

HPC Compute Time Application

”‘Title of your Project”’

Your Name

Date

*Note: Fill-out hints are given in italic. Please remove in the final version. If you are unsure or have questions please contact* *pc2-support@uni-paderborn.de**.*

*This template is for* ***normal or large projects that apply for a single year or multiple years and don’t have a scientific review yet****.*

*Projects that have already been* ***scientifically review in a peer-review process*** *(e.g. DFG, BMBF,.., details at* [*https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents/simplifications*](https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents/simplifications)*) can use a greatly simplified detailed description template available at* [*https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents*](https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents)*.*

***Project extensions*** *can use the simplified version available at* [*https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents*](https://pc2.uni-paderborn.de/hpc-services/our-services/forms-documents)*.*

*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, the external scientific reviewers, the NHR Nutzungsausschuss which is a joint NHR board that approves large NHR projects as well as the NHR Geschäftsstelle (for reporting purposes).*

**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)*

**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 | Program B | …. |
| 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 PC² 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 % 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/de/hpc-services/our-services/forms-documents/well-known-programs***](https://pc2.uni-paderborn.de/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*](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(Nref)/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 |
| 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. In case of a multi-year project, please make a table for each year.*

|  |  |  |
| --- | --- | --- |
| Project month | Run types | Resources |
| 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?*

**References**

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