HPC Compute Time Application
"'Title of your Project"'

Your Name

March 2, 2022

Note: Fill-out hints are given in italic. If you are unsure or have questions please contact `pc2-support@uni-paderborn.de`*. The information provided here will not be made public. It will only be accessible for PC² staff for the review process and support, the ressource allocation board of PC² and the external scientific reviewers. In case of NHR proposals (normal and large proposals) also the NHR Nutzungsausschuss which is a joint NHR board that approves large NHR projects as well as the NHR Geschäftsstelle (for reporting purposes) will have access to the submitted proposal.*

1 Introduction

Describe the general scientific background of your project. Introduce the scientific questions addressed by the project. Highlight the importance of the project. Include appropriate citations here.
(about 0.5-1 page)

2 Preliminary Work

Provide a brief summary of your preliminary work in connection with the proposed project. Include appropriate citations here.
(about 0.5-1 pages)
If this is a continuation or followup project describe the resources used so far in the project and explain the need for the continuation/follow-up.

3 Description of the Project

Describe what you specifically try to do in the frame of THIS project with the compute time you apply for. If appropriate, you can structure your project in sub-projects. Include appropriate citations here.

Please address at least the following questions because they are relevant for the external scientific review:

- *Scientific questions you want to address*
- *Scientific objectives*
- *Computational objectives*
- *Approach and expected outcome*
- *Expected impact on the research area*
- *Scientific and technical impact*
- *Progress beyond the state-of-the-art*

(about 2-4 pages)

4 Numerical Methods and Algorithms

Outline the numerical methods and algorithms that you plan to use in your project. If you plan to improve, extend or develop methods or algorithms, please shortly describe the starting point and your planned work in this regard. Include appropriate citations here.
(0.5-1 page)

5 Related Computational Work

Describe the related computational work here. Is your computational method successfully applied elsewhere? What size of simulation is state of the art? Are there any other computational methods or programs available to treat the scientific question? Explain the advantage or disadvantages of your selected method or program with respect to the scientific challenge?
(0.5-1 page)

6 Personnel and previous HPC Experience

Describe the experience of key persons involved in the project with large-scale computer simulations. What platforms and what size of computing jobs have you worked with?
(about 0.5 page)

7 Computational Methods and Programs

7.1 Program Summary

For each program that you plan to use in the project please add a column in the following table and answer the questions if applicable:

	Program A	...
name		
version number		
web page		
Citation or reference		
License model		
Usage conditions		
Is the source code publicly available? If yes, give link to code here.		
Is it a commercially licensed software? If yes, do you have a license that is useable on PC^2 systems?		
How is the code parallelized (pure MPI, hybrid MPI/OpenMP, Pthreads, CUDA,...)?		
Which programming language is used?		
Which libraries are required to compile it?		
Are there other special requirements for the program?		
Are you a developer, collaborator or end user of the program or library?		
Which hardware will be used (CPUs, GPUs (which type) or FPGAs)		
In which job type will this program be used (e.g. independent jobs, chained jobs, workflow,...)?		
Estimated resource share in % of the total planned CPU-Core-hours		
Estimated resource share in % of the total planned GPU-hours		
Estimated resource share in % of the total planned FPGA-hours		

7.2 Parallel Efficiency and Scaling

For each *program with a resource share larger than 10 % that is not listed at* `https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents/well-known-programs` *please describe the code performance and parallel efficiency for the jobs that you plan to run in*

this project. You can also use results from similar calculations or results obtained from comparable HPC systems. If you don't have comparable results you can also use publicly available benchmark results from the program (for example from a publication) or request a test project from PC² to benchmark your program. Please make sure that the result you present here are representable for the planned calculations in terms of parameter sets, problem size, method used and other aspects.

Note: For the programs listed at *https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents/well-known-programs* ***NO scaling analysis is required.***

A tutorial for creating scaling plots and scaling tables can be found at *https://hpc-wiki.info/hpc/Scaling_tutorial*

Please use the following section as a template.

7.2.1 Description of Parallel Efficiency for Program A

Job description: *Shortly describe the benchmark job here.*

Benchmark system:

Cluster location	
Cluster name	
CPUs per node	
CPU type	
main memory per node	
Interconnect	
accelerators used (such as GPUs)	
number of MPI processes per node	
number of threads per MPI process (e.g. OpenMP threads)	

Scaling Table:
Speedup(N) = T(1)/T(N)
parallel efficiency = Speedup(N)/N
If your job doesn't run on one node or takes too long, you can use multiple nodes as the reference point for the speedup, i.e., Speedup=$T(N_{\text{ref}})/T(N)$

#nodes N	Absolute runtime T(N) [s]	Speedup	Parallel efficiency
1			
2			
4			

Scaling Plot: *Plot the speedup versus the number of nodes from the previous table.*

Discussion: *Discuss the measured parallel efficiency in the context of the scientific problem addressed by the project. If you have insight into your algorithm or your code in terms of the models such as the Roofline model, demonstrate this insight in the discussion. Even codes or algorithms with an unfavorable parallel scaling can be granted computation time if the large HPC systems offered by PC2 are required to achieve progress for the given scientific problem that would not be possible on smaller HPC systems. The same holds for an embarrassingly parallel problem that in its total computational needs requires a large HPC system offered by PC2.*

7.3 Workflow

Describe your computational workflow here. Do you have special requirements for your workflow such as database server, high-bandwidth connectivity to external sites, job dependency management, ...?

8 Justification of Requested Resources

8.1 Estimation of Resources

Justify here your requested resources by filling out the following table.

Run type			Total/sum
Total/sum			
Programs used			
Cluster name			
#runs			
#steps per run			
Wall time per step [hours]			
Type of resource (CPU type, GPU type, FPGA type)			
CPU-Core hours			
Accelerator-hours (GPUs or FPGAs)			
Disk storage in GB			
Comment			

8.2 Schedule for Resources Usage

Describe here the planned schedule for using the resources by filling out the table. We encourage a continuous usage of resources during the project runtime.

Project month	Run types	CPU-Core-Hours	GPU types and GPU-hours	FPGA types and FPGA-hours
1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
total				

9 Special Resource and Support Requirements

Discuss for example the following questions:

- *Will your application benefit from FPGAs or GPUs?*
- *What is the major bottle neck in your current use of HPC systems?*
- *Any special need for large scale pre- or postprocessing?*
- *Do you have special requirements for your workflow?*
- *Do you require special capacities for data transfer?*

10 Summary

Summarize your proposal.
(0.5 page)

References

[1] *Programming languages - C++, ISO/IEC 14882,*