

Call for PASC project proposals

Letter of Intent Submission deadline: **October 15th, 2020**

Full proposal Submission deadline: **November 15th, 2020**

1. Content and Goals

The Swiss National Supercomputing Center (CSCS) develops and provides key supercomputing capabilities required to solve important problems to science and society. 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 Swiss Platform for Advanced Scientific Computing (PASC; www.pasc-ch.org) fosters computational science at scale through dedicated investment in application software development and related computational tools. PASC is coordinated by CSCS in close collaboration with Swiss universities, including ETH Zurich and EPFL. In the period 2021 through 2024 PASC will be funded through the HPCN investment budget of CSCS.

The platform overarching goal for the 2021 to 2024 period is to position Swiss computational sciences in the emerging exascale era, and to ensure application readiness leading to Swiss allocations on EuroHPC platforms and other Tier 0¹ systems. Specifically, PASC will invest in the development, availability and quality of application software and tools on GPU supercomputing systems deployed at CSCS and the EuroHPC LUMI consortium (<https://www.lumi-supercomputer.eu/>). This will be pursued through (1) the present call for HPC application software development projects as well as (2) dedicated collaboration with the teams developing application software, and contributions to transversal numerical libraries and components of programming environment by CSCS required to support the applications running on its supercomputing platforms. The dedicated investments in libraries and programming environments will involve close collaborations with similar initiatives in the USA, Europe and Japan.

2. Call for HPC projects

In this call, PASC is seeking proposals for HPC software development projects that address the broad availability, the quality, and performance of software on GPU-accelerated supercomputing platforms. Eligible 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 commit with 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.

¹ Tier 0 systems are supercomputing infrastructures that can support allocations of 1 million node hours and more per year.

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

- Efficient vectorization, multi-threading, and in particular GPU-acceleration.
- Performance-portable, highly-optimized implementations across multiple node architectures, in particular with multiple GPUs per node, supporting GPUs from various vendors.
- Scalability to many nodes, both in a strong and weak scaling sense, and assuming a high-end network fabric.

While exploration of novel programming languages and environments is encouraged, projects should ascertain that the software runs on commonly supported software environments. These include

- C/C++ and Fortran as imperative programming languages, where the use of newly emerging parallel constructs of the C++ standard is highly encouraged, as well as Python for more high-level descriptive layers of the application software.
- Pthreads, OpenMP, Intel TBB, HPX-3, CUDA, HIP and OpenACC for on-node thread-based parallelism, including in particular the use of tasking.
- MPI for both on-node and distributed memory programming at scale, where exploration of RMA is specifically encouraged, or the use of lower level standard protocols such as libfabrics or UCX.
- Use of standardized/open technologies to support scalable I/O, such as HDF5 and similar solutions.
- Algorithmic re-engineering leading to significant performance increase are welcomed.

Project teams are encouraged to be interdisciplinary, consisting of researchers from the relevant application domains, computational science and applied mathematics, as well as computer science. The organization of the interactions between project members of the various disciplines and participating institutions should be clearly described in the project proposal. Ideally, interactions between different disciplines and institutions are a straightforward consequence of the work breakdown structure of the project. Potential interactions with the PASC core team of developers at CSCS should be described.

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. 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 (though copyright and publications) should be developed and it is advisable to hold copyright with as few institutions as possible.

Adoption of test-driven development is encouraged and use of automated unit and regression testing technologies with emphasis on reproducibility is mandatory. 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 have to discuss their plans for support of the software beyond the duration of this project.

2.1 Eligible applicants

Researchers with tenured positions at Swiss universities and institutes of the ETH Domain are eligible to submit HPC software development projects as principal investigators (PI). SNSF rules for personnel eligibility apply.

Researchers from other institutions, including private companies and colleges 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 such other institutions bear their own cost; the PASC Steering Committee may approve exceptions in justified cases

2.2 CSCS Contributions

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

- Updated information about targeted new technologies will be provided throughout project duration.
- Access to development platforms, which initially will include the Cray XC supercomputing systems with: the GPU accelerated partition of Piz Daint (Nvidia P100), x86_64 multi-core nodes, the successor of Piz Daint (GPU architecture), as well as the LUMI platform (GPU architecture).
- Access to emerging technologies such as new ARM-based processors, and GPUs from various vendors.
- 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.
- 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 **July 1, 2021** and will have to be concluded by **June 30, 2024** at the latest. Expected project duration will be two to three years. The initial budget allocation for this call for PASC HPC software development projects is CHF 5 million. PASC expects to support around 10 projects.

Typical budget of the PASC-supported portion of an HPC software development project is expected to be in the range of CHF 300 to 500 thousand; 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 for 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 under 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 is expected to submit annual progress reports. PIs and/or co-PIs are expected to participate in and give oral presentations at PASC project review meetings. 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 **October 15, 2020**. The letter 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 **November 15, 2020**. The PASC steering committee may establish other deadlines or decide on launching additional calls in the future, depending on program needs.

3.2 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
- The 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 have to 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. Proposed developments and where necessary research: goals, justification, product breakdown structure (PBS) and work breakdown structure (WBS)
 - c. Required resources, including personnel, development systems and software, as well as resources to support outreach and dissemination activities
 - d. Timeline and milestones that correspond to the PBS/WBS
 - e. Project organization and management plan, including a description of how interactions between domain scientists (product owners) and PASC-funded software developers is organized
 - f. Software dissemination plan and licensing, management of copyrights, as well as plans for future support (beyond the PASC project)
 - g. Expected impact of the developed application software on the scientific domains as well as 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.
 - h. References

3.4 Evaluation Criteria

Submitted proposals will first be subject to eligibility check by the project office. Eligible proposals will subsequently be evaluated by external peers and ranked by the PASC Scientific Advisory Board.

Final decision on funding will be adopted by the PASC Steering Committee upon proposition of the PASC Program Director. Final decision is expected in March 2021.

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?
- Will the project CI/CD be integrated with CSCS infrastructure, potentially leading to production quality software available to the User Lab?
- Does the proposed project address portability across GPUs from different vendors, multi-GPU nodes, and both current CSCS and LUMI systems?
- 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? Are the risks understood and mitigated?
- Are the requested resources adequate, both in terms of funding and from a human resources perspective?

4. Contacts

PASC Program Leadership

Prof. Dr. Thomas C. Schulthess, Swiss National Supercomputing Centre, via Trevano 131, CH-6900 Lugano; phone: +41 91 610 82 01; email: schulthess@cscs.ch

PASC Executive Management

Dr. Michele De Lorenzi, Swiss National Supercomputing Centre, Via Trevano 131, 6900 Lugano; phone: +41 91 610 82 08; email: michele.delorenzi@cscs.ch

Dr. Joost VandeVondele, Swiss National Supercomputing Centre, Via Trevano 131, 6900 Lugano; phone: +41 44 633 33 58; email: joost.vandevondele@cscs.ch

PASC Project Office

Ms. Paola Colferai, Swiss National Supercomputing Centre, Via Trevano 131, 6900 Lugano; phone: +41 91 610 82 93; email paola.colferai@cscs.ch