JARA Jülich Aachen Research Alliance

Project Proposal for HPC Access

Period
Give the granting period you apply for (month year - month year)

Project title
Title as given in the online proposal

Type of project
Either "new project" or "project extension"

HPC system(s)
Please name the HPC system(s)/module(s) for which you are applying

Project ID or Project Acronym
Please provide in case of a project extension

Principal investigator
Name, affiliation, address

Project contributor(s)
Name, affiliation, address

The length of the project description is restricted to 18 pages (font 12 pt)!

Contents

1 Introduction

Give a short outline of the scientific background of your research, including references.

(about 0.5 to 1 page)

2 Preliminary Work

Provide a brief summary of your preliminary work in connection with the proposed project, including references.

(about 1 to 2 pages)

3 Description of the Project

3.1 Project Details

Describe your research project in detail, structured in sub-projects, if applicable. Please include the following points:

- *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

...

(1 to 2 pages per sub-project)

3.2 Review Processes

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

4 Numerical Methods and Algorithms

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

(1 to 2 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, MICs, 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** (no general benchmark results are accepted). 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

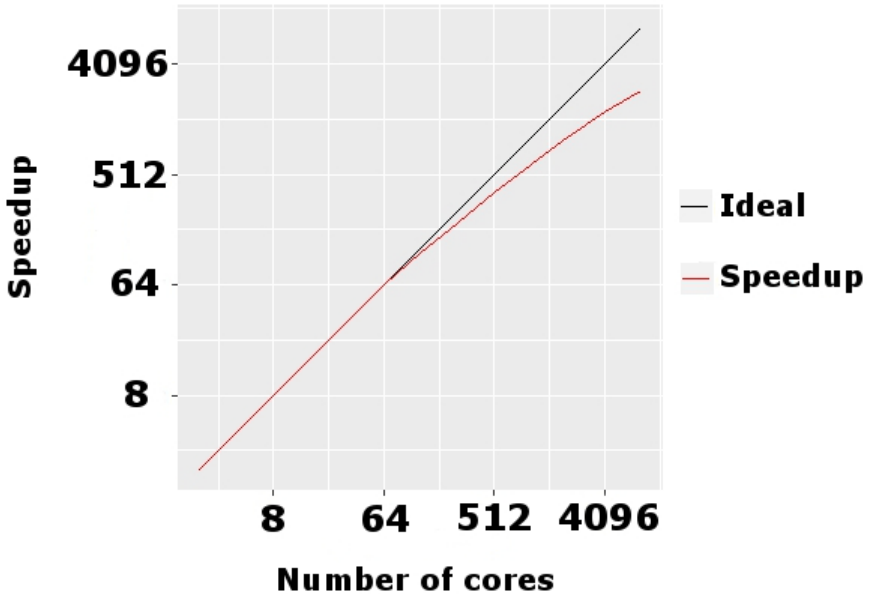

Figure 1: Scaling behavior of `code` on `architecture and system` at `location`. This data was obtained with a problem size of `size`.

(1 to 2 pages)

5.2 Justification of resources requested

Outline the amount of resources you request for the current granting period, structured in sub-projects, if applicable.

If you are requesting different types of resources (e.g. CPUs, GPUs, MICs, 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 core hours of the corresponding host CPUs. 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]	# host cores/ run	Total [core-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 to 1 page)

6 Resource Management and Work Schedule

6.1 Resource management

Describe how you intend to manage the resources you have requested. This should include a description of the methods you will deploy to monitor progress of the project and how project results are documented.

(0.5 to 1 page)

6.2 Work schedule

Please provide a short work schedule, structured in sub-projects, if applicable. Include a table and/or Gantt chart.

6.2.1 Sub-project 1

...

6.2.2 Sub-project 2

...

Example for a Gantt chart:

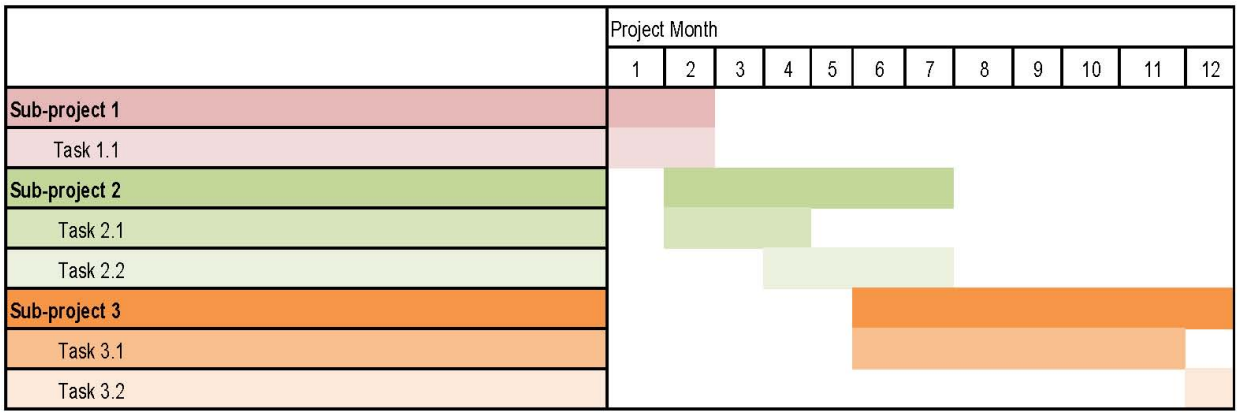

Figure 2: Work schedule for the project.

7 Key Personnel and Experiences

Give a short introduction of the key persons involved in the project and their experience (max 3 persons).

(half a page)

8 Bibliographic References

Provide recent/most important bibliographic references that are relevant to the project.