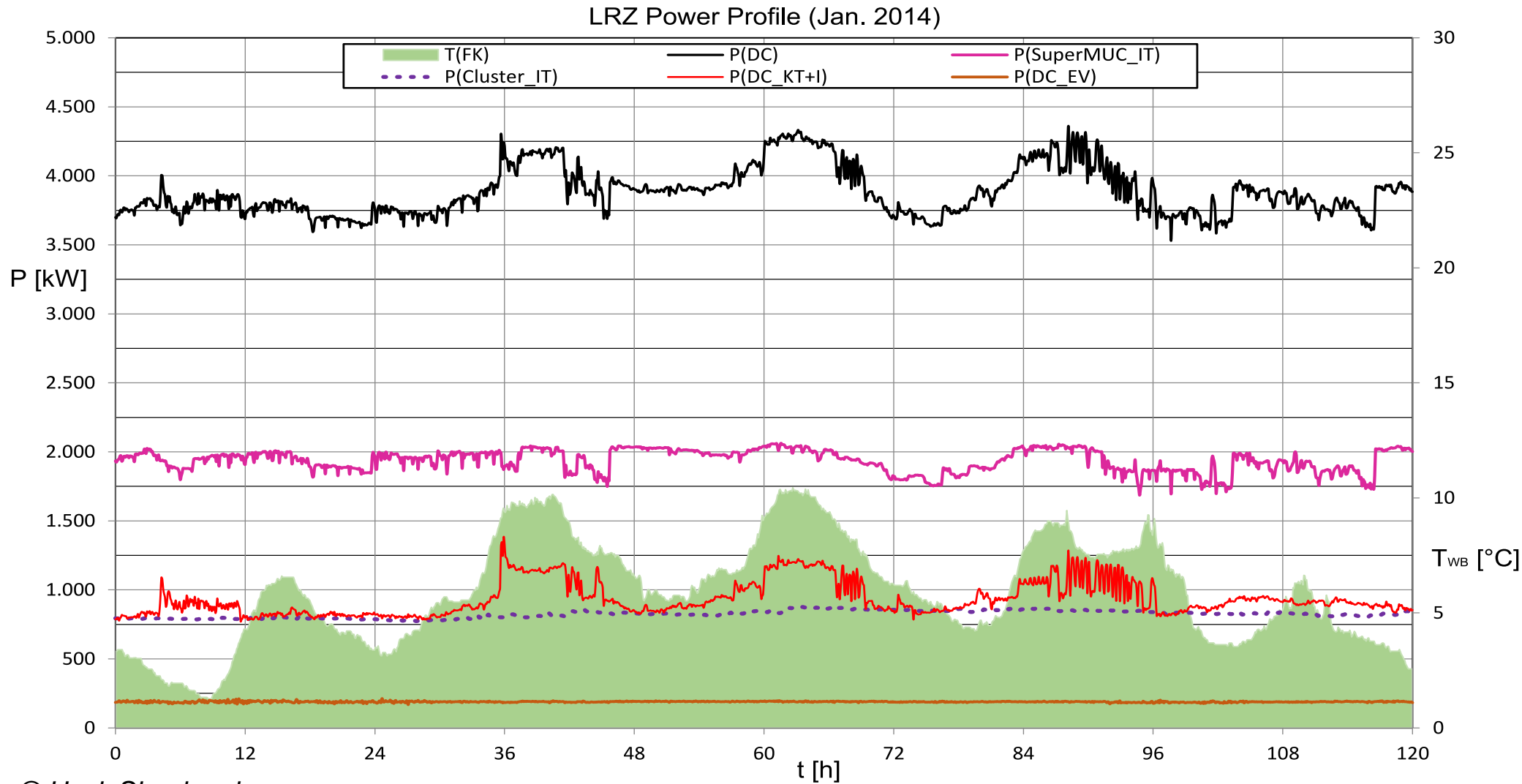


1kWh (2000)  $\approx$  0.07 €  
1kWh (2016)  $\approx$  0.161 €

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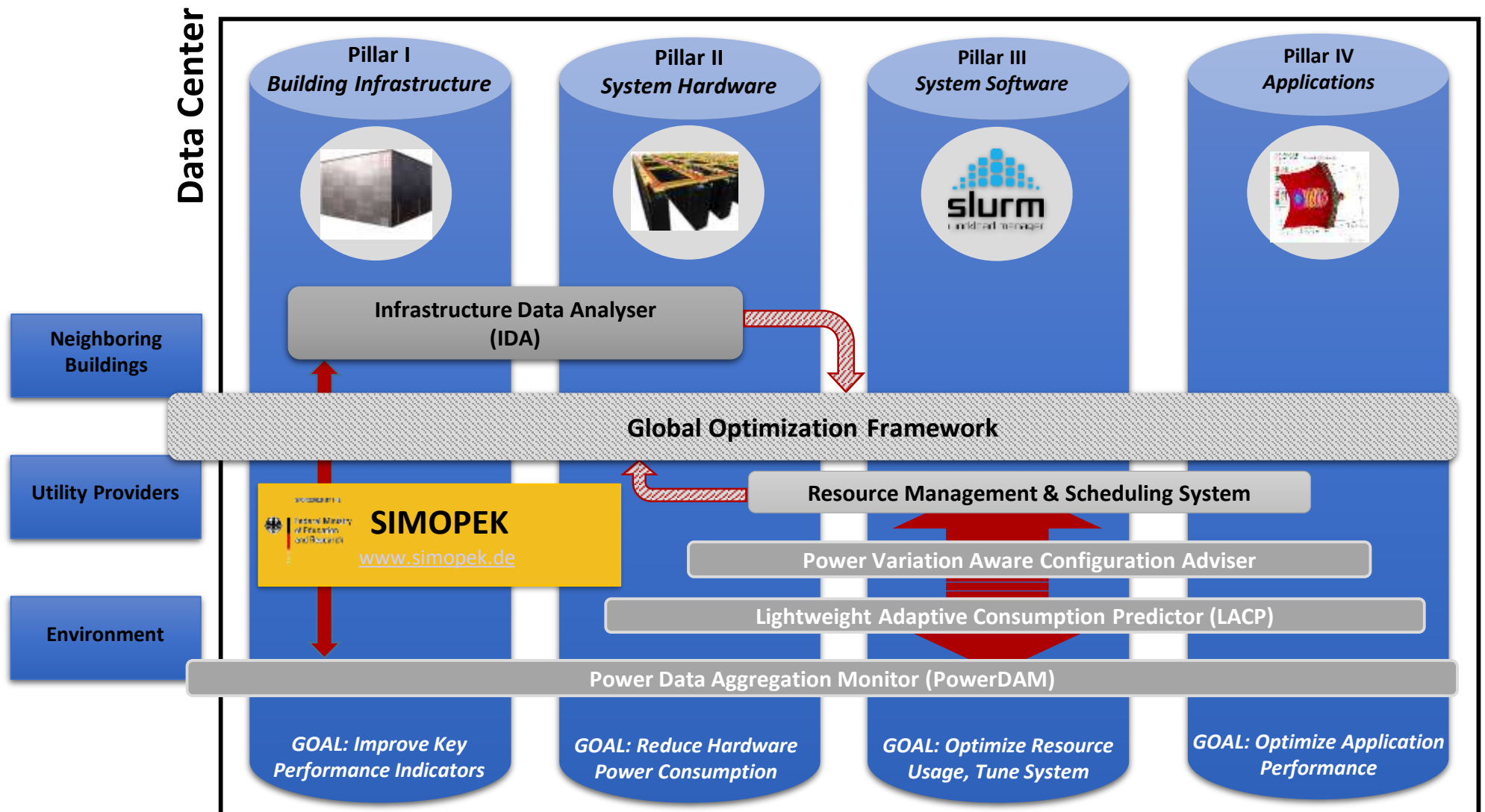


# Energy-Efficiency Challenges

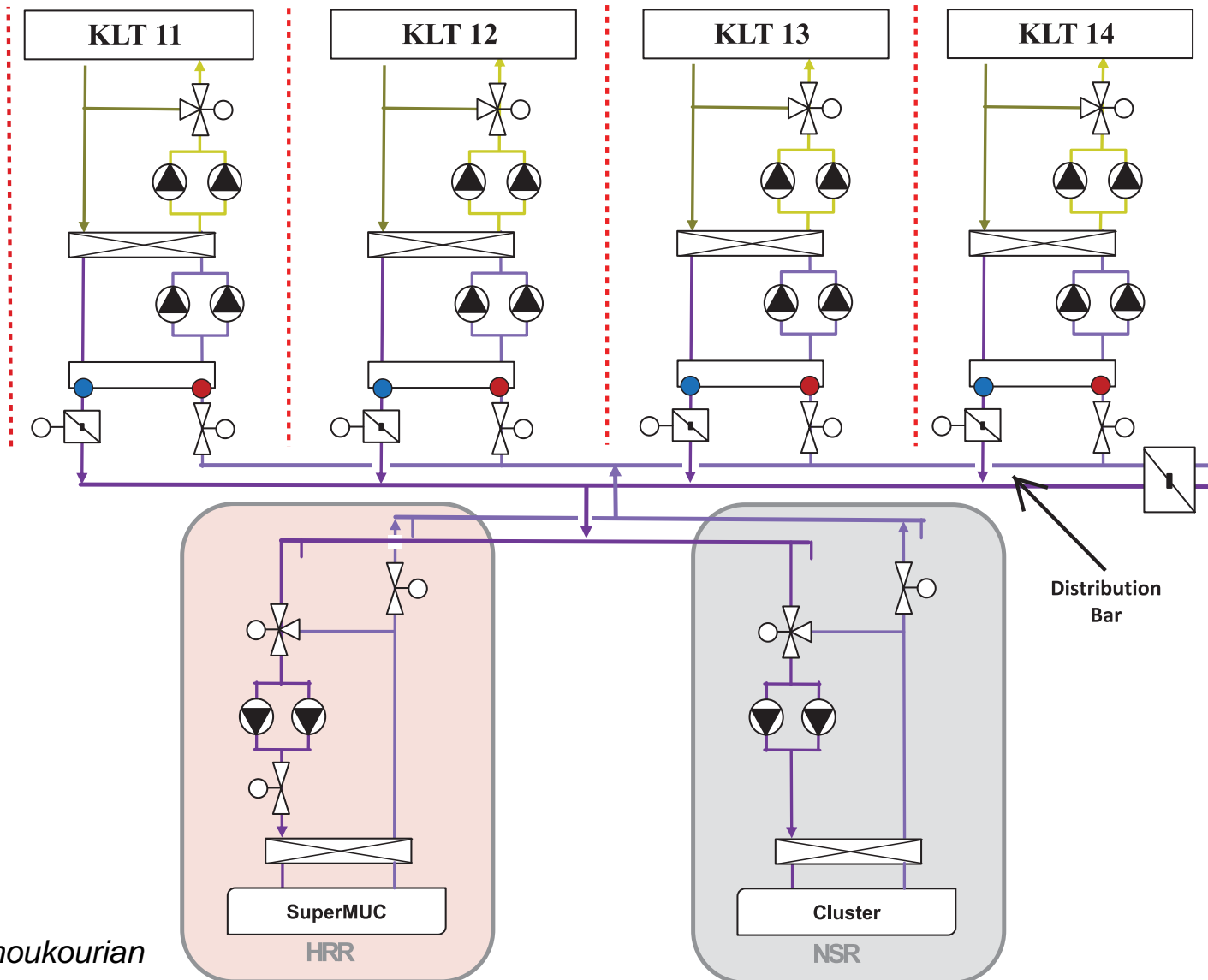


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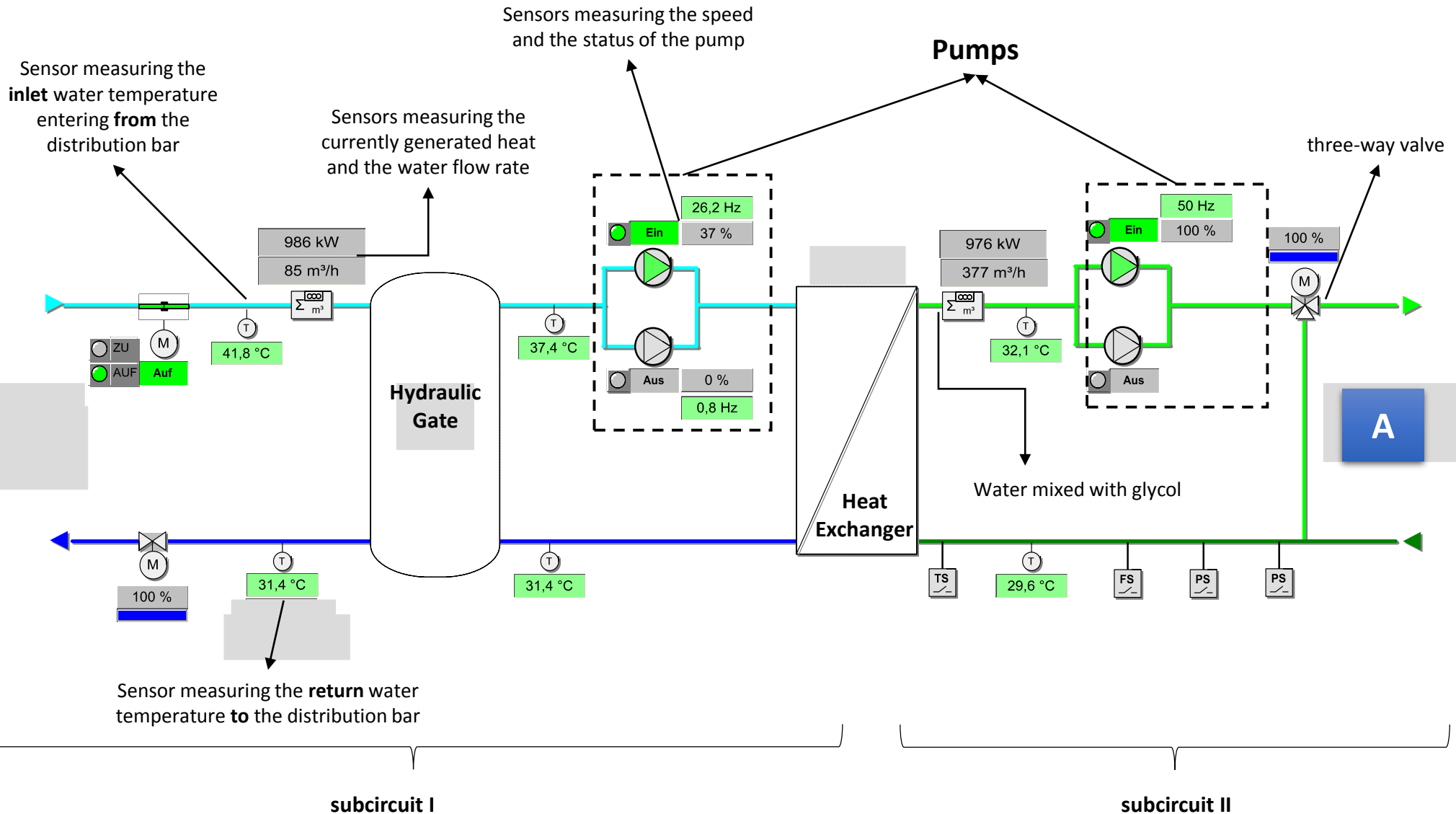
# Overview of Some EE R&D Activities @LRZ



# Schematic overview of LRZ's chiller-less cooling infrastructure



# Schematic overview of the hydraulic connection to the KLT14 cooling tower







# The Efficiency of Cooling Infrastructure

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$$COP = \frac{Q_{CoolingCircuits}}{P_{CoolingCircuits}}$$

$Q_{CoolingCircuits}$  - aggregated amount of cold generated by the four cooling circuits

$P_{CoolingCircuits}$  - aggregated amount of power consumed by the four cooling circuits

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# Predicting the Efficiency of Cooling Infrastructure Using Recurrent Neural Networks

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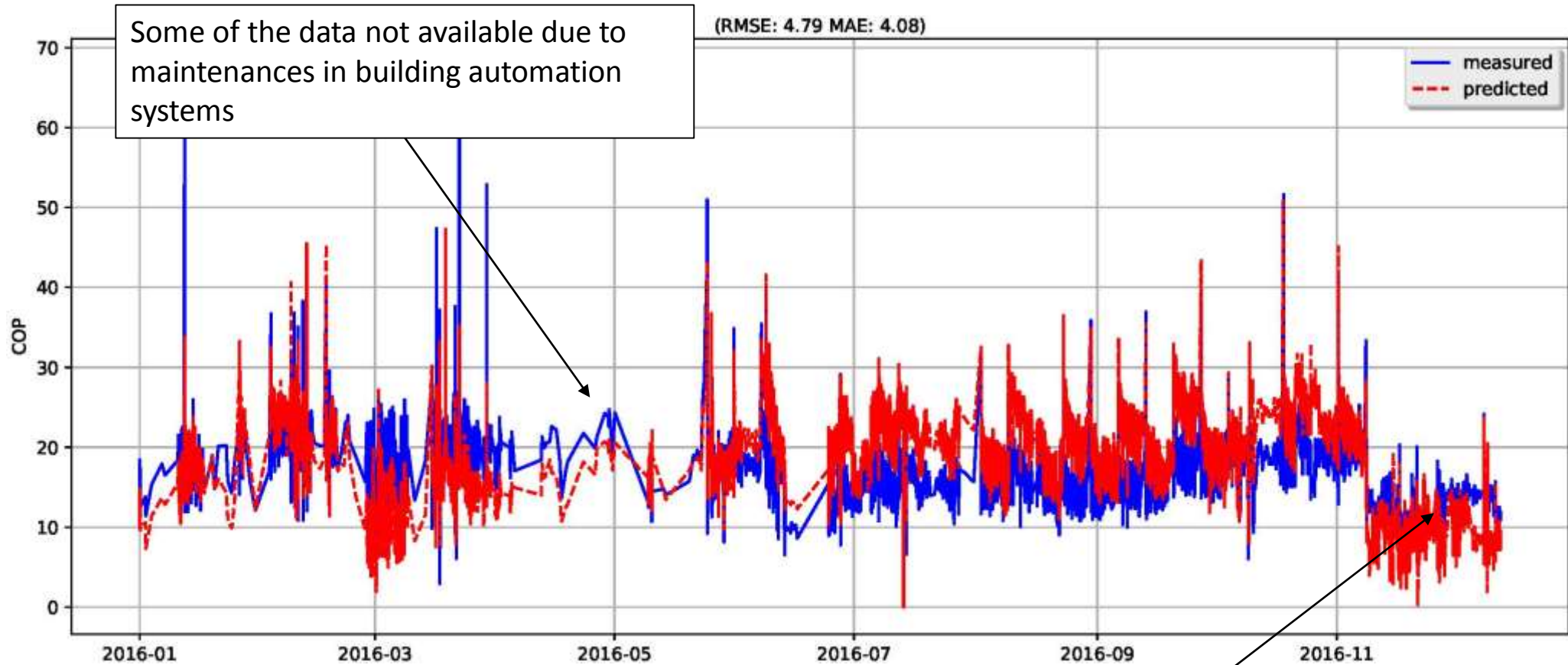
**Network Type:** LSTM (Long Short-Term Memory)  
**Software Package:** Keras | TensorFlow

- 12 Inputs:
  - aggregated amount of cold generated by each cooling circuit
  - aggregated amount of power consumed by the fans of each cooling circuit
  - number of active cooling towers
  - wet bulb temperature
  - **inlet** water temperature (to the distribution bar) **from** each cooling circuit (x 4)
  - **return** water temperature (to the distribution bar) **to** each cooling circuit (x 4)
- Output:
  - COP of warm water cooling infrastructure



# COP Prediction Results

(learned 2015 operational data – predicted for 2016)



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## GCS@LRZ summary

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- New procurement(s) for HPC in the context of GCS
- General purpose system, embedded into general IT infrastructure
  - visualization
  - „big data“
  - networking
- Research and Development in Energy Efficiency