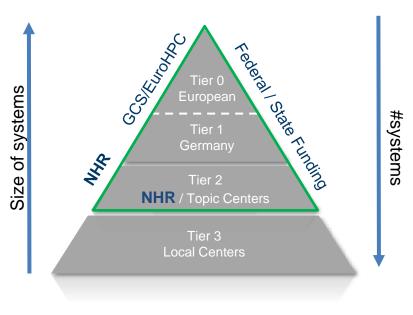


How to apply for computing resources in Germany and Europe

Georg Hager (NHR@FAU), Helmut Brüchle (LRZ Garching), Harald Köstler (NHR@FAU)

The HPC supply pyramid in Germany



EuroHPC Joint Undertaking (JU):
 EU-level legal and funding entity



• Funding: 7 B€ (2021-27)

 GCS: Gauss Centre for Supercomputing – three German national/EU-level centers at Garching, Stuttgart, Jülich



 NHR: A coordinated network of National High Performance Computing (NHR) centers at German universities funded by federal and state governments



- Total funding 625 M€ (2021-2030)
- Currently 9 NHR centers



Resources at NHR@FAU: Tier 3

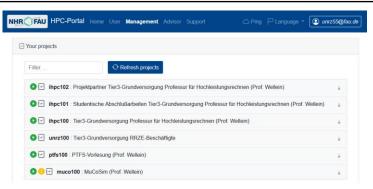


NHR@FAU: HPC Infrastructure

- HPC systems for FAU (local access only)
 - Approx. 17,000 cores (meggie, woody, tinyFAT)
 - Approx. 150 NVIDIA GPUs (tinyGPU)
- HPC systems accessible through NHR+FAU+BayernKI
 - Fritz: CPU-Cluster (11/2024: TOP500 #283): approx. 70,000 Intel cores
 - Alex: GPU-Cluster (11/2024: TOP500 #252): 304 A100 (+352 A40) NVIDIA
 - Helma: GPU-Cluster (11/2024: TOP500 #79): 384 H100 NVIDIA
- Central (online/offline) storage: 8 PB / >3300 tapes possible (NHR+FAU)
 - \$HOME, \$WORK, \$VAULT
 - Workspaces on NVME (5+ PB)

How to get access to Tier-3 systems (local supply)?

- Docs: <u>doc.nhr.fau.de/fau-tier3-application</u>
- New access for a group
 - PI (head of institute/group) logs into HPC portal (<u>portal.hpc.fau.de</u>) via SSO
 - Confirm export control guidelines
 - Delegate day-to-day tasks to Person(s) of Contact (known to the portal)
 - Request basic Tier-3 access for the institute via hpc.fau.de/application-for-fau-tier3-access
 - Wait
- If you are already part of a group that has access
 - Log into the HPC portal (portal.hpc.fau.de) via SSO
 - PI or PoC can then invite you to the project





BayernKI



BayernKI Wissenschaft

- www.ki-in-bayern.de
- Central infrastructure for the State of Bavaria to advance academic Al research
- LRZ & NHR@FAU cooperation
- Monthly BayernKI online Q&A
- Joint support team



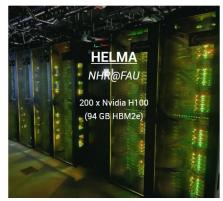












At NHR@FAU, BayernKI hardware is an integral part of Helma, but allocations for BayernKI users are also available on our clusters Fritz and Alex.



BayernKI hardware is an integral part of the <u>LRZ AI Systems</u>, but allocations for BayernKI users are also available on other LRZ AI Systems' partitions. Interested users can request access to LRZ's Cerebras CS-2 to experiment with this novel AI accelerator technology.

BayernKI – Wissenschaft

- Conditions
 - Only one project per group
 - One group can either have a project at LRZ or at NHR@FAU
- Massive extension of resources planned for 2026
- Resources are for AI research
 - Al services for the public sector (chatbot) available at www.stmfh.bayern.de/digitalisierung/ki
 - Inference services are not part of "BayernKI Wissenschaft"



Resources within the NHR Alliance: Tier 2



Nine NHR centers form the NHR alliance



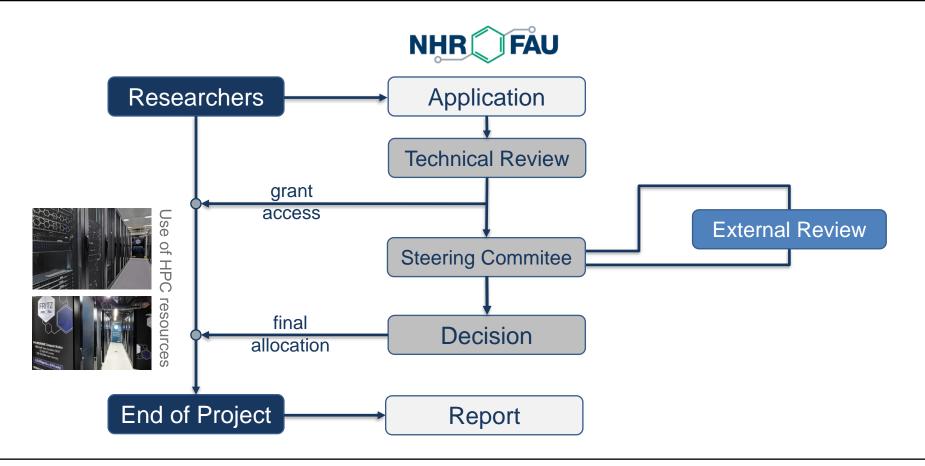
NHR provides

- HPC resources
- Scientific/technical project support
- Performance optimization support
- Example: Weekly Q&A and webinar series
 - AI From Laptop to Supercomputer
 - https://www.nhr-verein.de/en/aisupercomputers
 - Every Thursday 2:00 p.m.

Applying for NHR resources

- Docs: <u>doc.nhr.fau.de/nhr-application</u>
- NHR resources are open to researchers at German universities
 - No charge!
 - For detailed information see https://www.nhr-verein.de/en/computing-time
- Application for resources through central JARDS portal
 - Joint Application, Review, and Dispatch Service, developed since 2014 at JSC
 - Researchers have to choose an NHR center AND project category which meets their requirements best
 - https://jards.nhr-verein.de/
- Peer-review process
 - Scientific quality / need for Tier-2 resources must be proven
 - Simplified review process for projects already reviewed by DFG (and others)

Access to HPC resources beyond basic services



NHR@FAU project types and limits

Project type		imits ¹ I hrs) A100	CPU limits ¹ (mio. core-hrs)	Review	deadline
Test/Porting	< 3.000	< 3.000	< 0,5	technical	rolling call
Starter	< 10.000	< 10.000	< 1	technical	rolling call, only one time per group
Normal	6.000	4.000	1	technical rev. + 2 scientific rev.	rolling call
Pre-reviewed normal	60.000	40.000	30	technical rev. + resources/method	rolling call
Large Scale	60.000 - 180.000+	40.000 - 120.000+	30 - 100+	technical rev. + 2 scientific rev.	cut-off quarterly

¹Annual allocations

Admission to NHR and NHR@FAU systems

- Application evaluation process
 - Technical reviewing by NHR@FAU staff
 - You already get access to HPC resources!
 - Local Steering committee assigns reviewers (local and external)
 - Scientific reviewing by local/external reviewers
 - Allocation decision by local steering committee
 - Exception for Large Scale projects: approval by central NHR board necessary ("Zentraler NHR-Nutzungsausschuss") meets 4 times/year
 - Accepted projects get a project advisor / support expert assigned
- From application to decision: usually less than 3 months!



How to submit an application in JARDS



Which NHR center to choose?

https://www.nhr-verein.de/en/information-center-selection

Information for Center Selection

All NHR centers have up-to-date HPC hardware and offer best conditions for well-scaling applications. The following is a brief description of the centers' resources as well as the consulting services offered.

Center	Description	Details	Application Guidelines
NHR@FAU	NHR@FAU currently runs more than 70 000 of and offers extensive GPU resources for throu		<u>Link</u>
	calculations as well as moderately parallel appl	cations (up	
	to 8 GPUs). Available are 304 NVIDIA A100 (4	0/80 GB) as	https://doc.phr.fo.u.do/phr.application/
	well as 352 NVIDIA A40 cards; the latter are p	articularly	https://doc.nhr.fau.de/nhr-application/
	suitable for molecular dynamics simulations wi	th standard	
	packages such as GROMACS and AMBER.		
	User support is known for its expertise in perf	ormance	
	engineering for CPU and GPU nodes as well as	iterative	
	solvers. In application support, NHR@FAU has	a special	
	focus on atomistic simulations.		

JARDS

https://jards.nhr-verein.de/

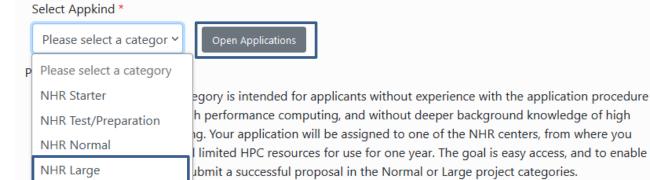
Start Page

Welcome to JARDS, please choose if you want to create an application or review submitted applications.

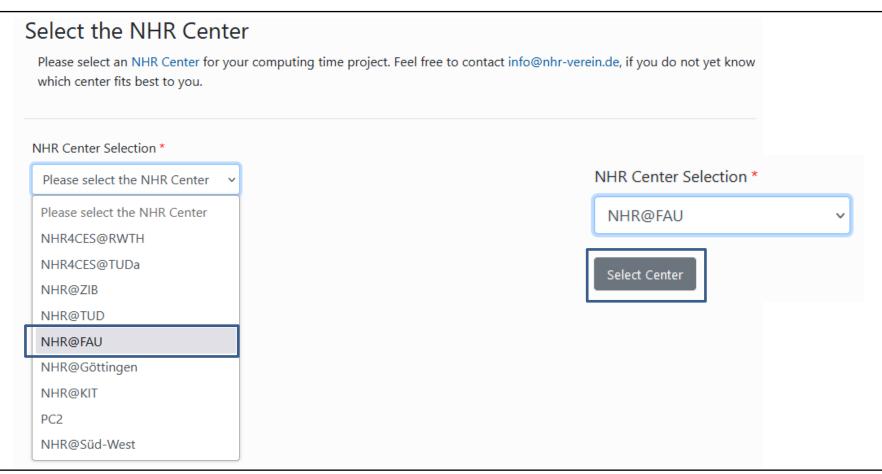
Applications

Please select an application kind to create an application. If you do not yet know which project category and/or NHR-center are appropriate for you, please first refer to the information on the NHR website.

2. NHR Test/Preparation Projects: This project category is mainly used to prepare an application; it can



JARDS



JARDS



Electronic project application form for NHR@FAU Compute Cl Category: NHR Large

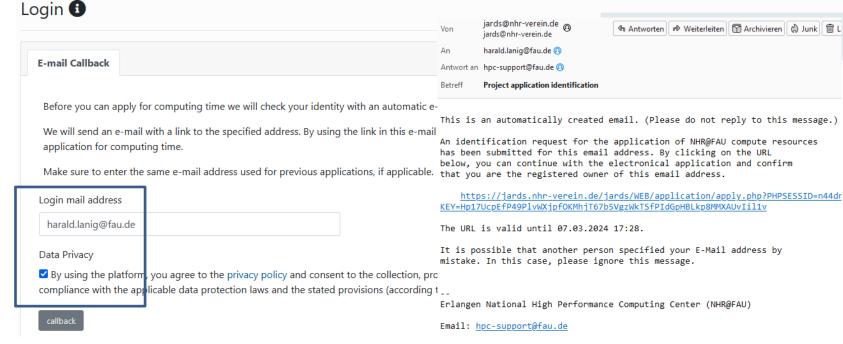
Mail sent to harald.lanig@fau.de

An E-mail for your identification is on the way.

This might take a few minutes. Please, also check your spam folder.

The link sent is valid for the next 30 minutes.

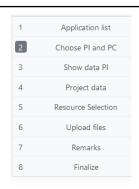
back



Further steps in JARDS

- Select project type (Starter, Normal, Large)
- Choose Principal Investigator (PI) and Person of Contact (PC)
 - Registration with JARDS platform is mandatory
- Enter project data (name, DFG category, amount and type of resources)
- Detailed scientific project description, supplementary material
- Further remarks

- Finalize application
 - It is possible to save an application mid-process and finish it later



Need Help?

We will **help you answering your questions** about the compute time application, the submission and the reviewing process

We will also **support you porting your applications** to run effectively on our systems

In any case, contact us via hpc-support@fau.de

After submitting the application and passing the technical review, you can immediately start doing calculations (via a test/porting project account)

Standard project runtime: 12 months



GCS Supercomputers

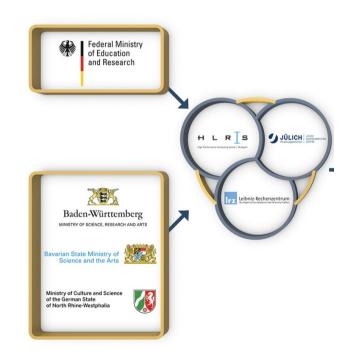
https://www.gauss-centre.eu/

The Gauss Centre for Supercomputing

SUPERCOMPUTING AT THE LEADING EDGE

Gauss Centre for Supercomputing

- Provision of state-of-the-art supercomputing resources
 featuring complementary system architectures to ensure the
 continual development of computer-aided science in Germany.
- Open access to GCS systems for all scientists and researchers through a peer-review process focused on evaluating a proposal's technical and scientific merit.
- In-depth user support for scientists and reseachers across all disciplines, personalized to fit the specific needs of the individual user.
- High-level education and training for current, past, or prospective users to ensure the most efficient use of GCS HPC resources
- Continually attracting and retaining highly qualified scientists and engineers by offering state-of-the-art HPC system infrastructures, services and support.
- Supporting Germany's leading position in the realms of scientific and industrial research in fields ranging from automotive research, medicine, climate and environment, fundamental research, and astronomy, among others.







HLRS - Hunter

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HPE Cray EX4000

48,1 PFlops

752 AMD Instinct MI300A, 512 AMD EPYC 9374F

In operation since Feb. 2025



https://www.hlrs.de

LRZ – SuperMUC-NG



	SuperMUC-NG Phase1 (general purpose)	SuperMUC-NG Phase 2 (accelerated)		
Number of compute nodes	6480	240		
Main memory	719 TB DDR4	123 TB DDR5		
Storage capacity	70 PB GPFS	1 PB DAOS		
Throughput memory to disk	500 GB/s	750 GB/s		
Data Science Archive (DSA) capacity	260 PB			
Throughput disk to tape	10 GB/s			
Network	Intel Omnipath	Mellanox HDR Infiniband		
Power consumption	2,7 MW	0,5 MW		

JSC - JUWELS

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CPU Partition

- 2511 nodes, 2x Intel Xeon Platinum 8168 (48 cores)
- 96-192 GB memory per node
- 122,768 compute cores in total

GPU Partition

- 56 nodes, 4x NVIDIA V100 per node
- 192 TB memory per node
- 224 GPUs in total



JSC – JUWELS Booster

SUPERCOMPUTING AT THE LEADING EDGE



Booster Partition

- 936 nodes, 2x AMD EPYC 7402 (48 cores)
- 512 GB memory per node
- 3744 GPUs in total



JSC – JUPITER Booster

SUPERCOMPUTING AT THE LEADING EDGE



Booster Partition

- ca. 6000 nodes,
- 4x NVIDIA GH200 Grace-Hopper Superchip
 - NVIDIA Grace (Arm Neoverse-V2), 72 cores at 3.1 GHz
 - 120 GB LPDDR5X memory
 - NVIDIA Hopper H100, 132 multiprocessors, 96 GB HBM3
 - ~24.000 GPUs in total
 - available in the Early Access Program
 - Current setup: Test system JEDI



Project types @LRZ

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Test Project:

- 300 K core-h on Phase 1 plus 900 GPU-h on Phase 2
- Typically one week after submission
- Up to 2 years duration

Regular Project:

- <45 M core-h on Phase 1, and/or < 140 K GPU-h on Phase 2
- Typically 6-8 weeks for scientific review
- Up to 2 years duration

Large-Scale Project:

- >45 M core-h on Phase 1, and/or >140 K GPU-h on Phase 2
- Call open twice per year
- Project start 1 May or 1 November
- Project duration 12 months

Project Extension:

- Any time for regular projects with or without additional compute budget (status report incl. justification of additional resources if requested)
- Large-Scale projects can only be extended in Large-Scale call (updated project description + status report)

Roles in a project

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Principal Investigator (PI):

- Proven scientific track record (e.g. PhD)
- Works at publicly funded German research institute
- Legally responsible
- Can also perform same tasks as PC

Person to Contact (PC):

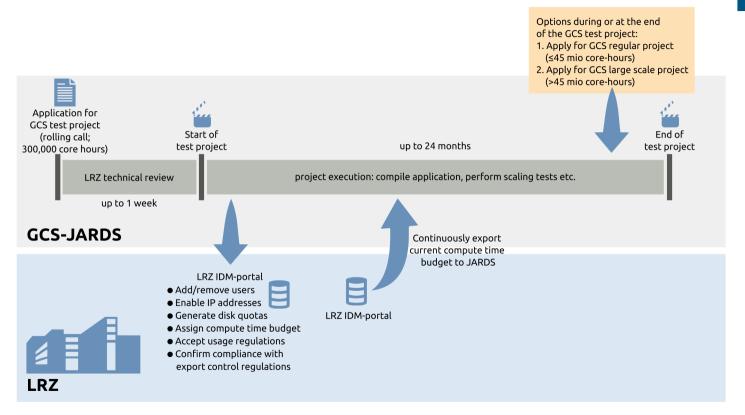
- Manages project: add/remove user, add/remove IP addresses
- Can apply for project application and extension
- Can upload status report and final report to GCS-JARDS

Project Partners:

- No limit on project partners
- Can come from anywhere
- Projet partners from industry possible (however: no industry relevant production runs; needs to be basic resarch to be published in peer reviewed journals)

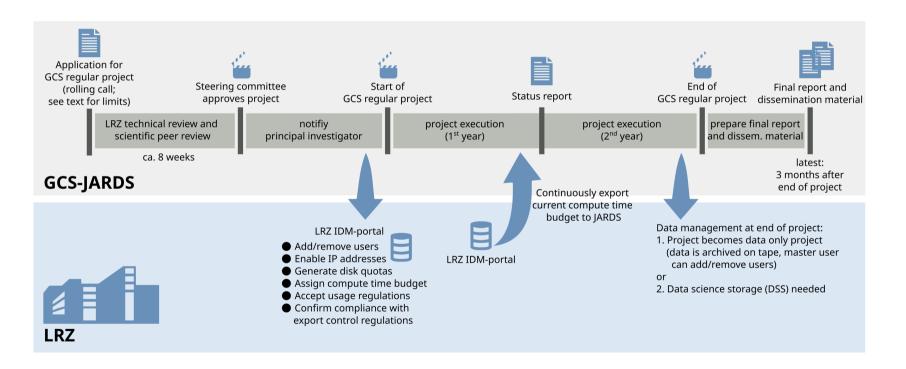
GCS test project @LRZ

GCS Gauss Centre for Supercomputing



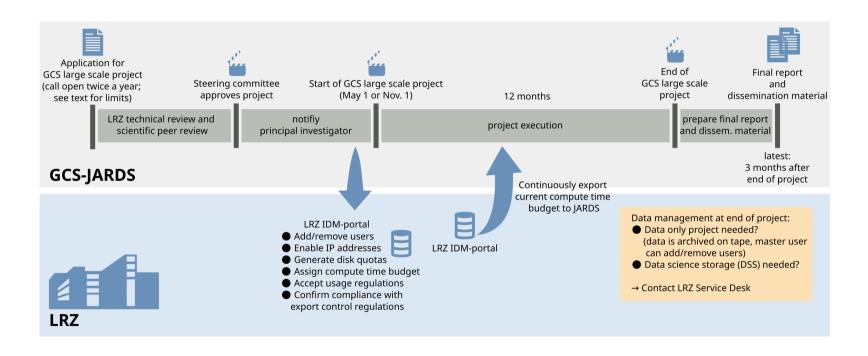
GCS regular project @LRZ





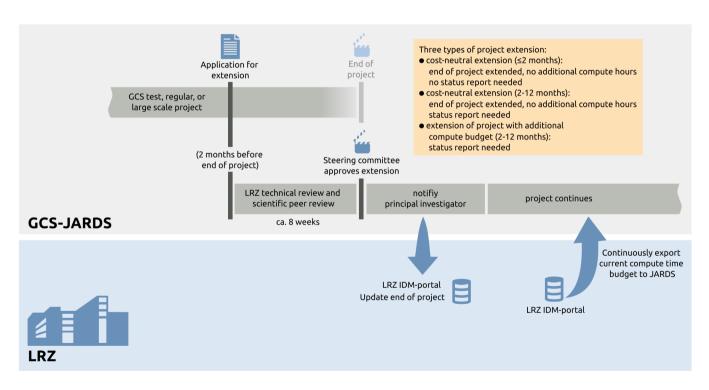
GCS Large-Scale project @LRZ





Project extension @LRZ





Application for a GCS project



- 1. Visit https://jards.gauss-centre.eu/gcshome/application
- 2. Select project type and GCS center
- 3. Create new application
- 4. Select PI (and potentially PC)
- 5. Add project partners with name and affiliation
- 6. Provide a project abstract (<1000 chars) and specific goals for the granting period (<500 chars)

Application Procedure (cont.)

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- 7. Request resources (compute time)
- 8. Characterize your jobs (applied codes, programming languages, software packages, job size)
- 9. Provide storage requirements, I/O strategy, I/O characteristics and data transfer
- 10. Upload a detailed project description, supporting material (for extensions: also status report)
- 11. Finalize submission
- 12. Print and sign PI agreement.

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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)

- Explain your science case as clearly as possible!
 Reviewers might not be from your direct field.
- Explain societal benefit! Why should the society spend considerable amounts of money for your case.
- Show that you know your field. Provide a concise introduction into the methodology and goals. Of course, not all preliminary work is yours.
- Checking the project members preliminary work ensures competent scientists get access to the resources.
- Preliminary work is not only papers, but can also be convincing intermediate result.
- Collected or evaluated datasets mark also an important preliminary work.

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3 Description of the Project

3.1 Project Details

Describe your research project in detail, structured in sub-projects, if applicable. Include discussion of the scientific questions that you are planning to address and the overall scientific goals of the project. It is important that you describe the innovative aspects, impact and topicality of the proposal.

- 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
- Progress beyond the state-of-the-art

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, ...) and the funding time frame. If possible, please provide the corresponding review report and upload it as supplemental material.

- Explain your science case as clearly as possible! Go into more detail: Provide what you want to do, which steps you plan like to perform, which methods to use.
- Explain why your result bring your scientific field forward! Explain what can be done if your approach works.
- Make your project easier tangible by breaking it down. Bring your work in a reasonable order.
- Compare also to the work schedule you provide in Sec. 6. which includes a Gantt chart
- Provide information about the **review process, that your project has already undergone.** Has the project already received grants from DFG, EU, etc.?

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• Briefly describe the numerics used, or the software package including dependencies, version numbers etc.

4 Numerical Methods and Algorithms

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

(1 to 2 pages)

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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 (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.)
- Describe memory requirements, requirements concerning the High Performance network and I/O requirements

Important: please consider 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. The presented scaling should range from a single core to the maximal possible number of cores. If this is not doable, the presented scaling should range from the lowest possible number to the maximal possible number of cores for your case. Please replace the text in Courier by the appropriate information.



- Show scaling data. Do not start with 1 core, but use
 the minimum number of nodes/cores/GPUs that are
 needed to fit a realistic test case. Then, show that the
 speed-up increases with additional nodes/cores/GPUs.
 Also useful is weak scaling: Increase the test case as
 well as the number of nodes/cores/GPUs
 (performance should stay constant).
- If you cannot use the general queue, describe your workflow. Can you use job farming, job arrays, etc.?

SUPERCOMPUTING AT THE LEADING EDGE



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, etc.), please provide the following information and table for <u>each</u> 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	Problem	# runs	# steps/	Wall time/	# cores/	Total
	of run	size		run	step [hours]	run	[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

- Provide a table that shows how many different runs you want to perform, how many cores/nodes/GPUs are used for each run.
- Estimate, how many hours one run or one timestep of one run takes (how many wall days does your longest simulation need to complete?).
- If you are using job farming, put the total number of cores/nodes/GPUs that can be used in one job in the table. Add a reference to 5.1, where you described how the resources are used by the workflow

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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

Provide tables and Gantt charts for a clear presentation of the work schedule, structured in sub-projects, if applicable.

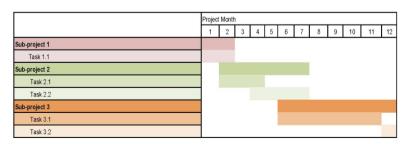
6.2.1 Sub-project 1

...

6.2.2 Sub-project 2

...

Example for a Gantt chart:



- Describe how your project proceeds. How does the project work in practice? Who communicates with whom and how?
- **Keep your schedule short.** The logical structure has already been explained.

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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.

- Make sure the relationship between the people and the planned project becomes apparent.
- Bibliography can be kept short. This is not a scientific paper, but the bibliography should help the reviewer find relevant literature.

Feel free to bring your questions to the LRZ "HPC Lounge":

https://doku.lrz.de/hpc-lounge-813636379.html





Questions?

Join us for the "HPC Lounge" (Virtual Zoom meeting)

Every Wednesday, 2pm-3pm



Details:

https://doku.lrz.de/hpc-lounge-813636379.html

Questions and answers

SUPERCOMPUTING AT THE LEADING EDGE



Contact:

GCS Coordination Office

c/o Jülich Supercomputing Centre

Forschungszentrum Jülich

52425 Jülich

Germany

E-mail: coordination-office@gauss-centre.eu

How to apply for EuroHPC Resources

Experiences and Best Practices

Overview Access Calls

- Benchmark/Development Access: develop, test and optimize your applications on the systems (preparation for Regular/Extreme Scale Access) (few thousand node hours)
- Regular Access: compelling cases that will enable scientific innovation in the domains covered (few hundred thousand node hours)
- Extreme Scale Access: extremely large allocations in terms of compute time, data storage and support resources (up to millions of node hours)
- Al Access: Al applications for science

Application Procedure

- 1. Submit form in portal (https://access.eurohpc-ju.europa.eu/)
 - For Benchmark/Development: continuously open
 - For Regular/Extreme Scale: two cut off dates per year
- 2. Wait for the review
 - For Benchmark/Development: a few days up to two weeks
 - For Regular/Extreme Scale: a few months up to half a year
- 3. Submit rebuttal (not for Benchmark/Development)
- 4. Get further information (e.g., access to HPC portal of the cluster) from the local compute center you have applied to via email
- 5. Submit project report (after the allocation period)

Experience with the Calls: Benchmark/Development

- Very light-weight review (easy accept)
- Decent compute time for scaling runs
- Pro tip: better apply for development access, because application process is the same, compute resources are the same, but allocation period is a year compared to three months in benchmark access

Experience with the Calls: Extreme Scale

- Resources awarded for 1 year
- Online form (like for Benchmark/Development) and project plan (20 pages) similar to NHR calls
- Three tracks: academia, industry and public sector
- Extensive review
- First: technical assessment (has the software been tested on the system, is the scaling fine, etc.)
- Second: three scientific reviews, each one awards up to 5 points per category (Excellence, Innovation and Impact, Quality and Efficiency of the Implementation)
- At least 3 points per category and 10 points in total are required to pass the review
- Even if you passed the review, there is still a chance that no or fewer resources are granted (not enough resources for all applications)