

Q1 What is your organisation's/project's name?

IT4Innovations national supercomputing center

Q2 Your organisation's/project's website

<http://www.it4i.cz/?lang=en>

Q3 Are you?

A research organisation

Q4 Your name

Q5 Your email address

Q6 Your contact phone number

Q7 Please summarise who you are and what you do

IT4Innovations national supercomputing center at VSB - Technical University of Ostrava is a large research e-infrastructure in the Czech Republic. In the framework of the national supercomputing center, the most powerful supercomputing facilities in the Czech Republic are operated and excellent research in HPC technologies is performed. IT4Innovations is currently operating two supercomputers. Anselm was installed in the summer of 2013 and its theoretical peak performance is 94 teraflops. Salomon was installed in the summer of 2015, and its theoretical peak performance is 2 petaflops. The supercomputer Salomon is ranked the 78th most powerful supercomputer worldwide and is the most powerful European supercomputer based on the first generation of the Intel Xeon Phi coprocessors (codenamed Knights Corner).

Q8 In what way would like to contribute to an EsD project? **An an application provider** ,
Other (please specify):
Hosting HPC center

Q9 What would be your contribution to an EsD project?

ETP4HPC - Extreme-Scale Demonstrators NETWORKING 2017

As an application provider, we would like to contribute the following results of the H2020 projects we were involved in the preceding H2020 work programmes.

HyperLoom, an open-source platform for defining and executing workflow pipelines in large-scale distributed environments developed within the H2020 ExCAPE project. Scientific pipelines, such as those in machine learning applications, usually compose of multiple interconnected data processing tasks whose processing can utilize thousands of computational cores in parallel.

HyperLoom users can easily define dependencies between computational tasks and create a pipeline which can then be executed on HPC systems. The high-performance core of HyperLoom dynamically orchestrates the tasks over available resources respecting task requirements. The entire system was designed to have a minimal overhead and to efficiently deal with varying computational times of the tasks. HyperLoom allows to execute pipelines that contain basic built-in tasks, user-defined Python tasks, tasks wrapping third-party applications or a combination of those.

HyperLoom has been successfully applied in the chemogenomics domain for modeling the activity of chemical compounds in the drug discovery phase of the pharmaceutical industry, where thousands of models were created using various parameterization and consequently cross-validated within a HyperLoom pipeline running on thousands of cores. In the next steps, we would like to continue evaluating HyperLoom scalability, extending it and apply it to other practical large-scale beyond use cases beyond the chemogenomics domain.

For more details see <https://code.it4i.cz/ADAS/loom>.

ESPRESO, an open-source ExaScale PaRallel FETI Solver for problems of engineering mechanics developed at IT4Innovations within the FP7 EXA2CT project. ESPRESO contains several FETI (Finite Element Tearing and Interconnecting) based domain decomposition algorithms including Hybrid Total FETI method suitable for parallel machines with tens or hundreds of thousands of cores. The solver is based on highly efficient communication layer on top of pure MPI. Its scalability has been tested up to almost 18,000 compute nodes of the Titan supercomputer at Oak Ridge National Laboratory. Moreover, it supports acceleration using GPUs and within the Intel Parallel Computing Center (IPCC) project at IT4Innovations the solver was accelerated using the Intel Xeon Phi coprocessors. An energy efficient version of ESPRESO is under development within the H2020 project READEX.

Future plans and extensions of ESPRESO: to develop massively parallel implementation of algorithms for extreme scale constrained optimization problems (e.g., extreme scale problems of contact mechanics) based on the state-of-the-art optimization methods. Further optimizations have to be applied to ensure scalability and performance on future platforms. These include, e.g., adaptation for the Knights Landing or Knights Hill Xeon Phi architecture (optimization for MCDRAM/DRAM memory hierarchy, optimization of the vectorization, etc.), exploitation of the NVM memory, or implementation of various communication hiding/avoiding algorithms (e.g., pipelined Krylov methods, double buffering methods for communication with accelerator, etc.).

For more details see <http://espresso.it4i.cz>.

As a hosting HPC center, we would like to participate in the co-design process and to manage system deployment during phase A, leveraging our links to application communities and the experience in mapping user requirements to system specifications. The infrastructure research laboratory at IT4Innovations would like to contribute towards integrating and customizing hardware and software components and sub-systems developed in the preceding R&D projects. Furthermore, we would like to operate the EsD, address numerical/extreme data challenges as well as characterization and contribute to system prototypes validation based on real use cases during phase B.

We are interested to deploy and operate the EsD and make it available to application owners for porting and development in phase B, and for regular usage in future. This will include providing advanced user support. These tasks are fully aligned with the mission of IT4Innovations and skills available at the IT4Innovations national supercomputing center.

Q10 What partners are you looking for?

Technology providers and system integrators to ensure the integration of the technologies, maintenance and service.

Application providers to contribute creation of rich software environment and to contribute to the assessment of the deployed EsD performance and usability.

Q11 Please include links to any additional material.

Information about the IT4Innovations national supercomputing center at <http://www.it4i.cz>

Information about IT4Innovations hardware and software at <https://docs.it4i.cz/>.

Q12 Other comments/ideas

Respondent skipped this question
