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# Detailed Description for Extensions of NHR Projects

[Project title here]

[PI/PC of the proposal here]

Version 9. October 2025

*Please note the following and remove this page in final version by removing the option **showhints** from the documentclass.*

***The length of the project description should not exceed 14 pages (font 11 pt, not including the references)!***

*Note: Fill-out hints are given in italic.* ***Please remove them in the final version by removing the option showhints from the documentclass.***

*Before using this template, please check at* `https://go-nhr.de/computing-time` *if a new version is available (this is version 9. October 2025).*

*When to use this template:*

- *for* ***extensions*** ***of NHR normal and NHR large projects***

*When* ***not*** *to use this template:*

- *Don't use this template for* ***short-term*** *extensions (up to three months). Contact your NHR center instead.*
- *Don't use this template for* ***new*** *NHR normal and NHR large projects. For new projects, please use the template available at* `https://go-nhr.de/computing-time`*.*
- ***Already reviewed research projects:*** *If you are applying for an NHR normal project and if your scientific project has already been successfully reviewed and approved by one of the accepted institutions (DFG, European Union, German Federal Ministries BM* (e.g. BMFTR; BMWK), Volkswagen Stiftung, another NHR or GCS center) depending on the NHR center you can use a simplified template available at* `https://go-nhr.de/computing-time`*.*

*In case of questions: If you are unsure or have questions please contact the center. The contacts can be found at* `https://www.nhr-verein.de/unsere-mitglieder`*.*
*The information provided here will be kept private. It will only be accessible to staff of the center you apply for, the resource allocation board of the center, the external scientific reviewers, the joint NHR resource allocation board (Nutzungsausschuss) which is a central NHR board that approves NHR large projects as well as the central NHR office (NHR Geschäftsstelle, for reporting purposes). The guidelines for confidentiality and neutrality of review processes apply.*

# 1 Progress Report

## 1.1 Short Summary (about 0.5 page)

*Shortly summarize the progress of the project in relation to the previous project proposal.*
*Please list here explicitly your publications that were using the HPC resources in the previous project period.*

## 1.2 Sub-project 2: [Sub-project title] (max. 1 page text per sub-project)

### 1.2.1 Project Progress

*Shortly describe the progress and accomplishments in the sub-project here including references to your publications.*

### 1.2.2 Project Challenges

*Please describe how the scientific challenges of the sub-project were tackled and solved here.*

### 1.2.3 Problems Encountered (optional)

*Please describe the technical, scientific or organizational problems encountered during the sub-project duration here. How did they influence the usage of your granted resource contingent?*

## 1.3 Sub-project 3: [Sub-project title] (max. 1 page text per sub-project)

# 2 Suggestions for Improvements of Services (optional)

*Please let us know here which hardware, software or services would have been helpful for your project or how else we could improve for you as a researcher.*

# 3 Description of the Project Extension

*Important: Please describe here all sub projects for which you want to request compute time in the extension. Descriptions of sub projects that are identical to the previous project phase can be copied.*

## 3.1 Sub-project 1: [Sub-project title] (1 page text max. per sub-project, 0.5 recommended)

*Please discuss relevant aspects of the project. The following points serve as a guideline, but in cases where they do not apply to your project, they can be omitted as you see fit.*

- *Scientific objectives*
- *Scientific and technical innovation potential and relevance*
- *Approach*
- *Computational objectives, types of calculations*
- *Which "types of runs" (see Chapter 4.3 Justification of Resources Requested) have you planned?*
- *Numerical methods and algorithms you want to use, improve, or design*
- *Progress beyond the state-of-the-art in terms of methods and calculations*
- *Expected outcome*

### 3.2 Sub-project 2: [Sub-project title] (1 page text max. per sub-project, 0.5 recommended)

...

## 4 Compute Resources

**Important note for applicants and reviewers: This section is only required in case there are relevant changes in the programs to be used or the properties of calculations compared to the previous proposal (e.g. relevant changes in system sizes that influences the scaling behavior). Otherwise remove sections 4.1 and 4.2.**

### 4.1 Code Overview

*Please use the following table to provide information on up to **three** software packages you plan to use in the project that will consume a relevant portion (each >=10%) of the requested compute time.*

| | Program A |
|---|---|
| Name | |
| Version number | |
| Web page | ... |
| Citation or reference | |
| Are you a developer, collaborator or end user of the program? | |
| Is the source code available? (publicly, upon request, no) | |
| Is it a commercially licensed software? If yes, do you already have a license that is useable at the requested NHR center? | |
| Are there usage limitation for this software like the maximal number of simultaneous runs, license server,...? | |
| How is the code parallelized (pure MPI, hybrid MPI/OpenMP, CUDA,...)? | |
| Which programming languages are used? (optional) | |
| Are there other further requirements (e.g. special libraries) for the program? (optional) | |

### 4.2 Code Benchmarks

*The purpose of benchmarks in the project proposal is to demonstrate an efficient use of parallel resources and to estimate the resources needed. The benchmark case(s) should be representative for your workload(s).*

*Even workloads with unfavorable parallel scaling can be granted computation time if the HPC systems offered by NHR are required to achieve progress for the given scientific problem that would not be possible with other HPC systems. The same holds for embarrassingly parallel workloads (high-throughput computing, e.g., parameter studies ) where the total computational need requires a large HPC system offered by NHR. In these cases, no scalability benchmarks are needed.*

*Fill out the benchmark section for each program listed section 4.1. Please refer to example evaluations on our website `https://go-nhr.de/computing-time`. The NHR centers offer NHR-test/NHR-preparation and NHR-starter projects that you can use to benchmark/test your programs on the desired NHR-center.*

*Some NHR centers offer a program-whitelisting procedure, meaning that no benchmarks/scaling tests are required for those codes and the following sections can be skipped. The lists can be found at* `https://go-nhr.de/computing-time`.
*If you want to provide an alternative demonstration (e.g. performance model) of parallel performance, please contact the respective center beforehand.*

#### 4.2.1 Program A: Program A Name (1 page text max. per relevant code, 0.5 recommended)

1. Benchmark Description

*Please provide a brief description of the calculations performed. If program A is used for a wide range of problem sizes (e.g., a factor of 10 or greater between problem sizes), then the benchmarks should cover the full range of problem sizes (PS1, ...).*

- *How does the benchmark problem size relate to the problem size in the respective subprojects?*
- *List the relevant execution parameters of the benchmark jobs (e.g., MPI ranks per node, OpenMP threads per MPI rank, ...)*
- *How is the code performance calculated? (runtime, TFLOPS,...)*

2. Benchmark System

*Please describe the computing systems used for the benchmarks. Typically, only benchmarks on one computing system are needed for the planned calculation. This compute system should be sufficiently similar to the resources/computing system requested in this proposal. Describe them all, if different systems are compared (e.g., to justify specific hardware requests like GPU hours instead of CPU hours).*

| | |
|---|---|
| Cluster location | |
| Cluster name | |
| CPUs per node | |
| CPU type | |
| Physical CPU-cores per CPU | |
| Main memory per node | |
| Interconnect | |
| Accelerators (such as GPUs) | |

3. Scaling Plot or Scaling Table

*Please present scaling plots as performance (e.g., steps/time, ns/day) on the y-axis against over used compute resources (e.g., cores, nodes) on the x-axis. Include a reference line for theoretical ideal scaling for a quick assessment of the parallel efficiency. Please include separate graphs for each relevant problem size (PS1,...).*
*Alternatively, show a scaling table (performance vs. used compute resources and ideal scaling).*

4. Discussion, Relevance to the Planned Calculations

*Discuss how the benchmarks inform your choice of parallel resources for the subprojects, and how that choice impacts your resource calculation. Do this for all problem sizes and different parallel resources.*

#### 4.2.2 Program B: Program B Name (1 page text max. per relevant code, 0.5 recommended)

### 4.3 Justification of Resources Requested

*Outline the amount of resources you request for the current proposal, structured in sub-projects, if applicable. For multiyear projects (not extensions), all years must be included. Please explain the # runs (R1,...) in the context of the subproject goals.*
*If you want to request resources not listed in the table, like FPGAs or other devices, please add them analogous to GPUs in the table below.*

**Run type:** *A one or two-word description of the calculation relating to the subprojects described above*

**Program used:** *The software used for the calculation should be listed in section 4.1.*

**Problem size (PS1,...):** *A metric of the investigated system that relates to the computing cost, e.g., number of atoms, number of cells, number of electrons, degrees of freedom*

**# runs (R1,...):** *The number of distinct calculation objectives you plan for this type and subproject, e.g., number of different starting configurations, different temperatures, different molecules*

**# steps per run (S1,...):** *Number of calculation steps needed for the planned run. This can be an estimate if the calculation is ended by e.g., convergence criteria or a fixed number if a step limit ends the calculation. If your simulation is not iterative, specify one here and the job runtime as wall time per step.*

**Wall time per step (W1,...):** *Calculation time required per step (S1,...) with the planned CPU-cores (C1,...) or GPUs (G1,...) per run. If a different metric better fits your situation, change as necessary.*

**# CPU-cores / run (C1,...):** *Number of CPU-cores you plan to use in this kind of calculation. This must be informed by the benchmarking of the respective program.*

**# GPUs / run (G1,...):** *Number of GPUs you plan to use in this calculation. This must be informed by the benchmarking of the respective program. Please note that you will also need some CPU-resources for GPU-jobs.*

*For molecular dynamics and similar simulations you can use the table ResourceTableMD instead, that uses*

**Simulation time in $\mu$s (T1,...):** *The desired simulation time in $\mu$s*

**Performance in ns/day (P1,...):** *The performance of the molecular dynamics simulation in ns/day with the chosen resources and workload.*

*and automatically calculates.*
*In case none of the automatic tables fit your situation, you can find a template for a manual table in the tex file.*

#### 4.3.1 CPU Resources:

| Sub-project | Run type | Programs used | Problem size | #runs | #steps per run | Wall time per step [hours] | #CPU-cores / run | Total [mio. CPU-core-hours] |
|---|---|---|---|---|---|---|---|---|
| 1 | Preproc | program A | $PS1$ | $R1$ | $S1$ | $W1$ | $C1$ | $R1 \cdot S1 \cdot W1 \cdot C1 \cdot 10^{-6}$ |
| ... | Type 1 | program B | $PS2$ | $R2$ | $S2$ | $W2$ | $C2$ | $R2 \cdot S2 \cdot W2 \cdot C2 \cdot 10^{-6}$ |
| 1 | Preproc | program A | N=1000 | 100 | 20 | 3.4 | 128 | 0.8704 |
| 1 | Type1 | program B | N=15000 | 1000 | 20 | 3.4 | 128 | 8.704 |
| 2 | Type2 | program C | N=100000 | 100 | 200 | 3.4 | 512 | 34.816 |
| TOTAL | - | - | - | - | - | - | - | 44.3904 |

#### 4.3.2 GPU Resources:

| Sub-project | Run type | Programs used | Problem size | #runs | #steps per run | Wall time per step [hours] | #GPUs / run | Total [thousand GPU-hours] |
|---|---|---|---|---|---|---|---|---|
| 1 | Preproc | program A | $PS1$ | $R1$ | $S1$ | $W1$ | $G1$ | $R1 \cdot S1 \cdot W1 \cdot G1 \cdot 10^{-3}$ |
| ... | Type 1 | program B | $PS2$ | $R2$ | $S2$ | $W2$ | $G2$ | $R2 \cdot S2 \cdot W2 \cdot G2 \cdot 10^{-3}$ |
| 1 | Type1 | program B | N=1000 | 100 | 20 | 3.4 | 4 | 27.2 |
| TOTAL | - | - | - | - | - | - | - | 27.2 |

## 5 Resource Management and Work Schedule (0.5 pages per year)

*Describe the planned resource usage by filling out the table below. In case of a multiyear project proposal (not an extension), please present one table per year. If you plan a roughly constant usage over time, you can skip the table(s) and state that a continuous usage is intended.*

| Project Months | Sub-project 1 | | Sub-project 2 | Sum | |
|---|---|---|---|---|---|
| | CPU [mio. CPU-core-hours] | GPU [thousand GPU-hours] | CPU [mio. CPU-core-hours] | CPU [mio. CPU-core-hours] | GPU [thousand GPU-hours] |
| 1 | 0.1 | 1.1 | 1.1 | 1.2 | 1.1 |
| 2 | 1.2 | 1.2 | 1.2 | 2.4 | 1.2 |
| 3 | 3.3 | 3.3 | 3.3 | 6.6 | 3.3 |
| 4 | 1.4 | 1.4 | 1.4 | 2.8 | 1.4 |
| 5 | 1.5 | 1.5 | 1.5 | 3 | 1.5 |
| 6 | 1.6 | 1.6 | 1.6 | 3.2 | 1.6 |
| 7 | 1.7 | 1.7 | 1.7 | 3.4 | 1.7 |
| 8 | 1.8 | 1.8 | 1.8 | 3.6 | 1.8 |
| 9 | 1.9 | 1.9 | 1.9 | 3.8 | 1.9 |
| 10 | 2.10 | 2.10 | 2.10 | 4.2 | 2.1 |
| 11 | 2.11 | 2.11 | 2.11 | 4.22 | 2.11 |
| 12 | 2.12 | 2.12 | 2.12 | 4.24 | 2.12 |
| Sum | 20.83 | 21.83 | 21.83 | 42.66 | 21.83 |

## 6 Special Requirements (optional) (maximum 0.5 page text)

- *Will your application benefit from FPGAs or GPUs?*
- *What is the major bottleneck in your current use of HPC systems?*
- *Is there any special need for large-scale pre- or postprocessing?*
- *Do you have any special requirements for your workflow?*
- *Do you require exceptional capacities for data transfer or data storage?*
- *Do you need help with a data management plan?*
- *Could we support you with our consulting offers or our scientific support?*

## 7 References

*You can place your reference in the bibtext file references.bib and cite them in this proposal as [1]. For more details on references in bibtex, have a look at* `https://www.overleaf.com/learn/latex/Bibliography_management_with_bibtex`. *Also, feel free to use other mechanisms like biblatex (see* `https://de.overleaf.com/learn/latex/Bibliography_management_with_biblatex`*) if you prefer them.*

[1] W. Kohn and L. J. Sham. Self-consistent equations including exchange and correlation effects. *Phys. Rev.*, 140:A1133–A1138, Nov 1965. doi: 10.1103/PhysRev.140.A1133. URL `https://link.aps.org/doi/10.1103/PhysRev.140.A1133`.