Application for a Computing Time Project on a System at

KIT | NHR

March 28, 2024

Period:	\<Compute period as given in the online proposal\>
Project Title:	\<Title as given in the online proposal\>
Project Extension:	\<Either "Yes" or "No"\>
Project ID:	\<Please only provide in case of a project extension = "Yes"\>
HPC Systems(s):	\<Either "HoreKa CPUs", "HoreKa GPUs" or both\>
Principal Investigator (PI):	\<Name of PI (needs to be a leading researcher (usually with doctorate), cf. eligibility)\> \<Affiliation\> \<Address\> \<EPPN (from the FELS portal)\>
Person to Contact (PC):	\<Name of (technical) contact person(s)\> \<Affiliation\> \<Address\> \<EPPN (from the FELS portal)\>
Confidentiality:	\<Is any part of the project covered by confidentiality? If YES, please give the reason for confidentiality. Nevertheless, by submitting the proposal, you accept that your project undergoes a scientific review process.\>

Abstract

Please give a short abstract of your project. NOTE: This abstract might be published on the NHR@KIT website after the approval of the computing time.

1 Introduction

Please give a short outline of the scientific background of your research (research of the PI!), which also should include references.

(max. 0.5 pages)

2 Preliminary Work

Provide a brief summary of your preliminary work in connection with the proposed project, including references documenting the experience and preliminary work of the PI and project contributors in the field.

It is absolutely necessary to describe which experience you already made with the simulation of the project topic. This can be the simulation of a smaller scaled problem on another machine, or on a system of NHR@KIT. Give some indicator numbers (e.g. numbers of DOF, control volumes, particles), to which you can reference by the description of the required resources in Section 5.

(max. 1-2 pages)

3 Description of the Project

3.1 Project Details

The scientific part in this section should be understandable for persons, who are related to the field of research, but not deeply involved!
Describe your proposed project in detail, structured in sub-projects, if applicable.
Please, include the following points:

- Research field (e.g. Physics, Chemistry, Electrical Engineering)
- Scientific questions you want to address
- Scientific objectives
- Computational objectives
- Approach and expected outcome
- Expected impact on the research area
- Scientific and technical innovation potential, impact and topicality

3.1.1 Sub-project 1

3.1.2 Sub-project 2

(max. 1 page per sub-project)

3.2 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 ...).

4 Numerical Methods and Algorithms

Describe the scientific and numerical methods and algorithms you are planning to use, improve, or develop.

(max. 0.5-1 pages)

5 Computer Resources

5.1 Code Performance and Workflow

Describe **all** codes, packages or libraries that you need to undertake the project, and how these will enable the research to be achieved. Include for **each** code to be used information about

- Which code will be used
- On which hardware the code will be used (CPUs, GPUs, etc. or combinations, if applicable)
- How the code is parallelized (pure MPI, mixed MPI/OpenMP, Pthreads, CUDA, etc.)
- The amount of memory necessary (per core, per node and in total)
- Scaling plots **and** tables with speedup results for runs with typical, parameter sets, problem size, and I/O **of the planned project**. Scaling data should start with the lowest number of cores possible
- Describe architecture, machine/system name, and problem size used for the scaling plots
- Current job profile (independent jobs, chained jobs, workflow, etc.)

Important: Please take into account the corresponding technical guidelines and requirements (e.g. required minimal code scalability, memory restrictions, etc.) of the chosen machine(s).

If you use third-party codes, include

- Name, version, licensing model and conditions
- Web page and other references
- Contact information of the code developers.

- Your relationship to the code (developer, collaborator to main developers, end user, etc.)

Here we give an example table and plot for presenting scaling and performance information. Let the scaling start with one core or, if not possible, with the lowest number of cores possible for your case. Please **replace** the text in `Courier` by the appropriate information.

Table 1: Scaling behavior of `code` on `architecture and system` at `location`. This test was performed with $5 \cdot 10^6$ particles, absolute timings per time step (s) and relative speedup normalized to 1 core are given.

#cores	absolute timing (s)	speedup	Performance per core [MFLOP/s]
1	3781.2	1.0	800
2	1890.6	2.0	800
4	945.3	4.0	800
8	472.7	8.0	800
16	236.3	16.0	800
32	118.1	32.0	800
64	59.1	64.0	800
128	32.8	115.2	720
256	18.4	204.8	640
512	10.5	358.4	559
1024	6.2	614.4	480
2048	3.7	1024.0	400
4096	2.3	1638.4	320

(1-2 pages)

5.2 Justification of Resources Requested

Outline the amount of resources you are requesting for the current granting period.

If you are requesting different types of resources (e.g. CPUs, GPUs, etc.), please provide the following information and table for each type of resource separately and use the unit core hours (core-h). For GPUs, please specify the resources in terms of GPU hours of the corresponding host systems. If you request resources on several HPC systems or modules, please justify why this is necessary for your project.

- *Type of run (e.g. pre- /post-processing run, production run, visualization, etc.)*
- *Problem size for planned runs (e.g. # particles or the like)*
- *Number of runs planned*
- *Number of steps per run*
- *Wall-clock time per run*
- *Number of cores used per run (for GPUs: number of cores of the host CPUs)*

- *Total amount of requested computing time in core-h*
- *Resources for data analytics, if applicable*

Table 2: The following CPU resources are requested

Sub-project	Type of run	Problem size	# runs	# steps/ run	Wall time/ step [hours]	# cores/ run	Total [core-h]
Sub-proj. 1	Preproc.	P1	R1	S1	W1	C1	R1·S1·W1·C1
	Type 1	P2	R2	S2	W2	C2	R2·S2·W2·C2
...					...		
TOTAL							sum of above

Table 3: The following GPU resources are requested

Sub-project	Type of run	Problem size	# runs	# steps/ run	Wall time/ step [hours]	# hosts/ run	Total [GPU-h]
Sub-proj. 1	MD 1	P3	R3	S3	W3	C3	R3·S3·W3·C3
	MD 2	P4	R4	S4	W4	C4	R4·S4·W4·C4
...					...		
TOTAL							sum of above

(0.5 - 1 pages)

5.3   Work schedule

Please provide a short work schedule, structured in sub-projects, if applicable. Include a table and/or Gantt chart.
In the last row, estimate the monthly core hour total (over all subprojects) in scientific notation.

Example for a Gantt chart:

	Project Month											
	1	2	3	4	5	6	7	8	9	10	11	12
Sub-project 1												
Task 1.1												
Sub-project 2												
Task 2.1												
Task 2.2												
Sub-project 3												
Task 3.1												
Task 3.2												

Figure 1: Work schedule for the project.

6   Key Personnel and Experiences

Give a short introduction of the key persons involved in the project and their experience (max 3 persons).
Furthermore, please provide at least five keywords stating the important topics the PI do research about (not the application topics but the PI research interests).

(max. 0.5 page)

7   Progress Report (MM-20YY – MM-20YY)

In case of an application for a **project extension**, please include here the report of the work done in the last period (structured in sub-projects, if applicable).

Please, include the following information:

- brief description of the (sub-) project

- scientific results obtained

- resources used

- performance, scaling behavior (if not already described in 1.6)

(about 1-4 pages)

7.1   Publications from project xxxx

Peer-reviewed Publications in form of DOIs published only.

- ...

- ...

7.2 Ph.D. theses completed within project xxxx

Please, give author's name and degree and the title of the thesis.

- ...

- ...

7.3 Additional references

- ...

7.4 Graphics suitable for the general public

In order to promote simulation science, we are interested in a short summary - suitable for a general audience – of your project and the achieved results. In particular, attractive color pictures of your results together a short description are desirable. We ask your permission to use this text and these pictures in publications.

8 Reviewers

Please, provide us with a list (at least three) of external reviewers from your field of research whom we can contact for a scientific review of the proposal.