
Detailed Project Description and/or (Final) Report ¹

of a Project at
Lichtenberg High Performance Computer
TU Darmstadt

This detailed project description should be 8 to 10 pages, for M- and L-project prolongation proposals. For S-Projects, and final reports of all project classes, you only have to give the information on the first page, and section 1 (Previous Project Period) The section 1.5 "Project Report" is very important, it is intended to publish this report in the internet (www.hkhlr.de/en/projects) and in the HPC-report Hessen. The scientific part in section 2 should be understandable for persons, who are related to the field of research, but not deeply involved.

Logo of your institution (if available):

Period: Please give the granting period you are applying for (yy-mm-dd to yy-mm-dd). The maximum granting period for a proposal is 12 months.

Project title: (As given in the online application)

Project ID at the Lichtenberg Cluster: (As given by the web form)

Previous Project IDs at the Lichtenberg Cluster for this project: (Please list all projects with a direct scientific continuation)

All current and previous Project IDs of the proposing project manager:

Director of the proposing institute: (= generally, the responsible professor. Title, name, affiliation)

Principal investigator: (= the supervisor of the project, if it is not the director. Title, name, affiliation)

Project manager/main researcher: (= generally, the corresponding person. Title, name, affiliation)

Research area: (according to "DFG-Fachsystematik", http://www.dfg.de/dfg_profil/gremien/fachkollegien/faecher/)

Confidentiality: Is any part of the project covered by confidentiality?

If YES, please give the reason for confidentiality:

By submitting the proposal, you accept that your project undergoes a scientific review process.

¹Please adapt this line to your requirements

1 Previous Project Period

1.1 Resources

Please, fill in the data you get by typing “csum” in a shell at the Lichtenberg Hochleistungsrechner. If the average of the used resources differs more than 20% of the granted/proposed, you are required to give a detailed explanation.

How many cores/cards was the maximum you used in parallel (for one run). Give a short description about the used resources in regard to the (sub)problem size(s).

Please also include the usage plot from your monthly Lichtenberg User Report.

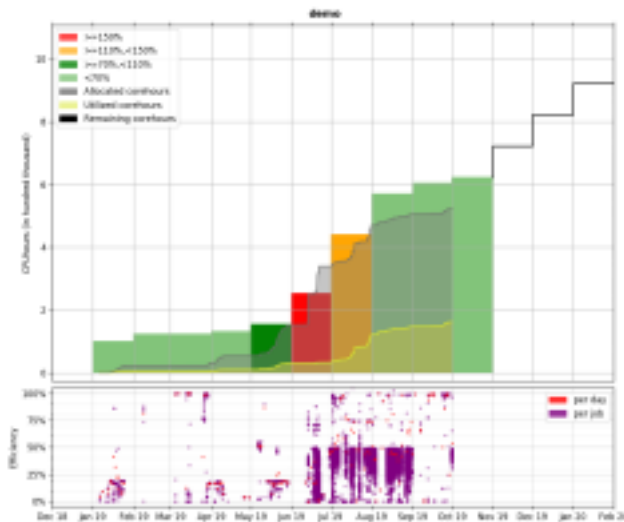


Figure 1: Example of usage plot.

1.2 Project Period

From yy-mm-dd to yy-mm-dd

1.3 Researchers of the project

List all researchers and cooperation partners of the previous project period:

Name	Title	Position Position	Affiliation (if not proposing institute)	Remark
Smith, Julia	M.Sc.	Scientific Staff member		Project manager
Meyer, Carlotta	Dr.	Post Doc		Supervisor
Nada, Otto		Student		Bachelor thesis
Ahmed, Jürgen	M.Sc.	External	RoRe GmbH	Cooperation partner

Table 1: Researchers

1.4 Previous Goals (only for M- and L-projects)

Have the goals of the previous project period been reached? If not, why, and what should be improved in the next period?

Subproject 1 (Simulations of 2HPE binding) was successfully completed.

Subproject 2 (Simulation of INS binding) was completed but yielded no positive results.

Subproject 3 (Dissociation simulations) was successfully completed, but required only half the computing time as we only had starting points from subproject 1, but not from subproject 2.

1.5 Project Report (To be published on the HKHLR website, or in the report “Hochleistungsrechnen in Hessen”).

*Please, give a short report, generally understandable, without using formulas or discipline specific abbreviations with the following subsections, and without references. This report should emphasize the motivation, **tasks** and special challenges (why do you need a High Performance Computer (HPC)?).*

1.5.1 Introduction

Short introduction which motivates the research topic and the use of HPC.

1.5.2 Methods

Short description of the used methods

1.5.3 Results

Results of the project (if the project is running for more than one year, please clarify which results were achieved in which phase of the project). Example: <https://www.hkhlr.de/projects/1218>). Further information will be published soon at www.hkhlr.de/en/projects

1.5.4 Discussion

Please discuss your results and give a short outlook.

1.5.5 Scientific Achievements/Publications

Please list all publications like articles, conference contributions, Bachelor-/Master-/PhD – thesis (standard bib references). If articles are submitted but still not published, please add the pdf. If possible, please provide a TUBiblio URL.

Publications

Juhl, P. Benjamin, et al. "Engineering of Candida antarctica lipase B for hydrolysis of bulky carboxylic acid esters." Journal of biotechnology 150.4 (2010): 474-480. URL: <https://doi.org/10.1016/j.jbiotec.2010.09.951>

Conference Contributions

Pöttgen, Philipp and Ederer, Thorsten and Pelz, P. F. : Examination and Optimisation of a heating circuit using TOR. In: EST 2015, 19-21 Mai 2015, Karlsruhe. [Conference or Workshop Item], (2015) URL: <http://tubiblio.ulb.tu-darmstadt.de/73625/>

Theses (Bachelor / Master / PhD)

Juhl, Benjamin. "Entwicklung und Anwendung einer flexiblen Dockingmethode für Enzyme und Substrate: Substrate-imprinted Docking." (2011). URL: <https://elib.uni-stuttgart.de/handle/11682/1346>

Others (Posters / Books / etc.)

Lorenz, U. and Ederer, T. and Juretzka, C. and Opfer, T. and Utz, M. and Weber, S.: Maple: Eine Einführung in das Computer-Algebra-System. RRZN [Book], (2011) URL: <http://tubiblio.ulb.tu-darmstadt.de/62188/>

1.5.6 Used Software

Please name the used software.

1.5.7 Keywords

Please, give 2-5 Keywords

1.5.8 Pictures

Please, add one or two meaningful pictures in a high quality. These pictures should not be under a copyright of a third party!

2 Next Project Period (only M-and L-Projects!)

The scientific part in this section should be understandable for persons, who are related to the field of research, but not deeply involved!

2.1 Description of the project (about 1 page)

Describe your research project in detail and include a discussion of the scientific questions that you are planning to address as well as the scientific goals of the project:

- *Scientific questions (please emphasize changes in the project tasks from the last period to the next one)*
- *Scientific objectives*
- *Computational objectives*
- *Approach and expected outcome*

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- *Expected impact on the research area*
 - *Scientific and technical innovation potential*
 - *Progress beyond the state of the art*

2.2 Other review processes

Has the underlying research project already (successfully) undergone a scientific review process? Is the project funded by external or public grants? If yes, please provide information about the funding source (e.g. State, BMBF, DFG ...).

2.3 Numerical methods and algorithms (about 1 page)

Please describe the numerical methods and algorithms that you are planning to use, improve, or develop.

3 Computer resources (about 0.5 to 1 pages)

3.1 Code performance and workflow

The description should give information about

- *Which code(s) will be used*
- *How is it parallelized (MPI, OpenMP, hybrid MPI/OpenMP, etc.)*
- *Necessary amount of memory (per core, per node, and in total)*
- *Problem size, and I/O (e.g. data size, bandwidth) of the planned project*
- *Scaling plots and tables with speedup results for runs with typical parameter sets, including the description of cpu-architecture, machine name, and problem size used. The scaling analysis must be relevant to your project, i.e., it must show a similar problem size, utilize at least as many cores as you want to request, and must be given for all software packages that you intend to use. If you need advise on how to create a scaling plot, or if you need computing resources for the test runs, please contact hhlr@hrz.tu-darmstadt.de.*
- *Information about third-party codes: Name, version, licensing model and conditions, web page, and other references.*

To motivate the required resources, please refer to section 1.

3.2 Justification of number of core hours requested

Please outline the amount of resources you are requesting for the current granting period. This should include information such as

- *Type of run (e.g. pre-/post-processing run, production run, etc.)*
- *Problem size for planned runs (e.g. # particles, # control volumes; refer to section 2.3)*
- *Number of runs planned. A run is a set of consecutive batch jobs (each job depends on the output of the previous one).*
- *Number of batch jobs per run*
- *Wall clock time per batch job. We strongly recommend a wall clock time per batch job of 24 hours or less.*
- *Number of cores (and accelerator cards) used in each batch job*
- *Total amount of requested computing time. This number should be calculated from the previous fields in each row (see PDF).*

Put the information into a table. You find an example in the PDF.

3.3 Work schedule

Please provide a short work schedule structured into sub-projects, and include a table or a Gantt chart. You find an example in the PDF.

4 Reviewers (Optionally, only for L-projects)

You may suggest external reviewers from your field of research whom we can contact for a scientific review of the proposal.

5 References