GCS
Gauss Centre for Supercomputing

29th Call for GCS Large-Scale Projects

Leading edge supercomputing

The Gauss Centre for Supercomputing (GCS) provides computing power and services of the highest performance class for computational sciences and engineering at its three member sites in Garching (Leibniz Supercomputing Centre, LRZ), Jülich (Jülich Supercomputing Centre, JSC), and Stuttgart (High Performance Computing Center Stuttgart, HLRS). To ensure an efficient utilisation of these highly valuable resources, GCS provides its users with world-leading support, education, and dissemination of best practices and methods in simulation science. Here, the three members focus on different topics with some overlap on the subjects due to the centres' traditional user base or specific system requirements. While LRZ supports all scientific fields equally, JSC focusses on fundamental and applied sciences and HLRS specialises in engineering sciences and global system science. GCS aims, in particular, at innovative and scientifically challenging large-scale projects that cannot be carried out within smaller infrastructures. Such projects will also gain most from the existing successful support structures within the GCS and from their continuous synchronisation and optimization. Please be aware of the different priorities of the GCS member sites when you apply for computing time.

State-of-the-art systems

The GCS offers highest-level computing and a networking infrastructure.
JSC provides computing time on the modular supercomputer JUWELS (Jülich Wizard for European Leadership Science). Its 2511 nodes on the Cluster Module are equipped with dual-socket Intel-Skylake Platinum 8168 CPUs. In addition, 56 Dual Intel Xeon Gold 6148 nodes are equipped with 4 additional NVIDIA Volta GPUs yielding a total performance of about 12 PF/s. Furthermore, the JUWELS Booster Module comprises 936 nodes each equipped with two AMD EPYC Rome 7402 CPUs with 512 GB DDR memory each and 4 NVIDIA Ampere A100 GPUs. This adds up to about 75 PF/s. JUWELS thus provides 87 PF/s in total to its users.
LRZ provides SuperMUC-NG, which features 6480 dual-socket nodes with Intel Xeon 8174 processors (48 cores/node). Out of these, 6336 "thin" nodes are equipped with a main memory of 96 GByte and 144 "fat" nodes with a main memory of 768 GByte. SuperMUC-NG delivers a peak performance of 26.9 PF/s.
HLRS provides the 5632-node Hawk system. Each node is equipped with two 2. generation AMD EPYC 7742 processors, offering 128 cores per node. All nodes have 256 GByte of main memory available. The nine-dimensional Hypercube network allows for applications using large partitions of Hawk. Last year, Hawk was extended by an AI-partition, named Hawk-I. This partition provides 24 nodes each equipped with 8 NVIDIA Ampere A100 GPUs. If you plan to make use of this extension within your projects workflow, please get in touch with your HLRS mentor or HLRS user support before submitting the proposal.
HLRS support for application porting is available and required support should be outlined in the project application.

The systems within the GCS are continuously being upgraded in a round robin fashion.

Large-Scale Projects

Large-scale projects and highly scalable parallel applications are characterised by large computing time requirements, not only for short time frames, but usually for longer time periods.

HLRS lrz JÜLICH Forschungszentrum

In detail, projects are classified as "Large-Scale" if they require 2% of the systems' annual production in terms of estimated availability. This requirement can be translated into different values. For the supercomputers Hawk and SuperMUC-NG we give the requirement in terms of core-hours. Thus, the projects' minimal requirements should be the following for these two systems:

- >= 100 million core-hours on **Hawk** or
- >= 45 million core-hours on **SuperMUC-NG**

Please note that the architecture and sustainable performance of a core of each system may differ widely and that the "core-hours" of the systems are not comparable or interchangeable.

JUWELS consists of two different modules with different hardware architectures. Thus, the minimal computing time requirements for GCS-LS projects cannot be coherently specified by use of core-hours but FLOP is used instead. The projects' minimal requirements summed over all requested modules should be:

- >= 45×10^{21} FLOP per year on **JUWELS**

Please note that FLOP refer to the peak performance. The applicant can apply for computing time either on one of JUWEL's modules or on both at the same time. Computing time requirements can be specified in FLOP or in core-hours. In the electronic questionnaire, these values will be converted into each other on the fly and displayed in due consideration of the requested modules. Resources will be allocated and accounted in core-hours only.

For these large-scale projects a competitive review and resource allocation process is established by the GCS. Requests above these limits will be processed according to joint procedures of the GCS and will be reviewed in a national context. Requests below these limits and requests for test projects will be directly processed by the individual member centres.

Call for Large-Scale Projects

A "Call for Large-Scale Projects" is published by the Gauss Centre twice a year. Dates for closure of calls are usually at the end of winter and at the end of summer. The current 29th call will be open

January 16th to February 13th 2023, 17:00 o'clock CET (strict deadline)

Eligible are applications from **German** universities and publicly funded **German** research institutions, e.g., Max-Planck Society, and Helmholtz Association.

Answering the Call

Leading, ground-breaking projects should deal with complex, demanding, innovative simulations that would not be possible without the GCS infrastructure and which can benefit from the exceptional resources provided by GCS.

Applications for a large-scale project may only be submitted by filling in the appropriate electronic application form that can be accessed from the GCS web page

https://www.gauss-centre.eu/for-users/hpc-access/

Please use the template for the project description of your GCS large-scale application which can be accessed from the above web page and are provided in pdf, docx, and LaTeX format.
Note that the regular application forms of the GCS member centres can be found here as well.

Please note:

- Projects with a running large-scale grant must **clearly indicate and justify this**.

- Projects targeting multiple GCS platforms must **clearly indicate and justify this**.
- Projects applying for an extension **must clearly indicate the differences to the previous applications** in the project description and must have submitted their reports of the previous application.
- Accepted large-scale projects **must fulfil their reporting obligations**.
- Project descriptions must not exceed 18 pages.
- **Existing grants or current applications to all German computer centres as well as PRACE have to be declared in the online application form**.

The proposals for large-scale projects will be reviewed with respect to their technical feasibility and peer-reviewed for a comparative scientific evaluation. On the basis of this evaluation by the GCS committee the projects will be approved for a period of one year and given their allocations.

Criteria for approvals

Applications for compute resources are evaluated only according to their scientific excellence and technical feasibility.

- The proposed scientific tasks must be scientifically challenging, and their treatment must be of substantial interest.
- Clear scientific goals and verifiable milestones on the way to reach these goals must be specified.
- The implementation of the project must be technically feasible on the available computing systems, and must be in reasonable proportion to the performance characteristics of these systems.
- The Principal Investigator must have a proven scientific record, and she/he must be able to successfully accomplish the proposed tasks. In particular, applicants must possess the necessary specialized know-how for the effective use of high-end computing systems. This has to be proven in the application for compute resources, e.g. by presenting work done on smaller computing system, scaling studies etc.
- The specific features of the high-end computers should be optimally exploited by the program implementations. This will be checked regularly during the course of the project.

Further help:

For further help please contact the member sites via https://www.gauss-centre.eu/service/contact/.