HPC.NRW

HPC.NRW in a Nutshell: HPC-Resources in NRW

A brief overview of what is available and who can use it

Martin Urban

GREAT COMPUTING COMES WITH GREAT SUPPORT.

Agenda

Key question: What is available?

AND

Who can use it?

HPC tier levels

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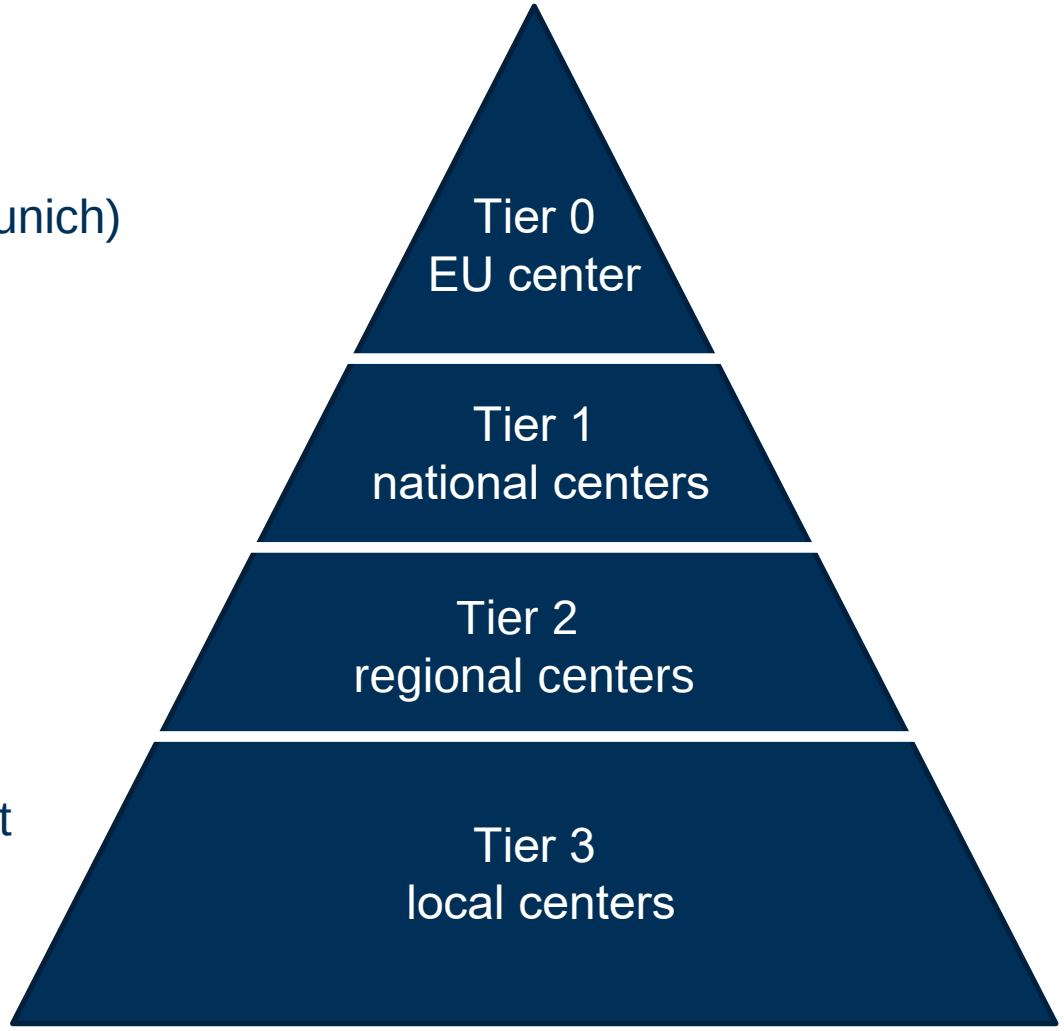
- Quick definition of different HPC tier levels
  - Tier 0-1
    - National supercomputer centers (e.g. Jülich, Stuttgart, Munich)
  - Tier 2
    - Regional computing centers
    - Federal user base
  - Tier 3
    - Local computing centers
    - Provides basic computing resources and for development



What is available

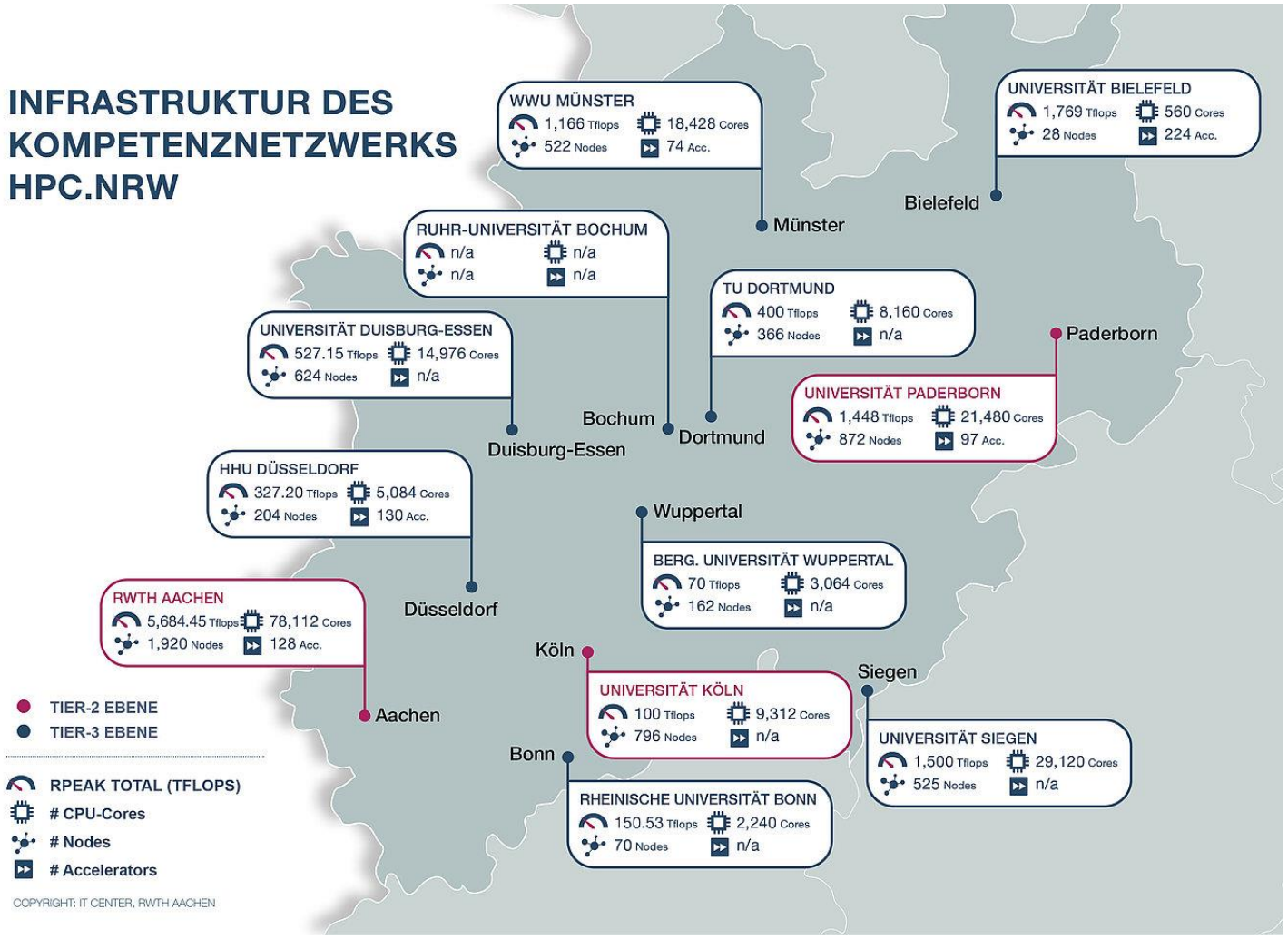
- 12 Partners in HPC.NRW
  - 3 x Tier 2
    - Aachen
    - Paderborn
    - Köln
  - 9 x Tier 3
    - Bielefeld
    - Bochum (currently no operational cluster)
    - Bonn
    - Duisburg-Essen
    - Düssledorf
    - Dortmund
    - Münster
    - Siegen
    - Wuppertal

What is available

- 12 partners in HPC.NRW
- Total numbers
  - 6089 Nodes
  - 190,536 CPU cores
  - Over 653 Accelerators
  - 13 142 Tflops

- Multiple new clusters are in planning and procurement

- Jülich center for supercomputing is part of NRW, but not HPC.NRW



How to choose?

Which cluster can I use?

And

Which cluster is the correct one for my needs?

Which cluster can I use to start with hpc?

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- I have an university with a hpc center at my location
  - Please contact your local universitary computing center
- I don‘t have an university with a hpc center at my location
  - Tier 2 centers offers a tier 3 substitute supply for universities of applied science
  - But: Which Tier 2 center is the best for my needs?

Which tier 2 is the best for my needs?

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- Aachen CLAIX
  - 1307 compute nodes
  - 62736 cores
  - 251 TB total main memory
  - 48 + 6 MPI-GPU nodes w/ 2 NVIDIA V100 GPUs
- Köln CHEOPS
  - 796 compute nodes
  - 9312 cores
  - 36 TB total main memory
  - 12 NVIDIA V100 GPUs
- Paderborn Noctua1
  - 270 compute nodes
  - 10880 cores
  - 52 TB total main memory
  - 32 Intel Straix-10 FPGAs
- Noctua2 (Q4 2021)
  - >1400 compute nodes
  - > 100 000 cores
  - 256 GB per node
  - >100 NVIDIA A100 GPUs
  - >60 FPGAs

Which Tier 2 is the best for my needs?

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Engineering	Life Science	Atomistic Simulations Optoelectronic and quantum photonics Machine learning for science and intelligent systems Accelerators for HPC

- GPUs
- >60 FPGAs

Which tier 2 is the best for my needs?

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- And software?

Which tier 2 is the best for my needs?

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- And software?

  A lot!

Software: Aachen

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no star - everyone can use this software.

★ software is restricted to members the RWTH University, external users - like members of the FH Aachen, the Research Center Jülich, etc. are NOT allowed to use this software.

★ software is restricted to employees and / or institutes, which means students are NOT allowed to use this software.

★ this software needs an additional user registration or a special license.

TECHNICS

- ★ abaqus
- ★ adams
- ★ ansys
- ★ cfx
- ★ comsol
- ★ dymola
- ★ dytran
- fds
- ★ fluent
- ★ hyperworks
- ★ icem
- ★ lsdyna
- ★ lsopt
- lsprepost
- ★ marc
- ★ nastran (MSC)
- openfoam
- ★ petromod
- ★ starcd
- ★ starccm
- superforge

CHEMISTRY

- abinit
- cp2k
- ★ cpmd
- dalton
- ★ gamess
- ★★ gaussian
- ★ gaussview
- gromacs, VMD
- lammps, liggghts
- meep
- ★ molcas
- openbabel
- openmx
- qe
- siesta
- ★ turbomole[-mpi|-smp]
- ★ vasp

MISC

- freerdp
- gnuplot
- ★ matlab
- opnet
- revolve
- tensorflow

GRAPHICS

- ★ ensight
- paraview
- ★ tecplot
- tecplotchorus
- visit
- wave

MATH

- gurobi
- ★ maple
- ★ mathematica

Check for updates !

https://doc.itc.rwth-aachen.de/display/CC/Installed+software

– Software: Köln

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abyss	diamond	mafft	openbabel	salmon
alps	eman	maple	opencv	sambamba
amber	examl	matlab	openfoam	samtools
ant	falcon	maxquant	orca	scilab
awscli	ffmpeg	mcl	orthofinder	smrttools
blast+	flye	meraculous-2d	partitionfinder	soapdenovo
bowtie	gaussian	mercurial	pasha	soapdenovo2
bowtie2	gaussian09	mira	phylobayes	sphire
bwamem2	gaussian16	molden	python	star
canu	gdal	mothur	pytorch	stata
cdo	grads	mpiblast	qe	tensorflow
cellprofiler	gromacs	mrbayes	R	trinity
cfour	hipmer	nbo6	raxml	turbomole
clustalo	hmmer	nco	ray	vmd
clustalw	iqtree	ncview	relion	xtb
comsol	jupyter	nonmem	rsem	
cp2k	keras	nwchem	rstudio	
cplex	khmer		ruby	
cryolo				

– Software: Paderborn

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- **Software Availability:**
  - Too much to be listed here
  - See https://wikis.uni-paderborn.de/pc2doc
  - Examples:

- Scientific and Technical Applications
  - ABAQUS - software suite for finite element analysis and computer-aided er
  - CAFFE - Deep Learning Framework
  - FEniCS Project - Automated Solution of Differential Equations by Finite Ele
  - Gurobi Solver for linear programming
  - LS-DYNA - A Strongly Coupled Multi-Physics Solver
  - MATLAB - Technical Computing
  - OpenFoam - Finite element Analysis
  - R-Project - Free software environment for statistical computing and graphic
  - Scilab - Open source software for numerical computation
  - SCIP - Solving Constraint Integer Programs
  - SIMULIA Abaqus - Unified Finite Element Analysis

- Chemical and Physical Applications
  - ABINIT - find total energy, charge density and electronic structure of systems made of electrons and nuclei within Density Functional Theory (DFT), using pseudop
  - BigDFT - Ab initio code based on Daubechies wavelet
  - CP2K - Open Source Molecular Dynamics
  - Dalton Suite - Dalton code, a powerful tool for a wide range of molecular properties at different levels of theory and LSDALTON, a linear-scaling HF and DFT code
  - ESPRESSO - Suite of Open-Source computer codes for electronic-structure calculations and materials modeling at nanoscale
  - GAMESS - General Atomic and Molecular Electronic Structure System. Ab initio quantum chemistry calculations.
  - Gaussian - Electronic Structure
  - Gromacs - Molecular Dynamics
  - HOOMD - General-purpose Particle Simulation Toolkit
  - LAMMPS - Open Source Molecular Dynamics Code, an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator.
  - MEEP - Finite-Difference Time-Domain (FDTD) Simulation
  - MPB - Electromagnetic Eigenmode Solver
  - NAMD - Scalable Molecular Dynamics
  - NWChem - Ab-initio and Semiempirical Computational Chemistry Package
  - ORCA - Electronic Structure Program Package
  - Turbomole - Ab-initio Electronic Structure Calculations
  - VASP - Ab-initio quantum-mechanical molecular dynamics
  - xTB - Semiempirical Extended Tight-Binding Program Package

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– Software: Paderborn

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But most important:
If you need a special software, you can ask us!

Paderborn Center for Parallel Computing

Contact informations

RWTH Aachen University	servicedesk@itc.rwth-aachen.de	https://www.itc.rwth-aachen.de/hpc-projects
Universität Bielefeld	gpucluster@physik.uni-bielefeld.de	https://www2.physik.uni-bielefeld.de/gpu-cluster.html
Ruhr-Universität Bochum	hpc@ruhr-uni-bochum.de	https://www.it-services.ruhr-uni-bochum.de/services/fowi/highperformancecomputing.html.de
Rheinische Friedrich-Wilhelms-Universität Bonn	hpca@uni-bonn.de (allgemeine HPC-Fragen) / bonna-support@hpc.uni-bonn.de (Fragen zum Rechner)	https://www.dice.uni-bonn.de/de/hpc (allgemein) / https://bonna.hpc.uni-bonn.de/ (zum Rechner, nur aus dem Uni-Netz)
Technische Universität Dortmund	service.itmc@tu-dortmund.de	https://www.lido.tu-dortmund.de/cms/de/home/Kontakt/index.html
Heinrich-Heine Universität Düsseldorf	hpc-support@hhu.de	https://www.zim.hhu.de/hpc
Universität Duisburg-Essen	hpc-support@uni-due.de	https://www.uni-due.de/css/sc_support.php
Universität zu Köln	hpc-mgr@uni-koeln.de (Cluster Support), rrzk-helpdesk@uni-koeln.de (Allgemeiner RRZK Helpdesk)	https://rrzk.uni-koeln.de/hpc-projekte/hpc
Westfälische Wilhelms-Universität Münster	hpc@uni-muenster.de	https://confluence.uni-muenster.de/display/HPC
Paderborn Center for Parallel Computing (PC^2), Universität Paderborn	pc2-support@uni-paderborn.de	https://pc2.uni-paderborn.de/go/access, https://wikis.uni-paderborn.de/pc2doc
Universität Siegen	hpc-support@uni-siegen.de	https://cluster.uni-siegen.de
Bergische Universität Wuppertal	lcg-admin@physik.uni-wuppertal.de	http://www.pleiades.uni-wuppertal.de/

And if I need more compute power?

Then please listen to the following talk!