

Call for PASC HPC software development project proposals

Submission deadline: November 13th, 2016

1. Context 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; <http://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 the Università della Svizzera italiana (USI), as well as other Swiss universities, including ETH Zurich and EPFL. In the period 2017 through 2020, PASC will be funded through the HPCN investment budget of CSCS.

The platform's overarching goal for the 2017 to 2020 period is to position Swiss computational sciences in the emerging exascale era. Specifically, PASC will invest in the development of application software and tools in order to support design and development of supercomputing systems deployed at CSCS at the end of this decade. This will be pursued through (1) the present call for *HPC application software development projects* as well as (2) dedicated contributions to 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 software development projects

In this call, PASC is seeking proposals for HPC software development projects that address the performance challenges on both current and newly emerging supercomputing platforms, both at node level and at scale. Eligible projects must be tied to application software that is related to important scientific problems that require high-end supercomputers to be solved. The proposed project will have to comprehensively address common performance issues at all levels, i.e.

- Efficient fine-grained SIMD and SIMT style parallelism at the level of individual cores or streaming multi-processors;
- Performance-portable, highly-optimized implementations across multiple node architectures; and
- 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 and OpenACC for on-node thread-based parallelism;
- MPI for both on-node and distributed memory programming at scale, where exploration of RMA is specifically encouraged.
- Use of standardized/open technologies to support scalable I/O, such as HDF5 and similar solutions.

Project teams should 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.

The products of these projects is software. Open-source developments, for example with publicly available source repositories, will be favored. Licensing models should be discussed and justified in the proposal.

Adoption of test driven development is encouraged and use of automated unit and regression testing technologies with emphasis on reproducibility is mandatory. 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: hybrid, GPU accelerated nodes (NVIDIA GP100, codename PASCAL); standard Intel Xeon multi-core processor nodes (code name Broadwell); Intel Xeon-Phi many-core processor nodes (codename Knightslanding)
- Access to emerging technologies such as new ARM-based processors and FPGA

- 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, as well as container based deployment technologies (i.e. Docker/Shifter)

2.3 Financial scope and duration

Projects will start on July 1, 2017 and will have to be concluded by June 30, 2020 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 a 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

Proposals have to be submitted before midnight Central European Time on November 13, 2016.

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

3.2 Proposal submission

Complete project proposals must be submitted in PDF format via email to projectoffice@pasc-ch.org.

Applicants are requested to submit the following information:

1. The proposal narrative (see section 3.3 for content and format)
2. The budget forms (see template)
3. The CV of PI and co-PIs
4. 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 shall 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, 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
 - h. References

3.4 Evaluation criteria

Submitted proposals will first be subject to eligibility check by the program secretariat.

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 2017.

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?
- To what extent can the applications and tools be adopted in other domains?
- Do the applicants have sound development, support and dissemination plans for the products they propose to develop?
- Does the proposed project address portability across new and emerging supercomputing architectures, e.g. hybrid CPU/GGPU systems, Intel Xeon Phi and ARM, and is it considering major supercomputing platforms not located at CSCS?
- 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?
- Are 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 from a human resources perspective?

4. Contacts

PASC Program Director

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 Project Office

Prof. Dr. Benedetto Lepori, Research Services, Università della Svizzera italiana, Via Lambertenghi 10, 6904 Lugano; phone: +41 58 666 46 14; email: blepori@usi.ch

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

Mrs. Paola Colferai, Research Services, Università della Svizzera italiana, Via Lambertenghi 10, 6904 Lugano; phone: +41 58 666 48 18 ; email: paola.colferai@usi.ch