Platform for Advanced Scientific Computing

Call for PASC project proposals 2025-2028

1. Content and Goals

The Swiss National Supercomputing Center (CSCS) develops and operates a high-performance computing and data research infrastructure that supports world-class science in Switzerland. It envisions to be the leading partner for extreme computing and data solutions that best serve the evolving needs of Science. The ETH Board funds high-end supercomputing infrastructure development and operations through the Swiss High-Performance Computing and Networking (HPCN) initiative and ETH Zurich. This infrastructure is available to domestic and international researchers through a transparent, peer-reviewed allocation process.

The Platform for Advanced Scientific Computing (PASC; www.pasc-ch.org) fosters computational science and data processing at scale through a dedicated investment in application software development and related computational tools. PASC is coordinated by CSCS in close collaboration with Swiss universities, including ETH Zürich and EPF Lausanne. In the period 2025 through 2028, PASC will be funded through the HPCN investment budget of CSCS, with matching funds from the awarded PIs.

The platform's overarching goal for the 2025 to 2028 period is to strengthen Swiss computational sciences in the exascale era, application driven machine learning, and to ensure application readiness leading to allocations on the Alps infrastructure at CSCS, on EuroHPC platforms (e.g. LUMI, in which Switzerland owns a share), and other Tier-0 systems[1]. Through PASC, HPC competence is fostered at Swiss universities, and CSCS obtains valuable insights into developing its next generation of systems. Specifically, PASC will invest in the development, availability and quality of application software and frameworks that are performant on GPUs, portable, scalable and sustainable. PASC strongly encourages open development and open-source licensing.

This will be pursued through (1) funding of HPC application software development projects through this call as well as (2) a core team at CSCS for dedicated collaboration with the teams developing application software and for contributions to transversal numerical libraries and components of user environments required to support the applications running on its supercomputing platforms. The dedicated investments in libraries and programming environments will involve collaborations with initiatives in the USA, Europe and Japan.

2. Call for HPC application software development projects

In this call, PASC is seeking proposals for software development projects that address the broad availability, the quality, and performance of software on GPU-accelerated

[1] Tier-0 systems are supercomputing infrastructures that can support allocations of minimum 1 million GPU hours per year.

supercomputing platforms. These projects can focus on simulation or data analysis using approaches from computational science or the machine learning field. Projects must lead to application software that is related to important scientific problems that require high-end GPU-accelerated supercomputers to be solved. The projects must present the science case that motivates the work and that would merit Tier-0 resources, or alternatively document the expected impact of the project on the user community as a whole at CSCS. Separately securing grants/resources on Tier-0 systems to tackle the science case during the course of the project is an important measure of success.

The proposed project will have to comprehensively address common performance issues at all levels, i.e.

- Efficient GPU-acceleration;
- Leveraging mixed-precision and specialized hardware where applicable;
- Performance-portable, highly optimized implementations, supporting GPUs from various vendors, typically with multiple GPUs per node;
- Scalability to many nodes, both in a strong and weak scaling sense;
- In-situ or online data analysis, or using scalable I/O solutions if storage is needed;
- Automated and robust workflows for complex simulations or training.

Efficient execution on GPUs often requires algorithmic re-engineering in order to expose sufficient parallelism. Project teams should be willing to re-implement legacy code when necessary to address the performance issues and to improve maintainability. Algorithmic re-engineering for performance is encouraged.

To reach the above-described goals, skills from various disciplines, including the application domain, computational science and/or machine learning, applied mathematics and computer science might be required. Potential collaboration with the PASC core team of software engineers at CSCS should be described. The core team offers software engineering experience and can actively participate in the project execution (see also section 2.2). In those cases where multiple scientific groups are involved in the project, the responsibilities and commitments of the various groups must be clearly described in the project proposal and must be a logical consequence of the work breakdown structure of the project. Regular meetings between these groups must be planned by the PI and be held as part of the management of the project.

While exploration of novel programming languages and environments is encouraged, projects should ascertain that the software runs on commonly supported software environments. We therefore recommend:

- C++ and Fortran as imperative programming languages, where the use of emerging parallel constructs of the C++ standard is highly encouraged, as well as Python for more high-level descriptive layers of the application software.
- The use of industry standard frameworks for machine learning.
- Pthreads, Kokkos, CUDA, or HIP for on-node parallelism, possibly using tasking.

- MPI for both on-node and distributed memory programming at scale, where exploration of RDMA/RMA (e.g. GPUdirect) is specifically encouraged. Lower level standard protocols such as libfabrics or UCX can be explored.
- Use of standardized/open technologies to support scalable I/O, such as HDF5, ADIOS, and similar solutions.
- The use of CMake and Spack to build software and manage dependencies, ideally within a container-first approach.

Adoption of test-driven development is encouraged and the use of automated unit and regression testing technologies with emphasis on reproducibility is mandatory. The proposal must describe one or two test cases that can, ideally, be used from the start, with the required data sets, to monitor the progress of the software towards the scientific goal. Projects are encouraged to run part of their CI/CD on CSCS infrastructure and to work together with CSCS to make their production quality software available to the CSCS user lab as a whole. Proposals must discuss their plans for support of the software beyond the duration of this project.

The product of these projects is software that can be modified, distributed and is broadly available for scientific use. During the development phase, availability of the software to the PASC core team should be guaranteed, open development is encouraged. A public release using an OSI approved license (https://opensource.org/licenses) as part of the deliverables of this project is strongly encouraged. Licensing models that are non-OSI approved should be discussed and justified in the proposal. A plan to manage intellectual property (through copyright and publications) should be developed.

2.1 Eligible applicants

Researchers with tenured positions at Swiss universities and institutes of the ETH Domain are eligible to submit PASC projects as principal investigators (PI). SNSF rules for personnel eligibility apply. Researchers from other institutions, including private companies and universities of applied sciences (Fachhochschulen), as well as non-Swiss universities and research institutes are eligible to participate in HPC software development projects. Typically, investigators from private companies or non-Swiss institutions bear their own cost; the PASC Steering Committee may approve exceptions in justified cases.

2.2 CSCS Contributions

PASC funds personnel with a focus on software development and provides limited (i.e. non-Tier-0) HPC resources for development. CSCS collaborates closely with the projects, with a core team of software engineers.

The following resources will be available at CSCS in support of the HPC software development projects:

- Access to development platforms, which will include the Cray EX system ALPS with Nvidia GH200 compute modules (ARM CPU with H100 GPU) and AMD MI300a GPUs, as well as the LUMI platform (GPU architecture).
- Updated information about targeted new technologies will be provided throughout project duration, with early access to novel hardware when possible.
- Coordination of necessary interactions between HPC software development project teams and manufacturers of supercomputing technologies.
- Consultancy, expertise and training in key aspects of emerging technologies and HPC software development, including building, testing and deploying.
- Support for automated testing and building tools (CI/CD), REST APIs for HPC access (FirecREST), cloud infrastructure (e.g. virtualized systems or object stores) as well as container-based deployment technologies (i.e. Docker/Sarus)

2.3 Financial Scope and duration

Projects will start on **January 1st 2025** and can plan for maximum three years of development. As a result of a mandatory review in year 3, an extension of the project by one year will be granted to those projects that are favorably reviewed on both past performance and an extension proposal. All projects must be concluded by **December 31st 2027** (no extension) or **December 31st 2028** (with extension)**.** PASC expects to support 10-15 projects. Typical budget of the PASC-supported portion of an HPC software development project is expected to be in the range of CHF 350.000-550.000 for 3 years; larger budgets of the PASC-supported portion will have to be well justified. Following federal regulations, each project team receiving PASC funds will have to provide matching funds. These can be in-kind and must be at least equal in value to funds requested from PASC. It is encouraged that PIs acquire additional funds in support of their HPC software development projects.

2.4 Eligible costs

The following costs will be eligible for support from PASC:

- Research and technical staff including post-doctoral fellows and PhD students; SNSF regulations concerning salaries and employment conditions will apply.
- Assistant professor positions will be funded only with a written confirmation of the hosting university, as well as a substantial share of co-funding from the university; professorial staff members employed by the host university at the time of submission are not eligible.
- Networking and dissemination activities, as well as participation at international events (workshops, conferences, etc.) in the respective field.
- Stay of researchers at CSCS for joint activities.

2.5 Reporting and documentation

- The PI of a supported project must submit annual progress reports.
- PIs and/or co-PIs must participate in and give oral presentations at the PASC project review meeting held in year 3.
- Members of the PASC project are expected to actively disseminate their results in the annual PASC conference, through poster or oral presentations, or the organization of mini-symposia.

Detailed guidelines with scientific requirements and notifications of the reporting deadlines will be given to PIs and co-PIs at least three months in advance.

3. Submission and proposal format

3.1 Timeline of this call

A letter, in which the intent for submitting a project proposal is expressed, should be submitted in PDF format to paola.colferai@cscs.ch at the latest by **April 30, 2024**. The letter (1-2 pages) should include:
(1) a preliminary title of the project;
(2) a brief description of the project ideas and the science domain it relates to;
(3) the contact information of the PI and co-PIs;
(4) suggestions for referees (following the usual SNSF rules for conflicts of interests).

Full proposals have to be submitted before midnight Central European Time on **June 10th, 2024.**

Tentatively, decisions on funding will be announced **October 31st, 2024**.

Project starting date should be **January 1st, 2025.**

The PASC steering committee may establish other deadlines or decide on launching additional calls in the future, depending on program needs.

3.2 Full Proposal submission

Complete project proposals must be submitted in PDF format via e-mail to paola.colferai@cscs.ch.
Applicants are requested to submit the following information:

- The proposal narrative;
- The budget forms (see template);
- The CV of PI and co-PIs;
- A list of five relevant publications in the domain of the PI and co-PIs.

Templates for submission will be available on the PASC website (www.pasc-ch.org).
All documents must be submitted in PDF format.

3.3 Format for proposal narrative

The proposal narrative should be structured as follows:

1. Cover page including basic project data (see template)
2. Project summary (max 2 pages)
3. International standing of applicant team
4. Proposal narrative (max 15 pages) with the following sections:
   a. Background and significance, including scientific motivations.
   b. Describe the state and capabilities, including limitations, of the relevant pre-existing software in the applicant's team.
   c. Proposed software developments: goals, justification, work breakdown structure (WBS). If the project goals involve research on novel methods, models, etc: distinction between research goals and improvements to implementations of existing algorithms. Describe the test-cases (including data) available to effectively monitor progress and correctness of the software towards the scientific goal.
   d. Required resources, including personnel, development systems and software, as well as resources to support outreach and dissemination activities.
   e. Timeline and milestones that correspond to the WBS.
   f. Project organization and management plan, including a description of how interactions between domain scientists (product owners) and PASC-funded software developers are organized, how co-PIs will interact, and their responsibilities.
   g. Software dissemination plan and licensing, management of copyrights, as well as plans for future application development and support (beyond the PASC project).
   h. Expected impact of the developed application software on the scientific domains as well as on CSCS' next generation supercomputing platforms, including a timeline to submit proposals for Tier-0 resources, or alternatively document the expected impact of the project on the user community as a whole at CSCS.
   i. References.

3.4 Evaluation Criteria

Submitted proposals will first be subject to an eligibility check by the project office. Eligible proposals will subsequently be evaluated technically by CSCS and on excellence by external peers and ranked by the PASC Scientific Advisory Board. The final decision on funding will be adopted by the PASC Steering Committee upon the proposition of the PASC Program Director.

Proposals will be evaluated against the following criteria:

- Do the applicants demonstrate a good understanding of the main challenges in the respective scientific domains?
- Will the proposed project deliver demonstrably accelerated applications and tools, and how significant will they be to address the scientific challenges of a particular domain?
- Will the project lead to Tier-0 applications or significantly impact the User Lab as a whole?
- Do the applicants have sound development, support and dissemination plans for the products they propose to develop? Are the codes available under an OSI-approved license and how are they managing copyright/IP?
- Are the applicants willing to change existing (legacy-)codes? If the proposed developments involve community codes, do they have enough standing in the community to integrate updates into the main version?
- Will the project CI/CD be integrated with CSCS infrastructure, potentially leading to production quality software available to the User Lab? Are the described test-cases suitable?
- Does the proposed project address portability across GPUs from different vendors, multi-GPU nodes, and both current CSCS and LUMI systems? Is the technical approach suitable?
- Are the scientific theories and models on which the proposed developments are based state-of-the-art? Should competing approaches be considered? (e.g. for risk mitigation purposes)
- Is the team credible in terms of its competences in the relevant science domain and does it hold sufficient competence in high-performance computing, computational methods, and software engineering to reach the project goals?
- Is the management approach, work breakdown and the timeline realistic to achieve the project's goals and deliver on the product plan? Are the milestones and deliverables meaningful and well-articulated, with clearly assigned tasks between partners? Are the risks understood and mitigated?
- Are the requested resources adequate, both in terms of funding as well as from a human resources perspective?

4. Contacts

PASC Program Leadership

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