Quick Reference Card for
HPC.NRW (general information)

Guidelines for the Application, Approval and Allocation
of HPC-Resources at HPC.NRW (general information)
`https://hpc.dh.nrw`
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HPC.NRW

Project Preparation

1. Note that the concrete compute time application guidelines differ in detail for each site. Use the flow graph on the next page to figure out which HPC center fits best to your requirements.

2. Estimate the needed resources, if required (not always the case especially for Tier-3 centers). Most HPC centers (e.g, Tier-2, Tier-1) allocate resources in Mio-Core-h. However, effective computing power per Core-h differs between different systems. Thus, you might be requested to convert this to the amount of floating point operations (EFLOP) during the application process. Furthermore, the required amount of main memory and disk storage might be requested.

   Example Core-h: Using one compute node with 48 cores for one year (24/7):
   $$48 \text{ cores} * 24 \text{ h} * 365 \text{ days} = 0.42 \text{ Mio Core-h}$$
   Example Memory: Many HPC systems are equipped with 2-4 GB per core.

   If you are unsure, trial accounts might be requested first. In case of any questions, do not hesitate to contact your local support or helpdesk@hpc.nrw.

3. Refer to the guidelines of the selected HPC center. For many sites in NRW quick reference cards like this are available.

4. Identify a fitting project category in the selected HPC center.

5. Prepare a project description for your project category, if required. Templates can typically be found on the local website.

Proposal Submission

1. Use the local submission system (mostly online).

2. Typically at least the PI has to sign the application.

3. Send signed and scanned proposal to the specified contact of the selected center.

Formal Evaluation

In the formal evaluation the access criteria and formal aspects of a project are verified by members of the selected HPC center. At least the PI will be contacted if questions or problems show up. This process usually takes up 1-2 day.

Technical Review

HPC experts at the selected center will check your proposal for technical feasibility (e.g., availability of requested resources, software, etc.) and contact you in case of any problems. This process typically takes up to one week.

Scientific Review

The scientific evaluation is not required for most smaller compute centers at Tier-3 level or for small projects on Tier-2 systems. If required, typically one to three independent domain scientists from German universities or research facilities will review your project application (e.g., single-blind review). This process usually takes 4-6 weeks for the rolling calls and up to 10 weeks for calls with fixed deadlines (depending on the deadlines).

Resource Allocation and Monitoring

1. The RAB decides about the resources for the project and informs at least the PI.

2. Refer to the selected HPC center documentation to

   - generate an account (if not done already).
   - add members to the approved compute project.
   - prepare and submit job scripts for the project.
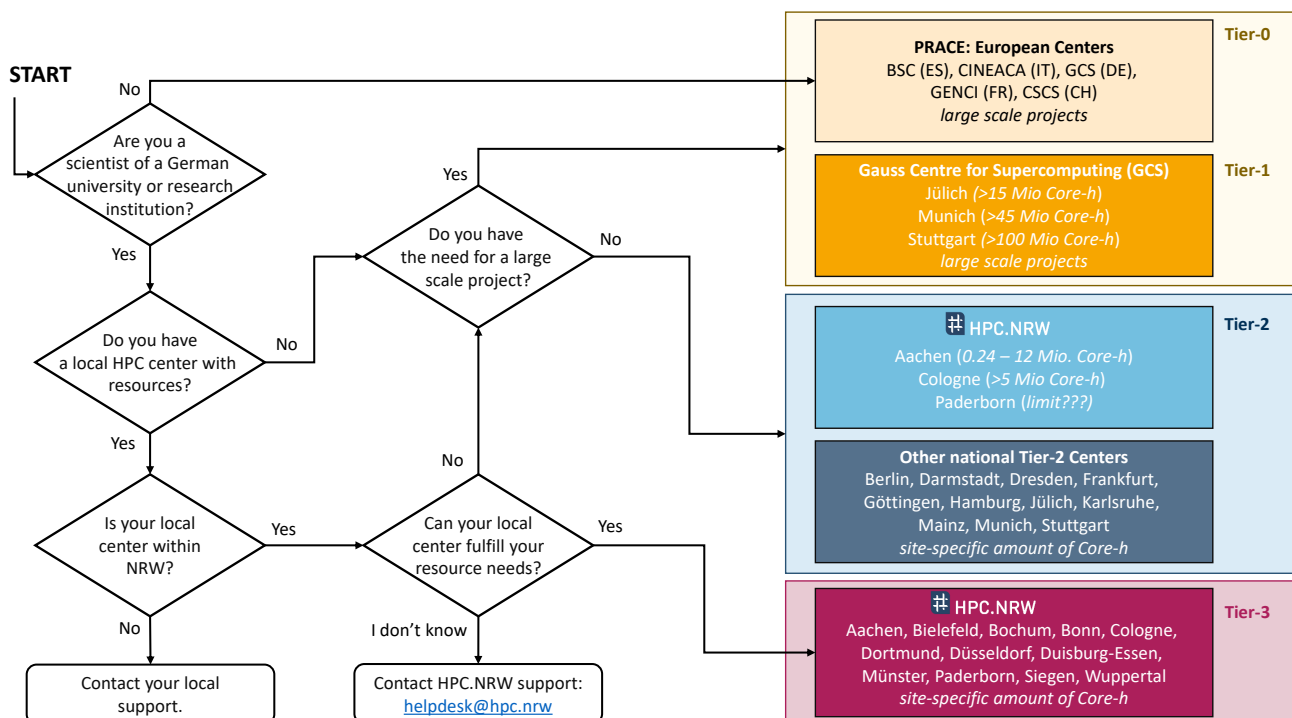   - obtain the project account information (quota, usage, etc.)

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Scientists from outside Germany need to apply for compute time via PRACE, a partnership that provides access to pan-European world-class HPC systems. German scientists should use their local resources if available and suitable. If you need less than a certain amount of resources per year, in most HPC centers there is no need to write a full compute time application, because you can use your personal default quota (e.g., fair-share). If you require more resources than your center can provide, you don't have a local HPC center or you identify special needs (e.g. larger memory, more Cores/CPU, GPUs), you may contact an other HPC center or apply for compute time at a higher level (e.g., Tier-2/Tier-1). Only very experienced users with well-scaling codes and high demands on compute time should apply for large scale projects on Tier-1/Tier-0 level. Please ensure to spend the granted compute time within the project period, preferably evenly distributed. Please refer to the documentation and quick reference card of the individual HPC centers for details on their configuration and application process.

PRACE: European Centers — Tier-0
BSC (ES), CINEACA (IT), GCS (DE),
GENCI (FR), CSCS (CH)
large scale projects

Gauss Centre for Supercomputing (GCS) — Tier-1
Jülich (*>15 Mio Core-h*)
Munich (*>45 Mio Core-h*)
Stuttgart (*>100 Mio Core-h*)
large scale projects

⊞ HPC.NRW — Tier-2
Aachen (*0.24 – 12 Mio. Core-h*)
Cologne (*>5 Mio Core-h*)
Paderborn (*limit???*)

Other national Tier-2 Centers
Berlin, Darmstadt, Dresden, Frankfurt,
Göttingen, Hamburg, Jülich, Karlsruhe,
Mainz, Munich, Stuttgart
site-specific amount of Core-h

⊞ HPC.NRW — Tier-3
Aachen, Bielefeld, Bochum, Bonn, Cologne,
Dortmund, Düsseldorf, Duisburg-Essen,
Münster, Paderborn, Siegen, Wuppertal
site-specific amount of Core-h

Flowchart:
START → Are you a scientist of a German university or research institution? (No → PRACE: European Centers; Yes →) Do you have a local HPC center with resources? (No → Do you have the need for a large scale project?; Yes →) Is your local center within NRW? (No → Contact your local support.; Yes →) Can your local center fulfill your resource needs? (I don't know → Contact HPC.NRW support: helpdesk@hpc.nrw; Yes → Tier-3). Do you have the need for a large scale project? (Yes → Gauss Centre for Supercomputing; No → HPC.NRW Tier-2).

Contact your local support.

Contact HPC.NRW support:
helpdesk@hpc.nrw

Glossary of Terms and Definitions

Core-h A Core-Hour (Core-h) is a unit used for the accounting of compute cluster resources. One core-hour equals one CPU core being used for the duration of one hour of execution time. The latter is always measured as the elapsed wall clock time from the job start to the job finish and not as the actual CPU time. For exclusively scheduled jobs (i.e., jobs using the complete node), the used core-hours usage are always equal to the total number of CPU cores on the allocated nodes times the execution time, regardless of the actual number of node slots allocated to the job.

EFLOP A exaFLOP (EFLOP) is a unit used for the accounting of compute cluster resources. This unit is based on theoretical peak performance of a core, which enables a better comparability between different HPC systems. Usually it is proportional to Core-h for a given machine type.

PI The Principal Investigator (PI) has to take responsibility for the project application and the project execution. He/She has to be a senior researcher (a leading scientist with a Dr./PhD degree or a permanent position) or (junior) professor at a university (depends on local rules). Often he agrees to also act as a reviewer for other submissions of computing project applications or otherwise to nominate and supervise a delegate who is able to thoroughly take part in the reviewing process. He/She has to sign the paper version of the application and he/she is also responsible for any due status or final reports. Furthermore, the PI is responsible for granting access to further project members. He has to make sure that citizens of countries that are subject to the export control policy of the German Federal Government have an additional authorization from the German Federal Office for Economic Affairs and Export Control (BAFA) before they are allowed to use the HPC system.

RAB The Resource Allocation Board (RAB) is a committee that decides on the acceptance/refusal of project proposals and allocation of compute resources based on the rating of the scientific reviewers. The review process typically follows the recommendations of the Gauss-Alliance for High-Performance-Computing in Germany.

single-blind review A review process in which the reviewers know the identity of the authors of the proposal, but the author does not know the identities of the reviewers.